



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:45 PM UTC

PDB ID : 2I14 / pdb_00002i14
Title : Crystal structure of nicotinate-nucleotide pyrophosphorylase from *Pyrococcus furiosus*
Authors : Shin, D.H.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2006-08-12
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

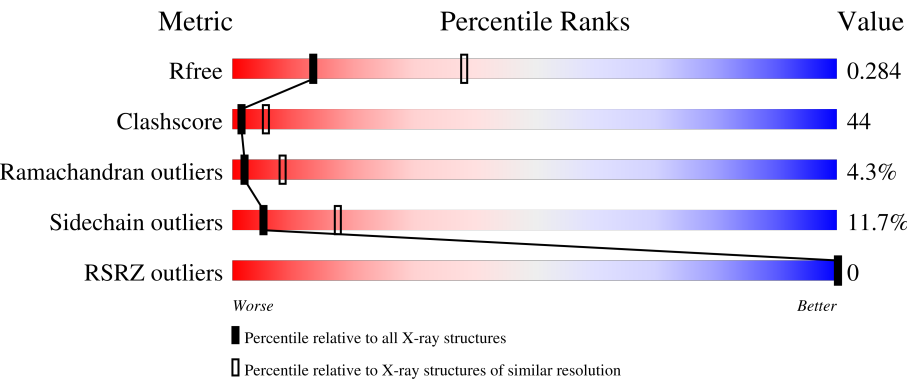
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	395	38%49%10%..
1	B	395	36%50%10%..
1	C	395	38%49%11%..
1	D	395	36%50%10%..

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Mol	Chain	Length	Quality of chain
1	E	395	 37% 50% 10% . .
1	F	395	 36% 50% 11% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18539 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nicotinate-nucleotide pyrophosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	B	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	C	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	D	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	E	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	F	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	cloning artifact	UNP Q8TZS9
A	-4	GLY	-	cloning artifact	UNP Q8TZS9
A	-3	GLY	-	cloning artifact	UNP Q8TZS9
A	-2	GLY	-	cloning artifact	UNP Q8TZS9
A	-1	GLY	-	cloning artifact	UNP Q8TZS9
A	0	GLY	-	cloning artifact	UNP Q8TZS9
B	395	GLY	-	cloning artifact	UNP Q8TZS9
B	396	GLY	-	cloning artifact	UNP Q8TZS9
B	397	GLY	-	cloning artifact	UNP Q8TZS9
B	398	GLY	-	cloning artifact	UNP Q8TZS9
B	399	GLY	-	cloning artifact	UNP Q8TZS9
B	400	GLY	-	cloning artifact	UNP Q8TZS9
C	995	GLY	-	cloning artifact	UNP Q8TZS9
C	996	GLY	-	cloning artifact	UNP Q8TZS9
C	997	GLY	-	cloning artifact	UNP Q8TZS9
C	998	GLY	-	cloning artifact	UNP Q8TZS9
C	999	GLY	-	cloning artifact	UNP Q8TZS9

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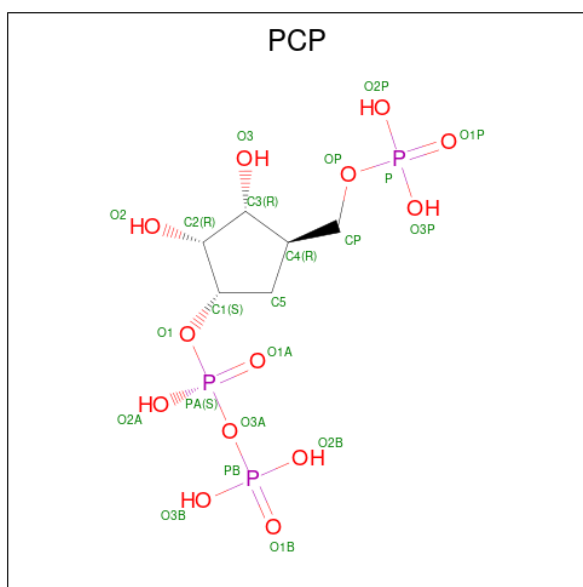
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1000	GLY	-	cloning artifact	UNP Q8TZS9
D	1395	GLY	-	cloning artifact	UNP Q8TZS9
D	1396	GLY	-	cloning artifact	UNP Q8TZS9
D	1397	GLY	-	cloning artifact	UNP Q8TZS9
D	1398	GLY	-	cloning artifact	UNP Q8TZS9
D	1399	GLY	-	cloning artifact	UNP Q8TZS9
D	1400	GLY	-	cloning artifact	UNP Q8TZS9
E	1995	GLY	-	cloning artifact	UNP Q8TZS9
E	1996	GLY	-	cloning artifact	UNP Q8TZS9
E	1997	GLY	-	cloning artifact	UNP Q8TZS9
E	1998	GLY	-	cloning artifact	UNP Q8TZS9
E	1999	GLY	-	cloning artifact	UNP Q8TZS9
E	2000	GLY	-	cloning artifact	UNP Q8TZS9
F	2395	GLY	-	cloning artifact	UNP Q8TZS9
F	2396	GLY	-	cloning artifact	UNP Q8TZS9
F	2397	GLY	-	cloning artifact	UNP Q8TZS9
F	2398	GLY	-	cloning artifact	UNP Q8TZS9
F	2399	GLY	-	cloning artifact	UNP Q8TZS9
F	2400	GLY	-	cloning artifact	UNP Q8TZS9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is 1-ALPHA-PYROPHOSPHORYL-2-ALPHA,3-ALPHA-DIHYDROXY-4-BETA-CYCLOPENTANE-METHANOL-5-PHOSPHATE (CCD ID: PCP) (formula: C₆H₁₅O₁₃P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			22	6	13	3		
3	B	1	Total	C	O	P	0	0
			22	6	13	3		
3	C	1	Total	C	O	P	0	0
			22	6	13	3		
3	D	1	Total	C	O	P	0	0
			22	6	13	3		
3	E	1	Total	C	O	P	0	0
			22	6	13	3		
3	F	1	Total	C	O	P	0	0
			22	6	13	3		

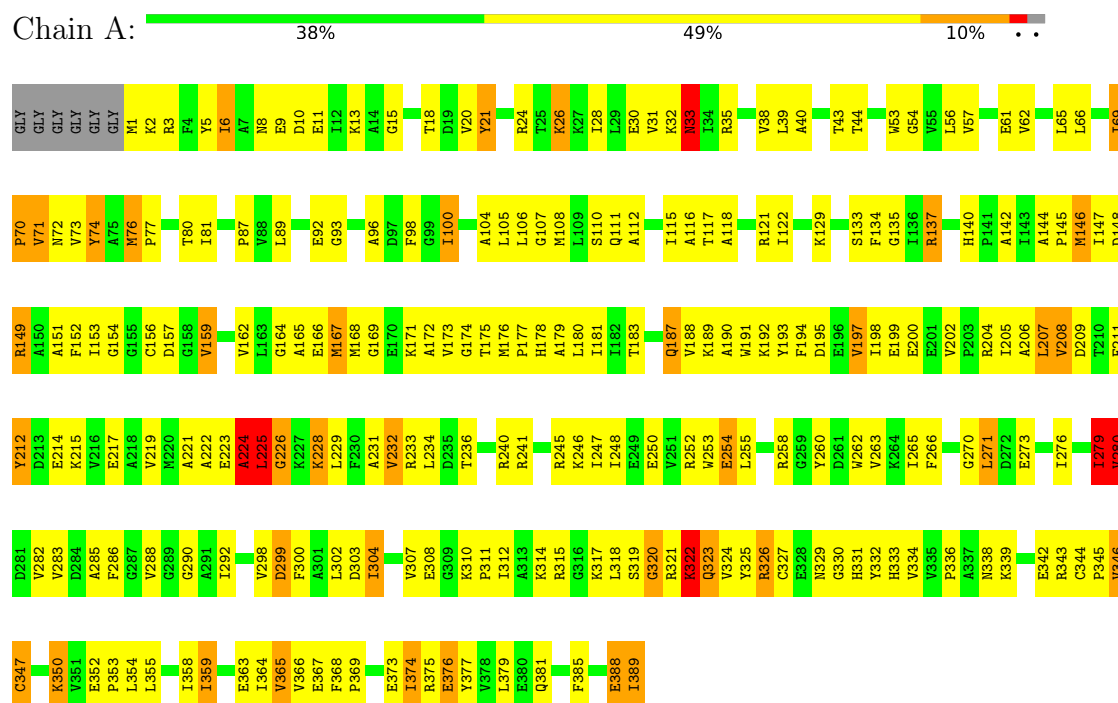
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	10	Total	O	0	0
			10	10		
4	C	9	Total	O	0	0
			9	9		
4	D	10	Total	O	0	0
			10	10		
4	E	16	Total	O	0	0
			16	16		
4	F	12	Total	O	0	0
			12	12		

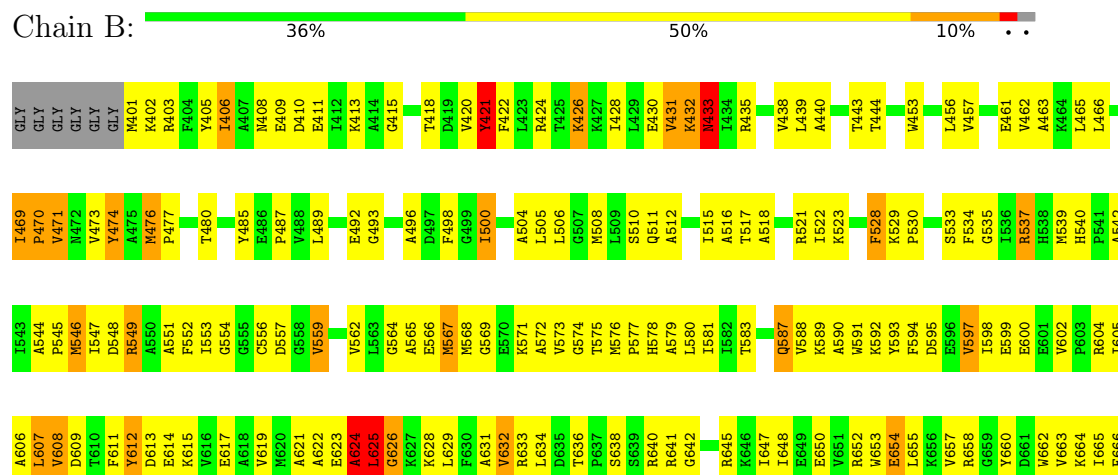
3 Residue-property plots

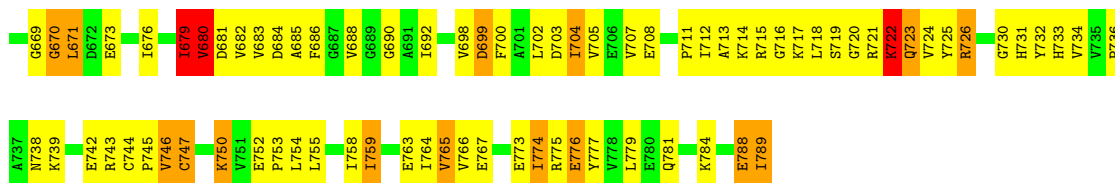
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Nicotinate-nucleotide pyrophosphorylase



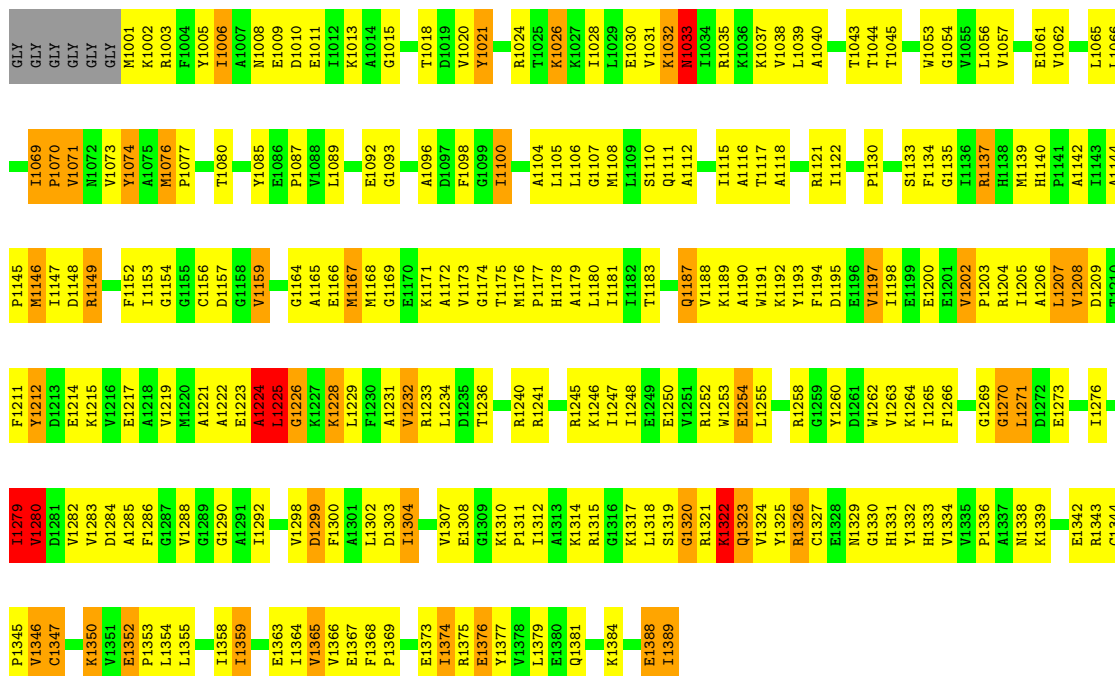
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase





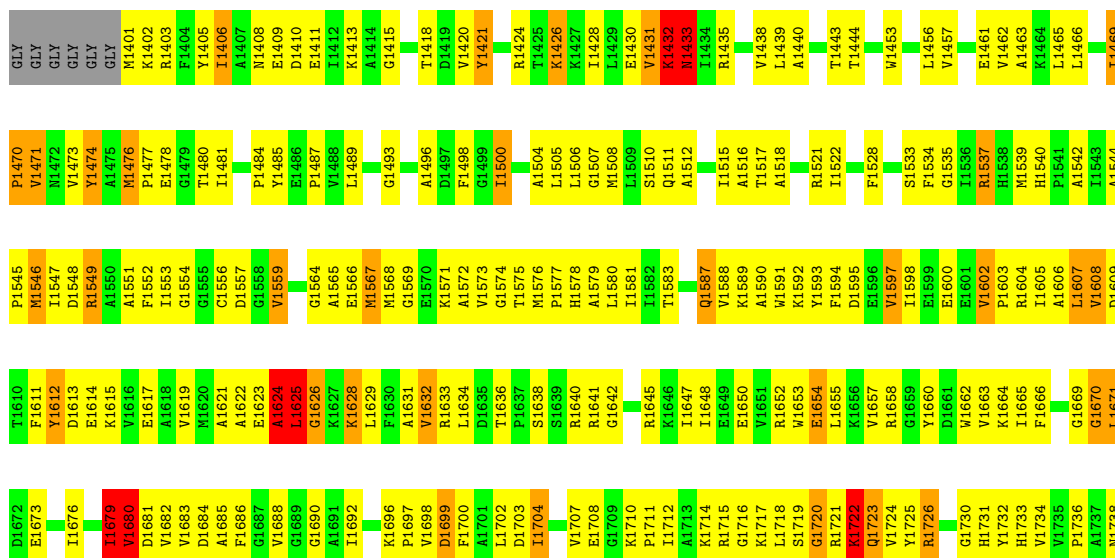
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

Chain C: 38% 49% 11% ..



• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

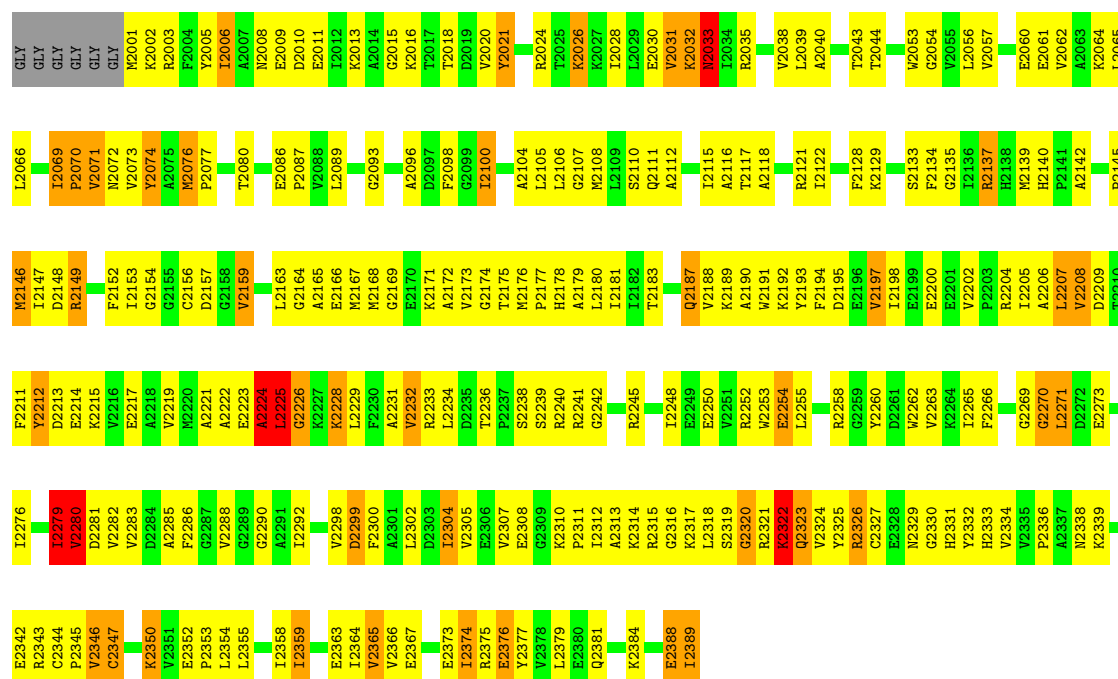
Chain D: 36% 50% 10% ..





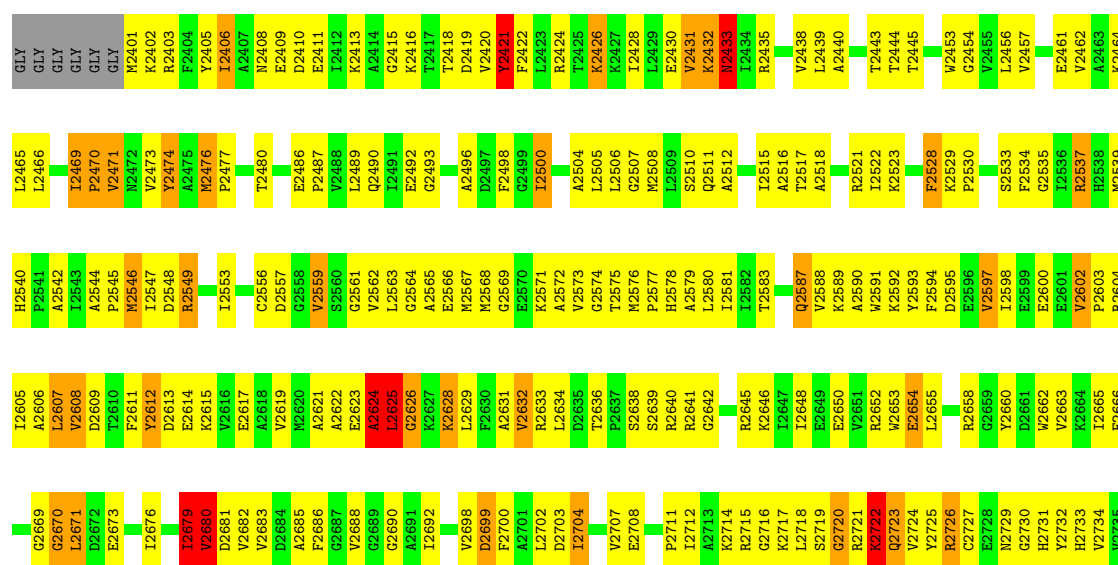
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

Chain E: 37% 50% 10% . .



• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

Chain F: 36% 50% 11% . .



P2736	A2737	N2738	K2739
E2742	R2743	C2744	P2745
V2746	C2747	K2750	V2751
E2752	P2753	L2754	L2755
12758	12759	E2763	12764
V2765	V2766	E2767	E2773
12774	R2775	E2776	V2777
L2778	L2779	E2780	Q2781
K2784	E2788	12789	

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	111.48Å 111.48Å 178.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.3 (19.99-2.90) 94.9 (19.99-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.282 0.250 , 0.284	Depositor DCC
R_{free} test set	5584 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.478 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18539	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2409e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/3117	1.02	21/4211 (0.5%)
1	B	0.53	0/3117	1.02	18/4211 (0.4%)
1	C	0.51	0/3117	1.02	20/4211 (0.5%)
1	D	0.52	0/3117	1.02	19/4211 (0.5%)
1	E	0.53	0/3117	1.03	21/4211 (0.5%)
1	F	0.53	0/3117	1.03	21/4211 (0.5%)
All	All	0.52	0/18702	1.02	120/25266 (0.5%)

There are no bond length outliers.

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1135	GLY	N-CA-C	11.28	127.08	114.67
1	E	2135	GLY	N-CA-C	10.95	126.72	114.67
1	F	2535	GLY	N-CA-C	10.90	126.66	114.67
1	B	535	GLY	N-CA-C	10.47	126.83	114.16
1	D	1535	GLY	N-CA-C	10.34	126.67	114.16
1	A	135	GLY	N-CA-C	8.64	126.63	115.32
1	B	510	SER	N-CA-C	8.45	121.33	111.02
1	F	2510	SER	N-CA-C	8.25	121.08	111.02
1	E	2110	SER	N-CA-C	8.00	120.78	111.02
1	D	1469	ILE	CA-C-N	7.89	129.71	119.84
1	D	1469	ILE	C-N-CA	7.89	129.71	119.84
1	D	1510	SER	N-CA-C	7.83	120.57	111.02
1	A	110	SER	N-CA-C	7.81	120.54	111.02
1	B	469	ILE	CA-C-N	7.80	129.59	119.84
1	B	469	ILE	C-N-CA	7.80	129.59	119.84
1	C	1110	SER	N-CA-C	7.79	120.52	111.02
1	F	2469	ILE	CA-C-N	7.74	129.51	119.84
1	F	2469	ILE	C-N-CA	7.74	129.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2069	ILE	CA-C-N	7.71	129.48	119.84
1	E	2069	ILE	C-N-CA	7.71	129.48	119.84
1	A	69	ILE	CA-C-N	7.63	129.37	119.84
1	A	69	ILE	C-N-CA	7.63	129.37	119.84
1	C	1069	ILE	CA-C-N	7.46	129.16	119.84
1	C	1069	ILE	C-N-CA	7.46	129.16	119.84
1	F	2592	LYS	N-CA-C	-6.50	103.47	111.40
1	A	192	LYS	N-CA-C	-6.48	103.50	111.40
1	E	2192	LYS	N-CA-C	-6.45	103.53	111.40
1	D	1680	VAL	CB-CA-C	-6.43	103.65	111.88
1	C	1197	VAL	N-CA-C	6.42	117.16	110.62
1	B	680	VAL	CB-CA-C	-6.41	103.68	111.88
1	A	280	VAL	CB-CA-C	-6.32	103.79	111.88
1	A	290	GLY	N-CA-C	6.30	120.51	112.83
1	A	197	VAL	N-CA-C	6.29	117.07	110.72
1	B	597	VAL	N-CA-C	6.24	117.03	110.72
1	F	2597	VAL	N-CA-C	6.24	117.03	110.72
1	D	1592	LYS	N-CA-C	-6.24	103.79	111.40
1	C	1192	LYS	N-CA-C	-6.23	103.80	111.40
1	E	2280	VAL	CB-CA-C	-6.20	103.95	111.88
1	D	1597	VAL	N-CA-C	6.18	116.97	110.72
1	E	2322	LYS	N-CA-C	6.16	118.31	109.14
1	C	1322	LYS	N-CA-C	6.16	118.31	109.14
1	B	592	LYS	N-CA-C	-6.12	103.93	111.40
1	F	2722	LYS	N-CA-C	6.11	118.24	109.14
1	C	1290	GLY	N-CA-C	6.10	120.27	112.83
1	F	2680	VAL	CB-CA-C	-6.10	104.08	111.88
1	C	1202	VAL	N-CA-C	6.08	113.09	107.56
1	E	2197	VAL	N-CA-C	6.06	116.84	110.72
1	A	322	LYS	N-CA-C	6.05	118.15	109.14
1	F	2602	VAL	N-CA-C	6.01	113.03	107.56
1	C	1352	GLU	CA-C-N	6.00	125.96	119.78
1	C	1352	GLU	C-N-CA	6.00	125.96	119.78
1	C	1280	VAL	CB-CA-C	-5.97	104.24	111.88
1	E	2228	LYS	N-CA-C	-5.96	105.83	113.23
1	D	1471	VAL	N-CA-C	5.96	116.76	108.23
1	B	690	GLY	N-CA-C	5.96	120.10	112.83
1	D	1722	LYS	N-CA-C	5.95	118.01	109.14
1	D	1602	VAL	N-CA-C	5.91	112.94	107.56
1	C	1228	LYS	N-CA-C	-5.90	105.91	113.23
1	B	722	LYS	N-CA-C	5.90	117.93	109.14
1	E	2071	VAL	N-CA-C	5.89	116.66	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	774	ILE	N-CA-C	-5.89	104.99	110.53
1	D	1774	ILE	N-CA-C	-5.88	105.00	110.53
1	A	71	VAL	N-CA-C	5.86	116.60	108.23
1	D	1690	GLY	N-CA-C	5.86	119.97	112.83
1	C	1071	VAL	N-CA-C	5.84	116.59	108.23
1	E	2290	GLY	N-CA-C	5.83	119.94	112.83
1	B	471	VAL	N-CA-C	5.80	116.53	108.23
1	F	2476	MET	N-CA-C	-5.77	102.89	110.39
1	B	602	VAL	N-CA-C	5.76	112.80	107.56
1	E	2202	VAL	N-CA-C	5.75	112.79	107.56
1	F	2471	VAL	N-CA-C	5.72	116.41	108.23
1	F	2628	LYS	N-CA-C	-5.71	106.15	113.23
1	F	2690	GLY	N-CA-C	5.69	119.78	112.83
1	A	320	GLY	N-CA-C	5.68	118.66	112.29
1	A	202	VAL	N-CA-C	5.62	112.67	107.56
1	C	1076	MET	N-CA-C	-5.60	103.11	110.39
1	C	1320	GLY	N-CA-C	5.59	118.55	112.29
1	A	228	LYS	N-CA-C	-5.58	106.31	113.23
1	A	374	ILE	N-CA-C	-5.55	105.31	110.53
1	A	224	ALA	N-CA-C	-5.54	98.99	110.80
1	F	2445	THR	N-CA-C	-5.54	106.57	113.38
1	A	76	MET	N-CA-C	-5.49	103.26	110.39
1	F	2720	GLY	N-CA-C	5.49	118.43	112.29
1	B	752	GLU	CA-C-N	5.48	125.43	119.78
1	B	752	GLU	C-N-CA	5.48	125.43	119.78
1	A	352	GLU	CA-C-N	5.48	125.43	119.78
1	A	352	GLU	C-N-CA	5.48	125.43	119.78
1	D	1776	GLU	N-CA-C	-5.48	105.31	111.28
1	D	1624	ALA	N-CA-C	-5.46	99.16	110.80
1	E	2320	GLY	N-CA-C	5.44	118.39	112.29
1	E	2224	ALA	N-CA-C	-5.43	99.24	110.80
1	B	624	ALA	N-CA-C	-5.42	99.25	110.80
1	B	776	GLU	N-CA-C	-5.42	105.37	111.28
1	F	2624	ALA	N-CA-C	-5.42	99.26	110.80
1	C	1224	ALA	N-CA-C	-5.41	99.27	110.80
1	E	2076	MET	N-CA-C	-5.37	103.41	110.39
1	F	2752	GLU	CA-C-N	5.37	125.31	119.78
1	F	2752	GLU	C-N-CA	5.37	125.31	119.78
1	D	1752	GLU	CA-C-N	5.31	125.25	119.78
1	D	1752	GLU	C-N-CA	5.31	125.25	119.78
1	A	129	LYS	CA-C-N	-5.31	114.45	119.76
1	A	129	LYS	C-N-CA	-5.31	114.45	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2374	ILE	N-CA-C	-5.30	105.55	110.53
1	E	2376	GLU	N-CA-C	-5.28	105.52	111.28
1	F	2776	GLU	N-CA-C	-5.28	105.53	111.28
1	D	1476	MET	N-CA-C	-5.24	103.58	110.39
1	B	476	MET	N-CA-C	-5.21	103.61	110.39
1	A	376	GLU	N-CA-C	-5.15	105.67	111.28
1	C	1045	THR	N-CA-C	-5.13	107.06	113.38
1	C	1374	ILE	N-CA-C	-5.11	105.72	110.53
1	F	2774	ILE	N-CA-C	-5.10	105.74	110.53
1	C	1376	GLU	N-CA-C	-5.10	105.73	111.28
1	D	1720	GLY	N-CA-C	5.07	117.97	112.29
1	B	551	ALA	N-CA-C	-5.03	105.80	111.28
1	E	2129	LYS	CA-C-N	-5.03	114.73	119.76
1	E	2129	LYS	C-N-CA	-5.03	114.73	119.76
1	D	1628	LYS	N-CA-C	-5.01	107.02	113.23
1	E	2352	GLU	CA-C-N	5.00	124.93	119.78
1	E	2352	GLU	C-N-CA	5.00	124.93	119.78
1	F	2561	GLY	N-CA-C	5.00	118.03	111.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3055	0	3140	289	0
1	B	3055	0	3138	293	0
1	C	3055	0	3137	295	1
1	D	3055	0	3138	304	1
1	E	3055	0	3138	302	1
1	F	3055	0	3138	310	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2	0	0	0	0
3	A	22	0	10	2	0
3	B	22	0	10	1	0
3	C	22	0	10	1	0
3	D	22	0	10	2	0
3	E	22	0	10	1	0
3	F	22	0	10	1	0
4	A	8	0	0	0	0
4	B	10	0	0	0	0
4	C	9	0	0	2	0
4	D	10	0	0	0	0
4	E	16	0	0	1	0
4	F	12	0	0	1	0
All	All	18539	0	18889	1627	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (1627) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LYS:HG3	1:A:336:PRO:HA	1.23	1.19
1:E:2322:LYS:HG3	1:E:2336:PRO:HA	1.23	1.15
1:B:722:LYS:HG3	1:B:736:PRO:HA	1.21	1.14
1:F:2722:LYS:HG3	1:F:2736:PRO:HA	1.23	1.11
1:A:157:ASP:HA	1:A:375:ARG:HH12	1.16	1.09
1:C:1157:ASP:HA	1:C:1375:ARG:HH12	1.17	1.09
1:D:1722:LYS:HG3	1:D:1736:PRO:HA	1.22	1.09
1:C:1322:LYS:HG3	1:C:1336:PRO:HA	1.22	1.08
1:D:1557:ASP:HA	1:D:1775:ARG:HH12	1.17	1.08
1:F:2557:ASP:HA	1:F:2775:ARG:HH12	1.16	1.06
1:B:557:ASP:HA	1:B:775:ARG:HH12	1.18	1.05
1:E:2157:ASP:HA	1:E:2375:ARG:HH12	1.17	1.03
1:F:2724:VAL:HG12	1:F:2734:VAL:HG22	1.41	1.02
1:C:1346:VAL:HG22	1:C:1347:CYS:H	1.25	1.01
1:A:346:VAL:HG22	1:A:347:CYS:H	1.26	1.00
1:B:724:VAL:HG12	1:B:734:VAL:HG22	1.42	1.00
1:D:1746:VAL:HG22	1:D:1747:CYS:H	1.27	0.99
1:A:324:VAL:HG12	1:A:334:VAL:HG22	1.43	0.99
1:E:2324:VAL:HG12	1:E:2334:VAL:HG22	1.40	0.99
1:F:2746:VAL:HG22	1:F:2747:CYS:H	1.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1044:THR:HG21	1:C:1298:VAL:HG12	1.44	0.98
1:F:2444:THR:HG21	1:F:2698:VAL:HG12	1.45	0.98
1:D:1724:VAL:HG12	1:D:1734:VAL:HG22	1.42	0.98
1:B:746:VAL:HG22	1:B:747:CYS:H	1.27	0.98
1:E:2044:THR:HG21	1:E:2298:VAL:HG12	1.45	0.97
1:C:1324:VAL:HG12	1:C:1334:VAL:HG22	1.43	0.97
1:B:444:THR:HG21	1:B:698:VAL:HG12	1.45	0.96
1:E:2346:VAL:HG22	1:E:2347:CYS:H	1.27	0.96
1:D:1444:THR:HG21	1:D:1698:VAL:HG12	1.47	0.96
1:A:44:THR:HG21	1:A:298:VAL:HG12	1.45	0.95
1:D:1750:LYS:HE3	1:D:1750:LYS:H	1.32	0.95
1:B:721:ARG:C	1:B:722:LYS:HD2	1.92	0.94
1:B:476:MET:HE2	1:B:724:VAL:HG21	1.50	0.94
1:C:1350:LYS:H	1:C:1350:LYS:HE3	1.33	0.94
1:C:1321:ARG:C	1:C:1322:LYS:HD2	1.91	0.94
1:E:2321:ARG:C	1:E:2322:LYS:HD2	1.93	0.94
1:F:2721:ARG:C	1:F:2722:LYS:HD2	1.93	0.94
1:A:321:ARG:C	1:A:322:LYS:HD2	1.93	0.93
1:A:76:MET:HE2	1:A:324:VAL:HG21	1.50	0.93
1:B:750:LYS:HE3	1:B:750:LYS:H	1.32	0.93
1:F:2476:MET:HE2	1:F:2724:VAL:HG21	1.49	0.93
1:A:350:LYS:HE3	1:A:350:LYS:H	1.32	0.93
1:E:2350:LYS:HE3	1:E:2350:LYS:H	1.33	0.93
1:E:2076:MET:HE2	1:E:2324:VAL:HG21	1.50	0.93
1:D:1721:ARG:C	1:D:1722:LYS:HD2	1.93	0.92
1:D:1476:MET:HE2	1:D:1724:VAL:HG21	1.49	0.92
1:F:2750:LYS:H	1:F:2750:LYS:HE3	1.34	0.91
1:C:1076:MET:HE2	1:C:1324:VAL:HG21	1.51	0.91
1:C:1100:ILE:HD12	1:C:1100:ILE:H	1.35	0.89
1:B:500:ILE:H	1:B:500:ILE:HD12	1.37	0.89
1:E:2100:ILE:H	1:E:2100:ILE:HD12	1.38	0.89
1:A:100:ILE:HD12	1:A:100:ILE:H	1.36	0.89
1:F:2500:ILE:HD12	1:F:2500:ILE:H	1.39	0.86
1:E:2323:GLN:NE2	1:E:2353:PRO:HB3	1.91	0.86
1:D:1500:ILE:H	1:D:1500:ILE:HD12	1.37	0.86
1:F:2723:GLN:NE2	1:F:2753:PRO:HB3	1.90	0.85
1:B:723:GLN:NE2	1:B:753:PRO:HB3	1.92	0.85
1:C:1323:GLN:NE2	1:C:1353:PRO:HB3	1.92	0.85
1:D:1723:GLN:NE2	1:D:1753:PRO:HB3	1.91	0.85
1:E:2112:ALA:HA	1:E:2146:MET:HE1	1.58	0.84
1:E:2197:VAL:HB	1:F:2428:ILE:HD13	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2512:ALA:HA	1:F:2546:MET:HE1	1.59	0.84
1:A:112:ALA:HA	1:A:146:MET:HE1	1.61	0.83
1:A:323:GLN:NE2	1:A:353:PRO:HB3	1.91	0.83
1:F:2537:ARG:HG2	1:F:2537:ARG:HH11	1.43	0.83
1:A:254:GLU:OE1	1:D:1719:SER:HB2	1.77	0.83
1:C:1350:LYS:H	1:C:1350:LYS:CE	1.92	0.83
1:D:1750:LYS:H	1:D:1750:LYS:CE	1.92	0.83
1:E:2018:THR:HG21	1:E:2100:ILE:O	1.80	0.82
1:C:1346:VAL:HG22	1:C:1347:CYS:N	1.95	0.82
1:C:1112:ALA:HA	1:C:1146:MET:HE1	1.61	0.82
1:F:2612:TYR:HB2	1:F:2617:GLU:HG3	1.62	0.81
1:A:350:LYS:H	1:A:350:LYS:CE	1.92	0.81
1:B:719:SER:HB2	1:C:1254:GLU:OE1	1.79	0.81
1:E:2212:TYR:HB2	1:E:2217:GLU:HG3	1.62	0.81
1:E:2350:LYS:H	1:E:2350:LYS:CE	1.92	0.81
1:A:212:TYR:HB2	1:A:217:GLU:HG3	1.63	0.81
1:A:346:VAL:HG22	1:A:347:CYS:N	1.96	0.81
1:B:750:LYS:H	1:B:750:LYS:CE	1.93	0.81
1:E:2028:ILE:HD13	1:F:2597:VAL:HB	1.60	0.81
1:F:2750:LYS:H	1:F:2750:LYS:CE	1.93	0.80
1:B:512:ALA:HA	1:B:546:MET:HE1	1.62	0.80
1:A:225:LEU:HB2	1:A:228:LYS:HB2	1.63	0.80
1:B:746:VAL:HG22	1:B:747:CYS:N	1.96	0.80
1:D:1746:VAL:HG22	1:D:1747:CYS:N	1.96	0.80
1:D:1512:ALA:HA	1:D:1546:MET:HE1	1.62	0.80
1:C:1212:TYR:HB2	1:C:1217:GLU:HG3	1.63	0.79
1:C:1225:LEU:HB2	1:C:1228:LYS:HB2	1.64	0.79
1:A:197:VAL:HB	1:B:428:ILE:HD13	1.64	0.79
1:B:625:LEU:HB2	1:B:628:LYS:HB2	1.64	0.79
1:C:1319:SER:HB2	1:F:2654:GLU:OE1	1.82	0.79
1:F:2746:VAL:HG22	1:F:2747:CYS:N	1.96	0.79
1:D:1625:LEU:HB2	1:D:1628:LYS:HB2	1.63	0.79
1:D:1722:LYS:HG3	1:D:1736:PRO:CA	2.10	0.79
1:D:1612:TYR:HB2	1:D:1617:GLU:HG3	1.65	0.79
1:A:18:THR:HG21	1:A:100:ILE:O	1.82	0.78
1:F:2625:LEU:HB2	1:F:2628:LYS:HB2	1.64	0.78
1:B:438:VAL:HG12	1:B:707:VAL:HG13	1.66	0.78
1:B:612:TYR:HB2	1:B:617:GLU:HG3	1.65	0.78
1:C:1038:VAL:HG12	1:C:1307:VAL:HG13	1.66	0.78
1:B:722:LYS:HG3	1:B:736:PRO:CA	2.10	0.78
1:E:2137:ARG:HG2	1:E:2137:ARG:HH11	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2225:LEU:HB2	1:E:2228:LYS:HB2	1.65	0.78
1:C:1018:THR:HG21	1:C:1100:ILE:O	1.84	0.78
1:D:1418:THR:HG21	1:D:1500:ILE:O	1.84	0.78
1:F:2418:THR:HG21	1:F:2500:ILE:O	1.83	0.77
1:B:418:THR:HG21	1:B:500:ILE:O	1.84	0.77
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.49	0.77
1:C:1197:VAL:HB	1:D:1428:ILE:HD13	1.65	0.77
1:E:2331:HIS:ND1	1:E:2346:VAL:HG11	2.00	0.77
1:C:1137:ARG:HH11	1:C:1137:ARG:HG2	1.48	0.77
1:B:731:HIS:ND1	1:B:746:VAL:HG11	1.99	0.77
1:E:2254:GLU:HG3	1:E:2258:ARG:HH12	1.49	0.77
1:D:1438:VAL:HG12	1:D:1707:VAL:HG13	1.67	0.77
1:E:2038:VAL:HG12	1:E:2307:VAL:HG13	1.66	0.77
1:A:146:MET:HG3	1:A:147:ILE:N	2.01	0.76
1:A:319:SER:HB2	1:E:2254:GLU:OE1	1.84	0.76
1:A:38:VAL:HG12	1:A:307:VAL:HG13	1.67	0.76
1:B:546:MET:HG3	1:B:547:ILE:N	2.01	0.76
1:D:1549:ARG:HH11	1:D:1553:ILE:HD11	1.49	0.76
1:D:1628:LYS:HA	1:D:1628:LYS:HE2	1.67	0.76
1:C:1028:ILE:HD13	1:D:1597:VAL:HB	1.67	0.76
1:D:1546:MET:HG3	1:D:1547:ILE:N	2.01	0.76
1:E:2149:ARG:HH11	1:E:2153:ILE:HD11	1.51	0.76
1:B:549:ARG:HH11	1:B:553:ILE:HD11	1.51	0.76
1:C:1100:ILE:HD12	1:C:1100:ILE:N	2.00	0.76
1:C:1228:LYS:HE2	1:C:1228:LYS:HA	1.68	0.76
1:F:2731:HIS:ND1	1:F:2746:VAL:HG11	2.00	0.76
1:E:2322:LYS:HG3	1:E:2336:PRO:CA	2.12	0.76
1:E:2346:VAL:HG22	1:E:2347:CYS:N	1.96	0.75
1:F:2546:MET:HG3	1:F:2547:ILE:N	1.99	0.75
1:A:228:LYS:HE2	1:A:228:LYS:HA	1.69	0.75
1:C:1331:HIS:ND1	1:C:1346:VAL:HG11	2.00	0.75
1:F:2654:GLU:HG3	1:F:2658:ARG:HH12	1.51	0.75
1:B:500:ILE:HD12	1:B:500:ILE:N	2.01	0.75
1:D:1731:HIS:ND1	1:D:1746:VAL:HG11	2.00	0.75
1:F:2438:VAL:HG12	1:F:2707:VAL:HG13	1.66	0.75
1:B:628:LYS:HA	1:B:628:LYS:HE2	1.67	0.75
1:E:2100:ILE:HD12	1:E:2100:ILE:N	2.02	0.75
1:D:1537:ARG:HG2	1:D:1537:ARG:HH11	1.51	0.75
1:B:615:LYS:HD3	1:B:650:GLU:OE1	1.87	0.74
1:F:2628:LYS:HE2	1:F:2628:LYS:HA	1.69	0.74
1:A:149:ARG:HH11	1:A:153:ILE:HD11	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:ASP:HB2	1:B:614:GLU:HG3	1.70	0.74
1:A:322:LYS:HG3	1:A:336:PRO:CA	2.11	0.74
1:D:1615:LYS:HD3	1:D:1650:GLU:OE1	1.87	0.74
1:F:2726:ARG:HH12	1:F:2781:GLN:HE21	1.33	0.74
1:A:100:ILE:HD12	1:A:100:ILE:N	2.03	0.74
1:D:1500:ILE:HD12	1:D:1500:ILE:N	2.02	0.74
1:F:2549:ARG:HH11	1:F:2553:ILE:HD11	1.50	0.74
1:D:1431:VAL:C	1:D:1433:ASN:H	1.96	0.74
1:D:1654:GLU:OE1	1:E:2319:SER:HB2	1.87	0.74
1:E:2031:VAL:C	1:E:2033:ASN:H	1.96	0.73
1:C:1031:VAL:C	1:C:1033:ASN:H	1.96	0.73
1:C:1215:LYS:HD3	1:C:1250:GLU:OE1	1.87	0.73
1:E:2146:MET:HG3	1:E:2147:ILE:N	2.02	0.73
1:A:331:HIS:ND1	1:A:346:VAL:HG11	2.02	0.73
1:F:2500:ILE:HD12	1:F:2500:ILE:N	2.02	0.73
1:C:1146:MET:HG3	1:C:1147:ILE:N	2.03	0.73
1:C:1149:ARG:HH11	1:C:1153:ILE:HD11	1.52	0.73
1:E:2228:LYS:HA	1:E:2228:LYS:HE2	1.69	0.73
1:B:650:GLU:OE2	1:F:2716:GLY:HA2	1.89	0.72
1:B:654:GLU:OE1	1:F:2719:SER:HB2	1.89	0.72
1:B:724:VAL:HG23	1:B:754:LEU:HB2	1.71	0.72
1:A:28:ILE:HD13	1:B:597:VAL:HB	1.69	0.72
1:C:1003:ARG:HG2	1:D:1409:GLU:OE2	1.89	0.72
1:E:2215:LYS:HD3	1:E:2250:GLU:OE1	1.89	0.72
1:E:2044:THR:HG21	1:E:2298:VAL:CG1	2.18	0.72
1:F:2609:ASP:HB2	1:F:2614:GLU:HG3	1.71	0.72
1:A:215:LYS:HD3	1:A:250:GLU:OE1	1.89	0.72
1:B:537:ARG:HG2	1:B:537:ARG:HH11	1.52	0.72
1:F:2615:LYS:HD3	1:F:2650:GLU:OE1	1.89	0.72
1:A:322:LYS:HZ1	1:A:336:PRO:HB3	1.54	0.72
1:F:2431:VAL:C	1:F:2433:ASN:H	1.97	0.72
1:A:255:LEU:HD13	1:A:263:VAL:CG2	2.20	0.72
1:B:726:ARG:HH12	1:B:781:GLN:HE21	1.38	0.72
1:C:1009:GLU:OE2	1:D:1403:ARG:HG2	1.90	0.72
1:E:2209:ASP:HB2	1:E:2214:GLU:HG3	1.72	0.72
1:A:31:VAL:C	1:A:33:ASN:H	1.97	0.71
1:B:444:THR:HG21	1:B:698:VAL:CG1	2.19	0.71
1:A:254:GLU:HG3	1:A:258:ARG:HH12	1.55	0.71
1:C:1044:THR:HG21	1:C:1298:VAL:CG1	2.19	0.71
1:B:431:VAL:C	1:B:433:ASN:H	1.95	0.71
1:C:1209:ASP:HB2	1:C:1214:GLU:HG3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1609:ASP:HB2	1:D:1614:GLU:HG3	1.70	0.71
1:D:1724:VAL:HG23	1:D:1754:LEU:HB2	1.72	0.71
1:E:2255:LEU:HD13	1:E:2263:VAL:CG2	2.20	0.71
1:E:2326:ARG:HH12	1:E:2381:GLN:HE21	1.37	0.71
1:A:9:GLU:OE2	1:B:403:ARG:HG2	1.89	0.71
1:B:655:LEU:HD13	1:B:663:VAL:CG2	2.20	0.71
1:D:1588:VAL:HA	1:D:1591:TRP:NE1	2.06	0.71
1:F:2655:LEU:HD13	1:F:2663:VAL:CG2	2.21	0.71
1:F:2724:VAL:HG23	1:F:2754:LEU:HB2	1.73	0.71
1:A:3:ARG:HG2	1:B:409:GLU:OE2	1.90	0.71
1:A:209:ASP:HB2	1:A:214:GLU:HG3	1.71	0.71
1:C:1324:VAL:HG23	1:C:1354:LEU:HB2	1.72	0.71
1:C:1322:LYS:HG3	1:C:1336:PRO:CA	2.11	0.70
1:C:1322:LYS:HZ2	1:C:1336:PRO:HB3	1.55	0.70
1:D:1726:ARG:HH12	1:D:1781:GLN:HE21	1.38	0.70
1:E:2188:VAL:HA	1:E:2191:TRP:NE1	2.06	0.70
1:E:2254:GLU:HG3	1:E:2258:ARG:NH1	2.06	0.70
1:D:1650:GLU:OE2	1:E:2316:GLY:HA2	1.90	0.70
1:F:2571:LYS:HG3	1:F:2571:LYS:O	1.91	0.70
1:F:2588:VAL:HA	1:F:2591:TRP:NE1	2.07	0.70
1:C:1255:LEU:HD13	1:C:1263:VAL:CG2	2.21	0.70
1:D:1655:LEU:HD13	1:D:1663:VAL:CG2	2.21	0.70
1:B:738:ASN:C	1:B:739:LYS:HD2	2.17	0.70
1:E:2171:LYS:O	1:E:2171:LYS:HG3	1.92	0.70
1:F:2654:GLU:HG3	1:F:2658:ARG:NH1	2.07	0.70
1:F:2444:THR:HG21	1:F:2698:VAL:CG1	2.20	0.69
1:A:324:VAL:HG23	1:A:354:LEU:HB2	1.73	0.69
1:B:588:VAL:HA	1:B:591:TRP:NE1	2.06	0.69
1:C:1188:VAL:HA	1:C:1191:TRP:NE1	2.08	0.69
1:D:1444:THR:HG21	1:D:1698:VAL:CG1	2.22	0.69
1:D:1654:GLU:HG3	1:D:1658:ARG:HH12	1.56	0.69
1:D:1738:ASN:C	1:D:1739:LYS:HD2	2.18	0.69
1:F:2722:LYS:HG3	1:F:2736:PRO:CA	2.12	0.69
1:F:2557:ASP:HA	1:F:2775:ARG:NH1	2.01	0.69
1:C:1005:TYR:O	1:D:1545:PRO:HG2	1.93	0.68
1:B:654:GLU:HG3	1:B:658:ARG:HH12	1.59	0.68
1:A:188:VAL:HA	1:A:191:TRP:NE1	2.08	0.68
1:B:722:LYS:HZ2	1:B:736:PRO:HB3	1.58	0.68
1:C:1254:GLU:HG3	1:C:1258:ARG:HH12	1.58	0.68
1:F:2465:LEU:HD22	1:F:2508:MET:CE	2.24	0.68
1:A:44:THR:HG21	1:A:298:VAL:CG1	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:O	1:A:171:LYS:HG3	1.94	0.68
1:C:1137:ARG:HH11	1:C:1137:ARG:CG	2.07	0.68
1:F:2537:ARG:HH11	1:F:2537:ARG:CG	2.06	0.68
1:B:655:LEU:HD13	1:B:663:VAL:HG21	1.76	0.68
1:D:1595:ASP:HA	1:D:1604:ARG:HE	1.58	0.68
1:E:2324:VAL:HG23	1:E:2354:LEU:HB2	1.75	0.68
1:B:595:ASP:HA	1:B:604:ARG:HE	1.59	0.68
1:D:1655:LEU:HD13	1:D:1663:VAL:HG21	1.76	0.68
1:A:137:ARG:HH11	1:A:137:ARG:CG	2.07	0.67
1:B:489:LEU:HD23	1:B:489:LEU:C	2.20	0.67
1:F:2489:LEU:C	1:F:2489:LEU:HD23	2.18	0.67
1:E:2137:ARG:HH11	1:E:2137:ARG:CG	2.07	0.67
1:A:145:PRO:HG2	1:B:405:TYR:O	1.94	0.67
1:E:2065:LEU:HD22	1:E:2108:MET:CE	2.25	0.67
1:D:1465:LEU:HD22	1:D:1508:MET:CE	2.25	0.66
1:E:2255:LEU:HD13	1:E:2263:VAL:HG21	1.78	0.66
1:B:465:LEU:HD22	1:B:508:MET:CE	2.25	0.66
1:E:2089:LEU:C	1:E:2089:LEU:HD23	2.21	0.66
1:F:2465:LEU:HD22	1:F:2508:MET:HE2	1.77	0.66
1:A:173:VAL:HG22	1:A:174:GLY:N	2.11	0.66
1:A:338:ASN:C	1:A:339:LYS:HD2	2.20	0.66
1:B:571:LYS:O	1:B:571:LYS:HG3	1.95	0.66
1:A:65:LEU:HD22	1:A:108:MET:HE2	1.77	0.66
1:C:1255:LEU:HD13	1:C:1263:VAL:HG21	1.77	0.66
1:A:179:ALA:HA	1:B:704:ILE:HD11	1.78	0.66
1:A:254:GLU:HG3	1:A:258:ARG:NH1	2.11	0.66
1:C:1171:LYS:HG3	1:C:1171:LYS:O	1.93	0.66
1:F:2517:THR:O	1:F:2521:ARG:HG3	1.95	0.66
1:E:2338:ASN:C	1:E:2339:LYS:HD2	2.21	0.66
1:A:5:TYR:O	1:B:545:PRO:HG2	1.95	0.65
1:A:224:ALA:C	1:A:226:GLY:H	2.04	0.65
1:C:1065:LEU:HD22	1:C:1108:MET:CE	2.26	0.65
1:A:89:LEU:C	1:A:89:LEU:HD23	2.22	0.65
1:D:1517:THR:O	1:D:1521:ARG:HG3	1.97	0.65
1:C:1065:LEU:HD22	1:C:1108:MET:HE2	1.78	0.65
1:C:1117:THR:O	1:C:1121:ARG:HG3	1.95	0.65
1:E:2322:LYS:CG	1:E:2336:PRO:HA	2.15	0.65
1:C:1342:GLU:OE2	1:C:1342:GLU:HA	1.97	0.65
1:D:1742:GLU:HA	1:D:1742:GLU:OE2	1.96	0.65
1:E:2065:LEU:HD22	1:E:2108:MET:HE2	1.79	0.65
1:A:255:LEU:HD13	1:A:263:VAL:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1145:PRO:HG2	1:D:1405:TYR:O	1.97	0.65
1:D:1654:GLU:HG3	1:D:1658:ARG:NH1	2.11	0.65
1:F:2742:GLU:OE2	1:F:2742:GLU:HA	1.96	0.65
1:B:742:GLU:HA	1:B:742:GLU:OE2	1.96	0.65
1:D:1573:VAL:HG22	1:D:1574:GLY:N	2.12	0.65
1:A:157:ASP:CA	1:A:375:ARG:HH12	2.03	0.64
1:A:195:ASP:HA	1:A:204:ARG:HE	1.62	0.64
1:A:342:GLU:OE2	1:A:342:GLU:HA	1.97	0.64
1:D:1557:ASP:CA	1:D:1775:ARG:HH12	2.03	0.64
1:F:2722:LYS:CG	1:F:2736:PRO:HA	2.15	0.64
1:B:557:ASP:CA	1:B:775:ARG:HH12	2.03	0.64
1:D:1571:LYS:O	1:D:1571:LYS:HG3	1.96	0.64
1:C:1089:LEU:C	1:C:1089:LEU:HD23	2.22	0.64
1:C:1179:ALA:HA	1:D:1704:ILE:HD11	1.79	0.64
1:C:1338:ASN:C	1:C:1339:LYS:HD2	2.21	0.64
1:F:2595:ASP:HA	1:F:2604:ARG:HE	1.62	0.64
1:A:65:LEU:HD22	1:A:108:MET:CE	2.26	0.64
1:D:1537:ARG:HH11	1:D:1537:ARG:CG	2.10	0.64
1:D:1624:ALA:C	1:D:1626:GLY:H	2.05	0.64
1:F:2624:ALA:C	1:F:2626:GLY:H	2.05	0.64
1:D:1722:LYS:CG	1:D:1736:PRO:HA	2.14	0.64
1:E:2173:VAL:HG22	1:E:2174:GLY:N	2.13	0.64
1:B:573:VAL:HG22	1:B:574:GLY:N	2.13	0.64
1:F:2726:ARG:NH1	1:F:2781:GLN:HE21	1.96	0.64
1:A:157:ASP:HA	1:A:375:ARG:NH1	2.01	0.64
1:B:517:THR:O	1:B:521:ARG:HG3	1.98	0.64
1:C:1157:ASP:CA	1:C:1375:ARG:HH12	2.02	0.64
1:D:1557:ASP:HA	1:D:1775:ARG:NH1	2.02	0.64
1:E:2342:GLU:HA	1:E:2342:GLU:OE2	1.96	0.64
1:A:364:ILE:HG13	1:A:364:ILE:O	1.97	0.64
1:B:654:GLU:HG3	1:B:658:ARG:NH1	2.13	0.64
1:C:1224:ALA:C	1:C:1226:GLY:H	2.04	0.64
1:C:1254:GLU:HG3	1:C:1258:ARG:NH1	2.12	0.64
1:E:2224:ALA:C	1:E:2226:GLY:H	2.05	0.64
1:F:2738:ASN:C	1:F:2739:LYS:HD2	2.22	0.64
1:C:1100:ILE:H	1:C:1100:ILE:CD1	2.10	0.63
1:D:1465:LEU:HD22	1:D:1508:MET:HE2	1.80	0.63
1:B:465:LEU:HD22	1:B:508:MET:HE2	1.80	0.63
1:B:722:LYS:CG	1:B:736:PRO:HA	2.13	0.63
1:B:537:ARG:HH11	1:B:537:ARG:CG	2.12	0.63
1:C:1326:ARG:HH12	1:C:1381:GLN:HE21	1.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:H	1:A:100:ILE:CD1	2.11	0.63
1:B:521:ARG:CB	1:B:789:ILE:HD11	2.29	0.63
1:B:624:ALA:C	1:B:626:GLY:H	2.05	0.63
1:E:2195:ASP:HA	1:E:2204:ARG:HE	1.62	0.63
1:D:1489:LEU:HD23	1:D:1489:LEU:C	2.23	0.63
1:B:725:TYR:CE2	1:B:753:PRO:HG3	2.33	0.63
1:C:1173:VAL:HG22	1:C:1174:GLY:N	2.13	0.63
1:A:173:VAL:HG22	1:A:174:GLY:H	1.63	0.63
1:C:1157:ASP:HA	1:C:1375:ARG:NH1	2.02	0.63
1:C:1195:ASP:HA	1:C:1204:ARG:HE	1.62	0.63
1:A:117:THR:O	1:A:121:ARG:HG3	1.98	0.63
1:E:2117:THR:O	1:E:2121:ARG:HG3	1.99	0.63
1:A:121:ARG:CB	1:A:389:ILE:HD11	2.29	0.62
1:C:1364:ILE:HG13	1:C:1364:ILE:O	1.97	0.62
1:E:2245:ARG:N	1:E:2279:ILE:HD11	2.14	0.62
1:F:2764:ILE:HG13	1:F:2764:ILE:O	1.99	0.62
1:F:2573:VAL:HG22	1:F:2574:GLY:N	2.14	0.62
1:D:1774:ILE:O	1:D:1777:TYR:HB3	2.00	0.62
1:E:2197:VAL:HB	1:F:2428:ILE:CD1	2.29	0.62
1:A:245:ARG:N	1:A:279:ILE:HD11	2.15	0.62
1:D:1521:ARG:CB	1:D:1789:ILE:HD11	2.30	0.62
1:B:774:ILE:O	1:B:777:TYR:HB3	1.99	0.62
1:E:2005:TYR:O	1:F:2545:PRO:HG2	1.99	0.62
1:F:2655:LEU:HD13	1:F:2663:VAL:HG21	1.80	0.62
1:E:2364:ILE:O	1:E:2364:ILE:HG13	1.99	0.61
1:A:325:TYR:CE2	1:A:353:PRO:HG3	2.35	0.61
1:E:2326:ARG:NH1	1:E:2381:GLN:HE21	1.97	0.61
1:C:1322:LYS:CG	1:C:1336:PRO:HA	2.14	0.61
1:E:2145:PRO:HG2	1:F:2405:TYR:O	1.99	0.61
1:F:2579:ALA:O	1:F:2583:THR:HG23	2.01	0.61
1:E:2179:ALA:HA	1:F:2704:ILE:HD11	1.82	0.61
1:B:671:LEU:CD1	1:B:688:VAL:HG22	2.30	0.61
1:B:764:ILE:HG13	1:B:764:ILE:O	2.01	0.61
1:C:1194:PHE:HA	1:D:1428:ILE:CD1	2.31	0.61
1:D:1725:TYR:CE2	1:D:1753:PRO:HG3	2.35	0.61
1:E:2028:ILE:CD1	1:F:2597:VAL:HB	2.28	0.61
1:F:2539:MET:HE2	4:F:11:HOH:O	2.01	0.61
1:F:2717:LYS:HD3	1:F:2718:LEU:H	1.65	0.61
1:B:504:ALA:O	1:B:508:MET:HG3	2.01	0.61
1:D:1500:ILE:H	1:D:1500:ILE:CD1	2.12	0.61
1:F:2578:HIS:HE1	1:F:2609:ASP:O	1.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1053:TRP:CD1	1:C:1053:TRP:C	2.79	0.60
1:C:1317:LYS:HD3	1:C:1318:LEU:H	1.66	0.60
1:A:276:ILE:O	1:A:280:VAL:HG22	2.01	0.60
1:F:2500:ILE:H	1:F:2500:ILE:CD1	2.13	0.60
1:F:2557:ASP:CA	1:F:2775:ARG:HH12	2.03	0.60
1:B:717:LYS:HD3	1:B:718:LEU:H	1.66	0.60
1:D:1764:ILE:HG13	1:D:1764:ILE:O	2.00	0.60
1:F:2671:LEU:CD1	1:F:2688:VAL:HG22	2.31	0.60
1:A:233:ARG:HA	1:A:266:PHE:O	2.01	0.60
1:C:1194:PHE:HA	1:D:1428:ILE:HD12	1.84	0.60
1:A:346:VAL:CG2	1:A:347:CYS:H	2.06	0.60
1:D:1573:VAL:HG22	1:D:1574:GLY:H	1.67	0.60
1:E:2100:ILE:H	1:E:2100:ILE:CD1	2.11	0.60
1:F:2504:ALA:O	1:F:2508:MET:HG3	2.01	0.60
1:F:2731:HIS:ND1	1:F:2746:VAL:CG1	2.64	0.60
1:C:1325:TYR:CE2	1:C:1353:PRO:HG3	2.36	0.60
1:E:2327:CYS:SG	1:E:2329:ASN:N	2.71	0.60
1:E:2325:TYR:CE2	1:E:2353:PRO:HG3	2.37	0.60
1:F:2521:ARG:CB	1:F:2789:ILE:HD11	2.32	0.60
1:F:2725:TYR:CE2	1:F:2753:PRO:HG3	2.36	0.60
1:A:194:PHE:HA	1:B:428:ILE:CD1	2.32	0.60
1:A:326:ARG:HH12	1:A:381:GLN:HE21	1.48	0.60
1:B:500:ILE:H	1:B:500:ILE:CD1	2.12	0.60
1:D:1671:LEU:CD1	1:D:1688:VAL:HG22	2.32	0.60
1:D:1717:LYS:HD3	1:D:1718:LEU:H	1.67	0.60
1:B:573:VAL:HG22	1:B:574:GLY:H	1.67	0.60
1:E:2028:ILE:HD11	1:F:2598:ILE:HG12	1.84	0.60
1:E:2157:ASP:HA	1:E:2375:ARG:NH1	2.02	0.60
1:E:2173:VAL:HG22	1:E:2174:GLY:H	1.67	0.60
1:F:2774:ILE:O	1:F:2777:TYR:HB3	2.02	0.60
1:A:271:LEU:CD1	1:A:288:VAL:HG22	2.31	0.59
1:B:619:VAL:O	1:B:623:GLU:HG2	2.02	0.59
1:C:1374:ILE:O	1:C:1377:TYR:HB3	2.02	0.59
1:E:2317:LYS:HD3	1:E:2318:LEU:H	1.66	0.59
1:C:1104:ALA:O	1:C:1108:MET:HG3	2.01	0.59
1:E:2178:HIS:HE1	1:E:2209:ASP:O	1.84	0.59
1:E:2179:ALA:O	1:E:2183:THR:HG23	2.01	0.59
1:E:2271:LEU:CD1	1:E:2288:VAL:HG22	2.32	0.59
1:B:726:ARG:NH1	1:B:781:GLN:HE21	2.00	0.59
1:A:194:PHE:HA	1:B:428:ILE:HD12	1.85	0.59
1:C:1233:ARG:HA	1:C:1266:PHE:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2331:HIS:ND1	1:E:2346:VAL:CG1	2.64	0.59
1:B:731:HIS:ND1	1:B:746:VAL:CG1	2.65	0.59
1:E:2157:ASP:CA	1:E:2375:ARG:HH12	2.04	0.59
1:F:2444:THR:HG23	1:F:2700:PHE:CD2	2.38	0.59
1:E:2219:VAL:O	1:E:2223:GLU:HG2	2.02	0.59
1:A:179:ALA:O	1:A:183:THR:HG23	2.02	0.59
1:C:1121:ARG:CB	1:C:1389:ILE:HD11	2.32	0.59
1:C:1173:VAL:HG22	1:C:1174:GLY:H	1.67	0.59
1:C:1180:LEU:C	1:C:1180:LEU:HD23	2.28	0.59
1:E:2198:ILE:HG12	1:F:2428:ILE:HD11	1.83	0.59
1:E:2374:ILE:O	1:E:2377:TYR:HB3	2.02	0.59
1:C:1331:HIS:ND1	1:C:1346:VAL:CG1	2.65	0.59
1:E:2304:ILE:HD11	1:F:2579:ALA:HA	1.83	0.58
1:F:2515:ILE:HG23	1:F:2692:ILE:O	2.02	0.58
1:A:180:LEU:C	1:A:180:LEU:HD23	2.28	0.58
1:C:1271:LEU:CD1	1:C:1288:VAL:HG22	2.32	0.58
1:D:1726:ARG:NH1	1:D:1781:GLN:HE21	2.01	0.58
1:F:2619:VAL:O	1:F:2623:GLU:HG2	2.02	0.58
1:B:579:ALA:O	1:B:583:THR:HG23	2.02	0.58
1:F:2453:TRP:CD1	1:F:2453:TRP:C	2.81	0.58
1:A:44:THR:HG23	1:A:300:PHE:CD2	2.39	0.58
1:A:317:LYS:HD3	1:A:318:LEU:H	1.68	0.58
1:B:557:ASP:HA	1:B:775:ARG:NH1	2.03	0.58
1:E:2006:ILE:HD11	1:F:2409:GLU:OE1	2.03	0.58
1:C:1044:THR:HG23	1:C:1300:PHE:CD2	2.39	0.58
1:D:1731:HIS:ND1	1:D:1746:VAL:CG1	2.66	0.58
1:D:1504:ALA:O	1:D:1508:MET:HG3	2.03	0.58
1:E:2233:ARG:HA	1:E:2266:PHE:O	2.03	0.58
1:D:1633:ARG:HA	1:D:1666:PHE:O	2.03	0.58
1:A:344:CYS:SG	1:A:346:VAL:HG12	2.44	0.58
1:E:2121:ARG:CB	1:E:2389:ILE:HD11	2.33	0.58
1:A:331:HIS:ND1	1:A:346:VAL:CG1	2.67	0.58
1:B:744:CYS:SG	1:B:746:VAL:HG12	2.44	0.58
1:D:1444:THR:HG23	1:D:1700:PHE:CD2	2.39	0.58
1:E:2002:LYS:HD3	1:E:2006:ILE:HD12	1.86	0.58
1:B:402:LYS:HD3	1:B:406:ILE:HD12	1.86	0.58
1:D:1578:HIS:HE1	1:D:1609:ASP:O	1.86	0.58
1:F:2573:VAL:HG22	1:F:2574:GLY:H	1.69	0.58
1:D:1589:LYS:HG2	1:D:1593:TYR:CE1	2.39	0.57
1:F:2726:ARG:HH12	1:F:2781:GLN:NE2	2.02	0.57
1:C:1115:ILE:HG23	1:C:1292:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1402:LYS:HD3	1:D:1406:ILE:HD12	1.86	0.57
1:D:1619:VAL:O	1:D:1623:GLU:HG2	2.04	0.57
1:F:2645:ARG:N	1:F:2679:ILE:HD11	2.18	0.57
1:B:444:THR:HG23	1:B:700:PHE:CD2	2.37	0.57
1:B:682:VAL:HG12	1:B:682:VAL:O	2.05	0.57
1:A:133:SER:O	1:A:134:PHE:HD1	1.87	0.57
1:B:408:ASN:HB2	1:B:411:GLU:HG3	1.84	0.57
1:C:1006:ILE:HG21	1:C:1142:ALA:HB2	1.85	0.57
1:E:2006:ILE:HG21	1:E:2142:ALA:HB2	1.86	0.57
1:A:8:ASN:HB2	1:A:11:GLU:HG3	1.86	0.57
1:C:1304:ILE:HD11	1:D:1579:ALA:HA	1.85	0.57
1:C:1331:HIS:CG	1:C:1346:VAL:HG11	2.39	0.57
1:E:2146:MET:HE3	1:E:2146:MET:O	2.05	0.57
1:C:1178:HIS:HE1	1:C:1209:ASP:O	1.87	0.57
1:C:1208:VAL:HG13	1:C:1217:GLU:HB2	1.87	0.57
1:D:1408:ASN:HB2	1:D:1411:GLU:HG3	1.86	0.57
1:D:1579:ALA:O	1:D:1583:THR:HG23	2.03	0.57
1:A:53:TRP:CD1	1:A:53:TRP:C	2.82	0.57
1:C:1031:VAL:C	1:C:1033:ASN:N	2.62	0.57
1:C:1245:ARG:N	1:C:1279:ILE:HD11	2.19	0.57
1:A:178:HIS:HE1	1:A:209:ASP:O	1.88	0.57
1:D:1515:ILE:HD13	1:D:1547:ILE:HG23	1.86	0.57
1:D:1744:CYS:SG	1:D:1746:VAL:HG12	2.44	0.57
1:E:2053:TRP:CD1	1:E:2053:TRP:C	2.82	0.57
1:F:2476:MET:CE	1:F:2724:VAL:HG21	2.28	0.57
1:D:1676:ILE:O	1:D:1680:VAL:HG22	2.04	0.57
1:D:1682:VAL:HG12	1:D:1682:VAL:O	2.05	0.57
1:E:2076:MET:CE	1:E:2324:VAL:HG21	2.30	0.57
1:E:2276:ILE:O	1:E:2280:VAL:HG22	2.04	0.57
1:E:2373:GLU:OE2	1:E:2376:GLU:OE1	2.22	0.57
1:F:2773:GLU:OE2	1:F:2776:GLU:OE1	2.22	0.57
1:A:6:ILE:HG21	1:A:142:ALA:HB2	1.86	0.56
1:A:53:TRP:CZ3	1:A:388:GLU:O	2.58	0.56
1:A:225:LEU:O	1:A:228:LYS:N	2.31	0.56
1:C:1179:ALA:O	1:C:1183:THR:HG23	2.05	0.56
1:F:2633:ARG:HA	1:F:2666:PHE:O	2.04	0.56
1:B:515:ILE:HD13	1:B:547:ILE:HG23	1.86	0.56
1:B:578:HIS:HE1	1:B:609:ASP:O	1.87	0.56
1:E:2175:THR:OG1	1:E:2176:MET:N	2.38	0.56
1:F:2698:VAL:O	1:F:2700:PHE:N	2.39	0.56
1:A:2:LYS:HD3	1:A:6:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:C	1:A:33:ASN:N	2.62	0.56
1:A:219:VAL:O	1:A:223:GLU:HG2	2.06	0.56
1:B:406:ILE:HG21	1:B:542:ALA:HB2	1.87	0.56
1:B:540:HIS:HD2	1:B:542:ALA:CB	2.18	0.56
1:F:2731:HIS:CG	1:F:2746:VAL:HG11	2.40	0.56
1:B:613:ASP:OD1	1:E:2240:ARG:NH1	2.39	0.56
1:D:1406:ILE:HG21	1:D:1542:ALA:HB2	1.87	0.56
1:E:2008:ASN:HB2	1:E:2011:GLU:HG3	1.88	0.56
1:E:2324:VAL:HG23	1:E:2324:VAL:O	2.06	0.56
1:B:724:VAL:CG2	1:B:754:LEU:HB2	2.36	0.56
1:C:1008:ASN:HB2	1:C:1011:GLU:HG3	1.86	0.56
1:C:1053:TRP:CZ3	1:C:1388:GLU:O	2.58	0.56
1:C:1146:MET:HE3	1:C:1146:MET:O	2.06	0.56
1:C:1166:GLU:O	1:C:1169:GLY:N	2.39	0.56
1:D:1431:VAL:C	1:D:1433:ASN:N	2.61	0.56
1:E:2009:GLU:OE1	1:F:2406:ILE:HD11	2.05	0.56
1:E:2172:ALA:HB3	1:F:2420:VAL:CG1	2.36	0.56
1:E:2208:VAL:HG13	1:E:2217:GLU:HB2	1.88	0.56
1:F:2406:ILE:HG21	1:F:2542:ALA:HB2	1.86	0.56
1:A:5:TYR:HA	1:B:567:MET:HE1	1.86	0.56
1:A:374:ILE:O	1:A:377:TYR:HB3	2.05	0.56
1:E:2020:VAL:CG1	1:F:2572:ALA:HB3	2.36	0.56
1:D:1645:ARG:N	1:D:1679:ILE:HD11	2.20	0.56
1:E:2057:VAL:HG21	1:E:2116:ALA:HB2	1.86	0.56
1:E:2326:ARG:HH12	1:E:2381:GLN:NE2	2.03	0.56
1:A:331:HIS:CG	1:A:346:VAL:HG11	2.40	0.56
1:E:2189:LYS:HG2	1:E:2193:TYR:CE1	2.40	0.56
1:A:189:LYS:HG2	1:A:193:TYR:CE1	2.41	0.56
1:C:1282:VAL:HG12	1:C:1282:VAL:O	2.05	0.56
1:E:2282:VAL:HG12	1:E:2282:VAL:O	2.06	0.56
1:E:2331:HIS:CG	1:E:2346:VAL:HG11	2.41	0.56
1:A:282:VAL:HG12	1:A:282:VAL:O	2.05	0.55
1:B:453:TRP:CD1	1:B:453:TRP:C	2.83	0.55
1:C:1005:TYR:HA	1:D:1567:MET:HE1	1.87	0.55
1:C:1008:ASN:N	1:C:1008:ASN:HD22	2.04	0.55
1:C:1344:CYS:SG	1:C:1346:VAL:HG12	2.46	0.55
1:D:1453:TRP:CD1	1:D:1453:TRP:C	2.84	0.55
1:E:2115:ILE:HG23	1:E:2292:ILE:O	2.06	0.55
1:A:304:ILE:HD11	1:B:579:ALA:HA	1.88	0.55
1:E:2311:PRO:O	1:E:2312:ILE:HG13	2.07	0.55
1:F:2580:LEU:CD2	1:F:2590:ALA:HB1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ARG:HA	1:B:666:PHE:O	2.06	0.55
1:B:679:ILE:O	1:B:683:VAL:HG22	2.06	0.55
1:B:731:HIS:CG	1:B:746:VAL:HG11	2.40	0.55
1:C:1324:VAL:CG2	1:C:1354:LEU:HB2	2.37	0.55
1:A:26:LYS:HD3	1:A:100:ILE:HD11	1.87	0.55
1:B:431:VAL:C	1:B:433:ASN:N	2.61	0.55
1:D:1540:HIS:HD2	1:D:1542:ALA:CB	2.19	0.55
1:E:2031:VAL:C	1:E:2033:ASN:N	2.62	0.55
1:E:2044:THR:HG23	1:E:2300:PHE:CD2	2.41	0.55
1:F:2589:LYS:HG2	1:F:2593:TYR:CE1	2.42	0.55
1:F:2608:VAL:HG13	1:F:2617:GLU:HB2	1.89	0.55
1:F:2727:CYS:SG	1:F:2729:ASN:N	2.74	0.55
1:A:236:THR:HB	1:A:241:ARG:HG2	1.89	0.55
1:C:1187:GLN:HG2	1:C:1217:GLU:OE1	2.07	0.55
1:C:1189:LYS:HG2	1:C:1193:TYR:CE1	2.42	0.55
1:E:2140:HIS:H	1:F:2511:GLN:NE2	2.05	0.55
1:A:71:VAL:HG12	1:A:93:GLY:HA3	1.89	0.55
1:A:111:GLN:NE2	1:B:540:HIS:H	2.05	0.55
1:C:1111:GLN:NE2	1:D:1540:HIS:H	2.05	0.55
1:C:1326:ARG:NH1	1:C:1381:GLN:HE21	2.03	0.55
1:D:1476:MET:CE	1:D:1724:VAL:HG21	2.31	0.55
1:D:1608:VAL:CG2	1:D:1632:VAL:HG13	2.37	0.55
1:D:1613:ASP:OD1	1:F:2640:ARG:NH1	2.38	0.55
1:E:2026:LYS:HD3	1:E:2100:ILE:HD11	1.89	0.55
1:E:2140:HIS:HD2	1:E:2142:ALA:CB	2.19	0.55
1:F:2408:ASN:HB2	1:F:2411:GLU:HG3	1.89	0.55
1:F:2540:HIS:HD2	1:F:2542:ALA:HB3	1.72	0.55
1:A:57:VAL:HG21	1:A:116:ALA:HB2	1.89	0.55
1:A:121:ARG:HB3	1:A:389:ILE:HD11	1.89	0.55
1:E:2104:ALA:O	1:E:2108:MET:HG3	2.07	0.55
1:F:2711:PRO:O	1:F:2712:ILE:HG13	2.07	0.55
1:A:246:LYS:HD3	1:D:1485:TYR:OH	2.07	0.55
1:B:589:LYS:HG2	1:B:593:TYR:CE1	2.41	0.55
1:E:2180:LEU:CD2	1:E:2190:ALA:HB1	2.37	0.55
1:E:2298:VAL:O	1:E:2300:PHE:N	2.40	0.55
1:F:2402:LYS:HD3	1:F:2406:ILE:HD12	1.87	0.55
1:C:1026:LYS:HD3	1:C:1100:ILE:HD11	1.88	0.54
1:C:1028:ILE:CD1	1:D:1594:PHE:HA	2.37	0.54
1:C:1166:GLU:O	1:C:1168:MET:N	2.40	0.54
1:E:2140:HIS:HD2	1:E:2142:ALA:HB3	1.72	0.54
1:E:2315:ARG:NH1	1:F:2609:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ASN:N	1:A:8:ASN:HD22	2.04	0.54
1:A:197:VAL:HB	1:B:428:ILE:CD1	2.36	0.54
1:A:208:VAL:CG2	1:A:232:VAL:HG13	2.37	0.54
1:A:320:GLY:HA3	1:A:322:LYS:HE2	1.89	0.54
1:C:1276:ILE:O	1:C:1280:VAL:HG22	2.07	0.54
1:D:1679:ILE:O	1:D:1683:VAL:HG22	2.06	0.54
1:D:1731:HIS:CG	1:D:1746:VAL:HG11	2.42	0.54
1:A:224:ALA:O	1:A:226:GLY:N	2.40	0.54
1:A:322:LYS:CG	1:A:336:PRO:HA	2.15	0.54
1:A:326:ARG:NH1	1:A:381:GLN:HE21	2.06	0.54
1:B:473:VAL:HB	1:B:759:ILE:HB	1.90	0.54
1:C:1002:LYS:HD3	1:C:1006:ILE:HD12	1.87	0.54
1:E:2208:VAL:CG2	1:E:2232:VAL:HG13	2.37	0.54
1:E:2365:VAL:HG12	1:E:2365:VAL:O	2.08	0.54
1:F:2566:GLU:O	1:F:2569:GLY:N	2.41	0.54
1:F:2765:VAL:HG12	1:F:2765:VAL:O	2.08	0.54
1:D:1426:LYS:HD3	1:D:1500:ILE:HD11	1.89	0.54
1:F:2608:VAL:CG2	1:F:2632:VAL:HG13	2.37	0.54
1:D:1534:PHE:HB3	3:D:1792:PCP:H3	1.90	0.54
1:D:1724:VAL:CG2	1:D:1754:LEU:HB2	2.37	0.54
1:A:149:ARG:NH1	1:A:153:ILE:HD11	2.22	0.54
1:B:647:ILE:HD11	1:E:2239:SER:O	2.08	0.54
1:A:187:GLN:HG2	1:A:217:GLU:OE1	2.08	0.54
1:A:208:VAL:HG12	1:A:209:ASP:N	2.23	0.54
1:B:676:ILE:O	1:B:680:VAL:HG22	2.08	0.54
1:C:1219:VAL:O	1:C:1223:GLU:HG2	2.08	0.54
1:C:1320:GLY:HA3	1:C:1322:LYS:HE2	1.89	0.54
1:D:1608:VAL:HG13	1:D:1617:GLU:HB2	1.90	0.54
1:F:2546:MET:HE3	1:F:2546:MET:O	2.07	0.54
1:A:208:VAL:HG13	1:A:217:GLU:HB2	1.89	0.54
1:A:208:VAL:HG21	1:A:232:VAL:HG13	1.90	0.54
1:B:546:MET:HE3	1:B:546:MET:O	2.08	0.54
1:D:1660:TYR:HA	1:D:1662:TRP:CZ3	2.43	0.54
1:E:2317:LYS:HD3	1:E:2318:LEU:N	2.23	0.54
1:E:2324:VAL:CG2	1:E:2354:LEU:HB2	2.38	0.54
1:F:2722:LYS:HZ2	1:F:2736:PRO:HB3	1.72	0.54
1:A:198:ILE:HG12	1:B:428:ILE:HD11	1.90	0.54
1:C:1279:ILE:O	1:C:1283:VAL:HG22	2.08	0.54
1:C:1298:VAL:O	1:C:1300:PHE:N	2.40	0.54
1:C:1311:PRO:O	1:C:1312:ILE:HG13	2.08	0.54
1:F:2426:LYS:HD3	1:F:2500:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2717:LYS:HD3	1:F:2718:LEU:N	2.22	0.54
1:A:28:ILE:CD1	1:B:594:PHE:HA	2.38	0.54
1:A:365:VAL:HG12	1:A:365:VAL:O	2.08	0.54
1:B:765:VAL:HG12	1:B:765:VAL:O	2.08	0.54
1:D:1726:ARG:HH12	1:D:1781:GLN:NE2	2.05	0.54
1:E:2133:SER:O	1:E:2134:PHE:HD1	1.91	0.54
1:F:2540:HIS:HD2	1:F:2542:ALA:CB	2.20	0.54
1:B:645:ARG:N	1:B:679:ILE:HD11	2.22	0.53
1:B:766:VAL:HG12	1:B:767:GLU:N	2.23	0.53
1:C:1224:ALA:O	1:C:1226:GLY:N	2.41	0.53
1:E:2156:CYS:O	1:E:2375:ARG:NH1	2.41	0.53
1:F:2566:GLU:O	1:F:2568:MET:N	2.41	0.53
1:F:2724:VAL:HG23	1:F:2724:VAL:O	2.07	0.53
1:C:1208:VAL:CG2	1:C:1232:VAL:HG13	2.39	0.53
1:F:2457:VAL:HG21	1:F:2516:ALA:HB2	1.90	0.53
1:D:1580:LEU:C	1:D:1580:LEU:HD23	2.34	0.53
1:E:2209:ASP:OD2	1:F:2715:ARG:NH1	2.41	0.53
1:F:2724:VAL:CG2	1:F:2754:LEU:HB2	2.37	0.53
1:A:322:LYS:HD2	1:A:322:LYS:N	2.24	0.53
1:B:515:ILE:HG23	1:B:692:ILE:O	2.07	0.53
1:B:608:VAL:HG13	1:B:617:GLU:HB2	1.90	0.53
1:F:2722:LYS:HD2	1:F:2722:LYS:N	2.24	0.53
1:A:311:PRO:O	1:A:312:ILE:HG13	2.07	0.53
1:B:426:LYS:HD3	1:B:500:ILE:HD11	1.91	0.53
1:B:717:LYS:HD3	1:B:718:LEU:N	2.23	0.53
1:B:720:GLY:HA3	1:B:722:LYS:HE2	1.90	0.53
1:D:1625:LEU:CB	1:D:1628:LYS:HB2	2.38	0.53
1:E:2322:LYS:HD2	1:E:2322:LYS:N	2.23	0.53
1:E:2343:ARG:HG2	1:E:2343:ARG:HH11	1.74	0.53
1:F:2676:ILE:O	1:F:2680:VAL:HG22	2.09	0.53
1:B:580:LEU:C	1:B:580:LEU:HD23	2.34	0.53
1:C:1076:MET:CE	1:C:1324:VAL:HG21	2.32	0.53
1:F:2473:VAL:HB	1:F:2759:ILE:HB	1.90	0.53
1:F:2549:ARG:NH1	1:F:2553:ILE:HD11	2.22	0.53
1:F:2575:THR:OG1	1:F:2576:MET:N	2.41	0.53
1:B:587:GLN:HG2	1:B:617:GLU:OE1	2.09	0.53
1:B:653:TRP:CG	1:F:2718:LEU:HD22	2.44	0.53
1:D:1608:VAL:HG21	1:D:1632:VAL:HG13	1.90	0.53
1:D:1739:LYS:HD2	1:D:1739:LYS:N	2.23	0.53
1:F:2682:VAL:HG12	1:F:2682:VAL:O	2.08	0.53
1:A:140:HIS:HD2	1:A:142:ALA:CB	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:VAL:HG12	1:B:493:GLY:HA3	1.90	0.53
1:B:476:MET:CE	1:B:724:VAL:HG21	2.30	0.53
1:B:775:ARG:HE	1:B:779:LEU:HD11	1.73	0.53
1:D:1471:VAL:HG12	1:D:1493:GLY:HA3	1.89	0.53
1:E:2180:LEU:C	1:E:2180:LEU:HD23	2.34	0.53
1:F:2743:ARG:HG2	1:F:2743:ARG:HH11	1.74	0.53
1:B:739:LYS:HD2	1:B:739:LYS:N	2.23	0.53
1:C:1028:ILE:CD1	1:D:1597:VAL:HB	2.38	0.53
1:C:1140:HIS:HD2	1:C:1142:ALA:HB3	1.73	0.53
1:C:1197:VAL:HB	1:D:1428:ILE:CD1	2.37	0.53
1:D:1457:VAL:HG21	1:D:1516:ALA:HB2	1.90	0.53
1:D:1625:LEU:O	1:D:1628:LYS:N	2.32	0.53
1:E:2073:VAL:HB	1:E:2359:ILE:HB	1.91	0.53
1:F:2587:GLN:HG2	1:F:2617:GLU:OE1	2.09	0.53
1:F:2720:GLY:HA3	1:F:2722:LYS:HE2	1.91	0.53
1:A:6:ILE:HD11	1:B:409:GLU:OE1	2.09	0.53
1:B:625:LEU:O	1:B:628:LYS:N	2.33	0.53
1:E:2073:VAL:O	1:E:2358:ILE:HG12	2.09	0.53
1:E:2074:TYR:N	1:E:2074:TYR:CD1	2.76	0.53
1:A:146:MET:HE3	1:A:146:MET:O	2.09	0.52
1:B:474:TYR:CD1	1:B:474:TYR:N	2.77	0.52
1:C:1073:VAL:HB	1:C:1359:ILE:HB	1.90	0.52
1:C:1137:ARG:HB3	1:C:1137:ARG:NH1	2.23	0.52
1:C:1198:ILE:HG12	1:D:1428:ILE:HD11	1.90	0.52
1:F:2444:THR:HG22	1:F:2699:ASP:O	2.09	0.52
1:F:2474:TYR:CD1	1:F:2474:TYR:N	2.77	0.52
1:B:540:HIS:HD2	1:B:542:ALA:HB3	1.74	0.52
1:B:721:ARG:O	1:B:722:LYS:HD2	2.10	0.52
1:D:1548:ASP:HB3	1:D:1559:VAL:HG21	1.92	0.52
1:D:1717:LYS:HD3	1:D:1718:LEU:N	2.24	0.52
1:D:1746:VAL:CG2	1:D:1747:CYS:H	2.06	0.52
1:F:2608:VAL:HG21	1:F:2632:VAL:HG13	1.90	0.52
1:A:21:TYR:CD1	1:B:577:PRO:HG3	2.44	0.52
1:A:209:ASP:OD2	1:B:715:ARG:NH1	2.43	0.52
1:B:556:CYS:O	1:B:775:ARG:NH1	2.42	0.52
1:B:566:GLU:O	1:B:569:GLY:N	2.42	0.52
1:C:1140:HIS:HD2	1:C:1142:ALA:CB	2.22	0.52
1:F:2612:TYR:CD1	1:F:2612:TYR:N	2.77	0.52
1:A:134:PHE:HB3	3:A:392:PCP:H3	1.91	0.52
1:A:324:VAL:CG2	1:A:354:LEU:HB2	2.38	0.52
1:A:339:LYS:HD2	1:A:339:LYS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:PHE:HB3	3:B:792:PCP:H3	1.91	0.52
1:C:1365:VAL:HG12	1:C:1365:VAL:O	2.09	0.52
1:D:1723:GLN:HE21	1:D:1753:PRO:HB3	1.74	0.52
1:D:1775:ARG:HE	1:D:1779:LEU:HD11	1.73	0.52
1:E:2134:PHE:HB3	3:E:2392:PCP:H3	1.91	0.52
1:E:2194:PHE:HA	1:F:2428:ILE:HD12	1.92	0.52
1:E:2248:ILE:HD13	1:E:2283:VAL:CG1	2.40	0.52
1:F:2556:CYS:O	1:F:2775:ARG:NH1	2.42	0.52
1:B:666:PHE:CD2	1:B:685:ALA:HB3	2.45	0.52
1:D:1408:ASN:HD22	1:D:1408:ASN:N	2.08	0.52
1:D:1711:PRO:O	1:D:1712:ILE:HG13	2.10	0.52
1:E:2071:VAL:HG12	1:E:2093:GLY:HA3	1.92	0.52
1:E:2208:VAL:HG21	1:E:2232:VAL:HG13	1.90	0.52
1:A:180:LEU:CD2	1:A:190:ALA:HB1	2.40	0.52
1:A:317:LYS:HD3	1:A:318:LEU:N	2.25	0.52
1:C:1006:ILE:HD11	1:D:1409:GLU:OE1	2.10	0.52
1:D:1453:TRP:CZ3	1:D:1788:GLU:O	2.62	0.52
1:D:1587:GLN:HG2	1:D:1617:GLU:OE1	2.10	0.52
1:D:1743:ARG:HH11	1:D:1743:ARG:HG2	1.74	0.52
1:A:175:THR:OG1	1:A:176:MET:N	2.42	0.52
1:B:625:LEU:CB	1:B:628:LYS:HB2	2.38	0.52
1:C:1209:ASP:OD2	1:D:1715:ARG:NH1	2.43	0.52
1:C:1212:TYR:N	1:C:1212:TYR:CD1	2.78	0.52
1:D:1426:LYS:HG2	1:D:1430:GLU:OE1	2.10	0.52
1:D:1766:VAL:HG12	1:D:1767:GLU:N	2.24	0.52
1:E:2115:ILE:HD13	1:E:2147:ILE:HG23	1.92	0.52
1:E:2187:GLN:HG2	1:E:2217:GLU:OE1	2.09	0.52
1:F:2473:VAL:O	1:F:2758:ILE:HG12	2.09	0.52
1:F:2625:LEU:O	1:F:2628:LYS:N	2.35	0.52
1:A:148:ASP:HB3	1:A:159:VAL:HG21	1.92	0.52
1:B:608:VAL:CG2	1:B:632:VAL:HG13	2.39	0.52
1:B:660:TYR:HA	1:B:662:TRP:CZ3	2.45	0.52
1:C:1322:LYS:HD2	1:C:1322:LYS:N	2.23	0.52
1:D:1575:THR:OG1	1:D:1576:MET:N	2.42	0.52
1:D:1720:GLY:HA3	1:D:1722:LYS:HE2	1.91	0.52
1:E:2053:TRP:CZ3	1:E:2388:GLU:O	2.63	0.52
1:E:2236:THR:HB	1:E:2241:ARG:HG2	1.92	0.52
1:A:104:ALA:O	1:A:108:MET:HG3	2.09	0.52
1:A:323:GLN:OE1	1:A:355:LEU:HD23	2.10	0.52
1:C:1118:ALA:O	1:C:1122:ILE:HD13	2.10	0.52
1:C:1180:LEU:CD2	1:C:1190:ALA:HB1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:GLU:O	1:B:568:MET:N	2.43	0.52
1:C:1073:VAL:O	1:C:1358:ILE:HG12	2.09	0.52
1:D:1473:VAL:HB	1:D:1759:ILE:HB	1.91	0.52
1:E:2320:GLY:HA3	1:E:2322:LYS:HE2	1.92	0.52
1:A:166:GLU:O	1:A:169:GLY:N	2.42	0.51
1:B:726:ARG:HH12	1:B:781:GLN:NE2	2.06	0.51
1:E:2111:GLN:NE2	1:F:2540:HIS:H	2.07	0.51
1:E:2260:TYR:HA	1:E:2262:TRP:CZ3	2.45	0.51
1:A:156:CYS:O	1:A:375:ARG:NH1	2.43	0.51
1:A:212:TYR:N	1:A:212:TYR:CD1	2.78	0.51
1:A:323:GLN:HE21	1:A:353:PRO:HB3	1.74	0.51
1:C:1134:PHE:HB3	3:C:1392:PCP:H3	1.92	0.51
1:C:1156:CYS:O	1:C:1375:ARG:NH1	2.43	0.51
1:D:1624:ALA:O	1:D:1626:GLY:N	2.43	0.51
1:D:1765:VAL:HG12	1:D:1765:VAL:O	2.08	0.51
1:A:73:VAL:O	1:A:358:ILE:HG12	2.11	0.51
1:A:324:VAL:HG23	1:A:324:VAL:O	2.10	0.51
1:B:698:VAL:O	1:B:700:PHE:N	2.42	0.51
1:B:702:LEU:HD13	1:B:702:LEU:C	2.35	0.51
1:C:1009:GLU:OE1	1:D:1406:ILE:HD11	2.10	0.51
1:C:1208:VAL:HG12	1:C:1209:ASP:N	2.24	0.51
1:C:1236:THR:HB	1:C:1241:ARG:HG2	1.93	0.51
1:E:2009:GLU:OE2	1:F:2403:ARG:HG2	2.10	0.51
1:E:2224:ALA:O	1:E:2226:GLY:N	2.43	0.51
1:E:2339:LYS:HD2	1:E:2339:LYS:N	2.25	0.51
1:F:2679:ILE:O	1:F:2683:VAL:HG22	2.10	0.51
1:A:73:VAL:HB	1:A:359:ILE:HB	1.92	0.51
1:A:248:ILE:HD13	1:A:283:VAL:CG1	2.40	0.51
1:B:580:LEU:CD2	1:B:590:ALA:HB1	2.40	0.51
1:C:1115:ILE:HD13	1:C:1147:ILE:HG23	1.92	0.51
1:D:1474:TYR:CD1	1:D:1474:TYR:N	2.77	0.51
1:D:1647:ILE:HD11	1:F:2639:SER:O	2.11	0.51
1:E:2003:ARG:HB2	1:F:2464:LYS:HD3	1.92	0.51
1:F:2624:ALA:O	1:F:2626:GLY:N	2.43	0.51
1:B:518:ALA:O	1:B:522:ILE:HD13	2.10	0.51
1:B:743:ARG:HH11	1:B:743:ARG:HG2	1.76	0.51
1:C:1339:LYS:HD2	1:C:1339:LYS:N	2.25	0.51
1:D:1657:VAL:HG22	1:E:2322:LYS:HE3	1.92	0.51
1:E:2038:VAL:CG1	1:E:2307:VAL:HG13	2.40	0.51
1:E:2225:LEU:O	1:E:2228:LYS:N	2.34	0.51
1:A:140:HIS:HD2	1:A:142:ALA:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:VAL:O	1:A:300:PHE:N	2.43	0.51
1:D:1580:LEU:CD2	1:D:1590:ALA:HB1	2.41	0.51
1:F:2533:SER:O	1:F:2534:PHE:HD1	1.93	0.51
1:F:2580:LEU:HD23	1:F:2580:LEU:C	2.35	0.51
1:A:137:ARG:HB3	1:A:137:ARG:NH1	2.26	0.51
1:B:548:ASP:HB3	1:B:559:VAL:HG21	1.92	0.51
1:C:1021:TYR:HB2	1:D:1575:THR:O	2.10	0.51
1:C:1026:LYS:HG2	1:C:1030:GLU:OE1	2.11	0.51
1:C:1175:THR:O	1:D:1421:TYR:HB2	2.11	0.51
1:D:1556:CYS:O	1:D:1775:ARG:NH1	2.43	0.51
1:D:1588:VAL:HA	1:D:1591:TRP:HE1	1.74	0.51
1:E:2140:HIS:HE1	1:F:2461:GLU:OE1	1.94	0.51
1:F:2471:VAL:HG12	1:F:2493:GLY:HA3	1.93	0.51
1:F:2534:PHE:HB3	3:F:2792:PCP:H3	1.93	0.51
1:A:76:MET:CE	1:A:324:VAL:HG21	2.34	0.51
1:C:1317:LYS:HD3	1:C:1318:LEU:N	2.25	0.51
1:E:2212:TYR:N	1:E:2212:TYR:CD1	2.78	0.51
1:F:2431:VAL:C	1:F:2433:ASN:N	2.62	0.51
1:A:26:LYS:HG2	1:A:30:GLU:OE1	2.11	0.51
1:A:175:THR:O	1:B:421:TYR:HB2	2.10	0.51
1:A:366:VAL:HG12	1:A:367:GLU:N	2.25	0.51
1:C:1366:VAL:HG12	1:C:1367:GLU:N	2.25	0.51
1:D:1612:TYR:CD1	1:D:1612:TYR:N	2.79	0.51
1:F:2660:TYR:HA	1:F:2662:TRP:CZ3	2.46	0.51
1:F:2744:CYS:SG	1:F:2746:VAL:HG12	2.51	0.51
1:F:2775:ARG:HE	1:F:2779:LEU:HD11	1.76	0.51
1:A:302:LEU:HD13	1:A:302:LEU:C	2.36	0.51
1:B:612:TYR:CD1	1:B:612:TYR:N	2.79	0.51
1:C:1225:LEU:O	1:C:1228:LYS:N	2.33	0.51
1:C:1260:TYR:HA	1:C:1262:TRP:CZ3	2.46	0.51
1:D:1566:GLU:O	1:D:1569:GLY:N	2.44	0.51
1:D:1653:TRP:CG	1:E:2318:LEU:HD22	2.46	0.51
1:F:2515:ILE:HD13	1:F:2547:ILE:HG23	1.94	0.51
1:C:1057:VAL:HG21	1:C:1116:ALA:HB2	1.92	0.50
1:D:1666:PHE:CD2	1:D:1685:ALA:HB3	2.46	0.50
1:D:1721:ARG:O	1:D:1722:LYS:NZ	2.40	0.50
1:E:2344:CYS:SG	1:E:2346:VAL:HG12	2.51	0.50
1:C:1133:SER:O	1:C:1134:PHE:HD1	1.94	0.50
1:E:2166:GLU:O	1:E:2169:GLY:N	2.44	0.50
1:F:2739:LYS:HD2	1:F:2739:LYS:N	2.27	0.50
1:B:408:ASN:HD22	1:B:408:ASN:N	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:VAL:HG21	1:B:686:PHE:CZ	2.45	0.50
1:C:1148:ASP:HB3	1:C:1159:VAL:HG21	1.93	0.50
1:C:1248:ILE:CG2	1:C:1282:VAL:HG12	2.42	0.50
1:E:2137:ARG:CG	1:E:2137:ARG:NH1	2.73	0.50
1:E:2149:ARG:NH2	1:F:2405:TYR:CE1	2.79	0.50
1:E:2208:VAL:HG12	1:E:2209:ASP:N	2.26	0.50
1:F:2453:TRP:CZ3	1:F:2788:GLU:O	2.64	0.50
1:B:624:ALA:O	1:B:626:GLY:N	2.44	0.50
1:C:1071:VAL:HG12	1:C:1093:GLY:HA3	1.92	0.50
1:D:1621:ALA:O	1:D:1629:LEU:HD22	2.11	0.50
1:F:2408:ASN:N	1:F:2408:ASN:HD22	2.10	0.50
1:A:9:GLU:OE1	1:B:406:ILE:HD11	2.10	0.50
1:A:26:LYS:HD2	1:A:96:ALA:O	2.11	0.50
1:A:140:HIS:H	1:B:511:GLN:NE2	2.10	0.50
1:B:722:LYS:HD2	1:B:722:LYS:N	2.25	0.50
1:C:1028:ILE:HD12	1:D:1594:PHE:HA	1.92	0.50
1:D:1722:LYS:HD2	1:D:1722:LYS:N	2.26	0.50
1:B:426:LYS:HG2	1:B:430:GLU:OE1	2.10	0.50
1:B:521:ARG:HB3	1:B:789:ILE:HD11	1.92	0.50
1:B:575:THR:OG1	1:B:576:MET:N	2.45	0.50
1:F:2426:LYS:HG2	1:F:2430:GLU:OE1	2.11	0.50
1:A:248:ILE:CG2	1:A:282:VAL:HG12	2.41	0.50
1:B:426:LYS:O	1:B:430:GLU:HB2	2.12	0.50
1:B:465:LEU:HD22	1:B:508:MET:HE1	1.93	0.50
1:D:1608:VAL:HG12	1:D:1609:ASP:N	2.27	0.50
1:A:74:TYR:N	1:A:74:TYR:CD1	2.80	0.50
1:A:260:TYR:HA	1:A:262:TRP:CZ3	2.46	0.50
1:B:722:LYS:HG2	1:C:1253:TRP:CH2	2.46	0.50
1:C:1026:LYS:HD2	1:C:1096:ALA:O	2.12	0.50
1:C:1026:LYS:O	1:C:1030:GLU:HB2	2.12	0.50
1:C:1077:PRO:HG2	1:C:1080:THR:OG1	2.12	0.50
1:D:1465:LEU:HD22	1:D:1508:MET:HE1	1.94	0.50
1:E:2266:PHE:CD2	1:E:2285:ALA:HB3	2.46	0.50
1:F:2588:VAL:HA	1:F:2591:TRP:HE1	1.77	0.50
1:A:28:ILE:HD12	1:B:594:PHE:HA	1.94	0.50
1:B:426:LYS:HD2	1:B:496:ALA:O	2.12	0.50
1:B:453:TRP:CZ3	1:B:788:GLU:O	2.65	0.50
1:B:609:ASP:C	1:B:609:ASP:OD1	2.55	0.50
1:B:766:VAL:CG1	1:B:767:GLU:N	2.75	0.50
1:D:1636:THR:HB	1:D:1641:ARG:HG2	1.93	0.50
1:E:2028:ILE:HD12	1:F:2594:PHE:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2609:ASP:OD1	1:F:2609:ASP:C	2.55	0.50
1:A:77:PRO:HG2	1:A:80:THR:OG1	2.12	0.49
1:A:373:GLU:OE2	1:A:376:GLU:OE1	2.30	0.49
1:B:485:TYR:OH	1:C:1246:LYS:HD3	2.11	0.49
1:C:1037:LYS:NZ	4:C:16:HOH:O	2.44	0.49
1:D:1473:VAL:O	1:D:1758:ILE:HG12	2.11	0.49
1:E:2026:LYS:HD2	1:E:2096:ALA:O	2.12	0.49
1:E:2228:LYS:HA	1:E:2228:LYS:CE	2.41	0.49
1:F:2624:ALA:C	1:F:2626:GLY:N	2.70	0.49
1:A:28:ILE:CD1	1:B:597:VAL:HB	2.40	0.49
1:C:1266:PHE:CD2	1:C:1285:ALA:HB3	2.47	0.49
1:C:1323:GLN:OE1	1:C:1355:LEU:HD23	2.11	0.49
1:D:1609:ASP:C	1:D:1609:ASP:OD1	2.55	0.49
1:E:2061:GLU:OE1	1:F:2540:HIS:HE1	1.94	0.49
1:F:2477:PRO:HG2	1:F:2480:THR:OG1	2.12	0.49
1:C:1121:ARG:HB3	1:C:1389:ILE:HD11	1.93	0.49
1:C:1167:MET:HE1	1:D:1405:TYR:HA	1.94	0.49
1:C:1228:LYS:HA	1:C:1228:LYS:CE	2.40	0.49
1:D:1515:ILE:HG23	1:D:1692:ILE:O	2.12	0.49
1:F:2426:LYS:HD2	1:F:2496:ALA:O	2.12	0.49
1:F:2625:LEU:CB	1:F:2628:LYS:HB2	2.40	0.49
1:F:2683:VAL:HG21	1:F:2686:PHE:CZ	2.48	0.49
1:A:26:LYS:O	1:A:30:GLU:HB2	2.13	0.49
1:A:38:VAL:CG1	1:A:307:VAL:HG13	2.40	0.49
1:A:166:GLU:O	1:A:168:MET:N	2.45	0.49
1:A:221:ALA:O	1:A:229:LEU:HD22	2.12	0.49
1:B:588:VAL:HA	1:B:591:TRP:HE1	1.73	0.49
1:B:608:VAL:HG21	1:B:632:VAL:HG13	1.94	0.49
1:B:711:PRO:O	1:B:712:ILE:HG13	2.12	0.49
1:C:1283:VAL:HG21	1:C:1286:PHE:CZ	2.48	0.49
1:D:1426:LYS:HD2	1:D:1496:ALA:O	2.12	0.49
1:D:1521:ARG:HB3	1:D:1789:ILE:HD11	1.93	0.49
1:E:2069:ILE:HG23	1:E:2070:PRO:HD2	1.93	0.49
1:F:2608:VAL:HG12	1:F:2609:ASP:N	2.26	0.49
1:A:115:ILE:HD13	1:A:147:ILE:HG23	1.94	0.49
1:A:167:MET:HE1	1:B:405:TYR:HA	1.95	0.49
1:C:1208:VAL:HG21	1:C:1232:VAL:HG13	1.93	0.49
1:E:2121:ARG:NH1	1:E:2273:GLU:OE2	2.44	0.49
1:E:2194:PHE:HA	1:F:2428:ILE:CD1	2.42	0.49
1:E:2221:ALA:O	1:E:2229:LEU:HD22	2.12	0.49
1:E:2366:VAL:HG12	1:E:2367:GLU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2666:PHE:CD2	1:F:2685:ALA:HB3	2.47	0.49
1:A:253:TRP:HD1	1:A:254:GLU:OE2	1.96	0.49
1:A:279:ILE:O	1:A:283:VAL:HG22	2.13	0.49
1:B:457:VAL:HG21	1:B:516:ALA:HB2	1.94	0.49
1:B:537:ARG:NH1	1:B:537:ARG:HB3	2.28	0.49
1:D:1549:ARG:NH1	1:D:1553:ILE:HD11	2.23	0.49
1:F:2469:ILE:HG23	1:F:2470:PRO:HD2	1.94	0.49
1:A:105:LEU:HD12	1:A:106:LEU:N	2.26	0.49
1:B:444:THR:HG22	1:B:699:ASP:O	2.13	0.49
1:B:642:GLY:HA3	1:E:2238:SER:O	2.12	0.49
1:B:657:VAL:HG22	1:F:2722:LYS:HE3	1.93	0.49
1:D:1546:MET:HE3	1:D:1546:MET:O	2.13	0.49
1:E:2008:ASN:HD22	1:E:2008:ASN:N	2.10	0.49
1:A:253:TRP:CH2	1:D:1722:LYS:HG2	2.48	0.49
1:B:473:VAL:O	1:B:758:ILE:HG12	2.12	0.49
1:B:671:LEU:HD12	1:B:688:VAL:HG22	1.93	0.49
1:C:1166:GLU:C	1:C:1168:MET:N	2.70	0.49
1:C:1315:ARG:NH1	1:D:1609:ASP:OD2	2.46	0.49
1:E:2026:LYS:HG2	1:E:2030:GLU:OE1	2.12	0.49
1:F:2537:ARG:NH1	1:F:2537:ARG:HB3	2.27	0.49
1:A:118:ALA:O	1:A:122:ILE:HD13	2.12	0.49
1:A:315:ARG:NH1	1:B:609:ASP:OD2	2.46	0.49
1:D:1469:ILE:HG23	1:D:1470:PRO:HD2	1.95	0.49
1:D:1702:LEU:HD13	1:D:1702:LEU:C	2.38	0.49
1:E:2021:TYR:CD1	1:F:2577:PRO:HG3	2.47	0.49
1:E:2137:ARG:NH1	1:E:2137:ARG:HB3	2.27	0.49
1:F:2521:ARG:HB3	1:F:2789:ILE:HD11	1.95	0.49
1:A:137:ARG:CG	1:A:137:ARG:NH1	2.73	0.49
1:B:608:VAL:HG12	1:B:609:ASP:N	2.26	0.49
1:D:1683:VAL:HG21	1:D:1686:PHE:CZ	2.48	0.49
1:F:2621:ALA:O	1:F:2629:LEU:HD22	2.13	0.49
1:B:624:ALA:C	1:B:626:GLY:N	2.70	0.48
1:B:628:LYS:HA	1:B:628:LYS:CE	2.40	0.48
1:B:722:LYS:HZ2	1:B:736:PRO:CB	2.24	0.48
1:C:1074:TYR:N	1:C:1074:TYR:CD1	2.80	0.48
1:C:1193:TYR:HB3	1:D:1428:ILE:HG23	1.95	0.48
1:C:1322:LYS:HZ2	1:C:1336:PRO:CB	2.26	0.48
1:D:1766:VAL:CG1	1:D:1767:GLU:N	2.76	0.48
1:C:1221:ALA:O	1:C:1229:LEU:HD22	2.13	0.48
1:C:1271:LEU:HD12	1:C:1288:VAL:HG22	1.96	0.48
1:D:1444:THR:HG22	1:D:1699:ASP:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1628:LYS:HA	1:D:1628:LYS:CE	2.40	0.48
1:E:2003:ARG:HG2	1:F:2409:GLU:OE2	2.12	0.48
1:F:2723:GLN:HE21	1:F:2753:PRO:HB3	1.73	0.48
1:A:166:GLU:C	1:A:168:MET:N	2.72	0.48
1:C:1248:ILE:HD13	1:C:1283:VAL:CG1	2.43	0.48
1:C:1302:LEU:HD13	1:C:1302:LEU:C	2.39	0.48
1:E:2077:PRO:HG2	1:E:2080:THR:OG1	2.13	0.48
1:E:2166:GLU:O	1:E:2168:MET:N	2.45	0.48
1:F:2424:ARG:O	1:F:2428:ILE:HG12	2.14	0.48
1:A:15:GLY:O	1:A:18:THR:HG23	2.13	0.48
1:A:20:VAL:HG23	1:A:21:TYR:N	2.29	0.48
1:A:225:LEU:CB	1:A:228:LYS:HB2	2.39	0.48
1:B:636:THR:HB	1:B:641:ARG:HG2	1.95	0.48
1:C:1015:GLY:O	1:C:1018:THR:HG23	2.14	0.48
1:C:1165:ALA:HB2	1:C:1172:ALA:HB2	1.95	0.48
1:C:1324:VAL:HG23	1:C:1324:VAL:O	2.12	0.48
1:D:1698:VAL:O	1:D:1700:PHE:N	2.45	0.48
1:E:2148:ASP:HB3	1:E:2159:VAL:HG21	1.94	0.48
1:B:621:ALA:O	1:B:629:LEU:HD22	2.13	0.48
1:B:724:VAL:HG23	1:B:724:VAL:O	2.13	0.48
1:C:1028:ILE:HG23	1:D:1593:TYR:HB3	1.95	0.48
1:C:1149:ARG:NH1	1:C:1153:ILE:HD11	2.23	0.48
1:D:1671:LEU:HD12	1:D:1688:VAL:HG22	1.95	0.48
1:D:1744:CYS:SG	1:D:1746:VAL:CG1	3.02	0.48
1:F:2469:ILE:O	1:F:2471:VAL:N	2.41	0.48
1:F:2723:GLN:OE1	1:F:2755:LEU:HD23	2.14	0.48
1:B:716:GLY:HA2	1:C:1250:GLU:OE2	2.13	0.48
1:B:744:CYS:SG	1:B:746:VAL:CG1	3.01	0.48
1:C:1069:ILE:HG23	1:C:1070:PRO:HD2	1.96	0.48
1:C:1105:LEU:HD12	1:C:1106:LEU:N	2.28	0.48
1:C:1175:THR:OG1	1:C:1176:MET:N	2.46	0.48
1:C:1209:ASP:C	1:C:1209:ASP:OD1	2.57	0.48
1:D:1722:LYS:HZ2	1:D:1736:PRO:HB3	1.78	0.48
1:E:2149:ARG:NH1	1:E:2153:ILE:HD11	2.23	0.48
1:E:2209:ASP:C	1:E:2209:ASP:OD1	2.56	0.48
1:A:21:TYR:HB2	1:B:575:THR:O	2.14	0.48
1:A:69:ILE:HG23	1:A:70:PRO:HD2	1.95	0.48
1:A:248:ILE:HG22	1:A:282:VAL:HG12	1.96	0.48
1:A:266:PHE:CD2	1:A:285:ALA:HB3	2.49	0.48
1:C:1021:TYR:CD1	1:D:1577:PRO:HG3	2.48	0.48
1:C:1137:ARG:CG	1:C:1137:ARG:NH1	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1140:HIS:H	1:D:1511:GLN:NE2	2.11	0.48
1:D:1722:LYS:HZ2	1:D:1736:PRO:CA	2.27	0.48
1:A:180:LEU:HD23	1:A:181:ILE:N	2.29	0.48
1:B:648:ILE:HD13	1:B:683:VAL:CG1	2.44	0.48
1:C:1205:ILE:HA	1:C:1231:ALA:O	2.14	0.48
1:D:1566:GLU:O	1:D:1568:MET:N	2.47	0.48
1:D:1642:GLY:HA3	1:F:2638:SER:O	2.12	0.48
1:E:2064:LYS:HD3	1:F:2403:ARG:HB2	1.95	0.48
1:E:2322:LYS:HZ2	1:E:2336:PRO:HB3	1.79	0.48
1:E:2330:GLY:O	1:E:2332:TYR:HD1	1.97	0.48
1:F:2619:VAL:HG11	1:F:2658:ARG:HD2	1.96	0.48
1:A:343:ARG:HG2	1:A:343:ARG:HH11	1.79	0.48
1:A:375:ARG:HE	1:A:379:LEU:HD11	1.79	0.48
1:C:1253:TRP:HD1	1:C:1254:GLU:OE2	1.97	0.48
1:D:1537:ARG:NH1	1:D:1537:ARG:HB3	2.29	0.48
1:E:2302:LEU:HD13	1:E:2302:LEU:C	2.39	0.48
1:D:1648:ILE:HD13	1:D:1683:VAL:CG1	2.44	0.48
1:E:2026:LYS:O	1:E:2030:GLU:HB2	2.14	0.48
1:E:2028:ILE:CD1	1:F:2594:PHE:HA	2.44	0.48
1:E:2107:GLY:HA3	1:F:2539:MET:O	2.14	0.48
1:E:2166:GLU:C	1:E:2168:MET:N	2.72	0.48
1:E:2321:ARG:O	1:E:2322:LYS:NZ	2.38	0.48
1:F:2648:ILE:HD13	1:F:2683:VAL:CG1	2.44	0.48
1:A:165:ALA:HB2	1:A:172:ALA:HB2	1.96	0.47
1:A:344:CYS:SG	1:A:346:VAL:CG1	3.01	0.47
1:B:477:PRO:HG2	1:B:480:THR:OG1	2.14	0.47
1:C:1219:VAL:HG11	1:C:1258:ARG:HD2	1.95	0.47
1:D:1724:VAL:HG23	1:D:1724:VAL:O	2.13	0.47
1:E:2105:LEU:HD12	1:E:2106:LEU:N	2.29	0.47
1:F:2766:VAL:HG12	1:F:2767:GLU:N	2.28	0.47
1:A:172:ALA:HB3	1:B:420:VAL:CG1	2.44	0.47
1:B:424:ARG:O	1:B:428:ILE:HG12	2.14	0.47
1:B:653:TRP:HD1	1:B:654:GLU:OE2	1.97	0.47
1:C:1069:ILE:HA	1:C:1070:PRO:HD3	1.78	0.47
1:D:1477:PRO:HG2	1:D:1480:THR:OG1	2.14	0.47
1:D:1533:SER:O	1:D:1534:PHE:HD1	1.97	0.47
1:E:2283:VAL:HG21	1:E:2286:PHE:CZ	2.49	0.47
1:B:648:ILE:CG2	1:B:682:VAL:HG12	2.44	0.47
1:D:1540:HIS:HD2	1:D:1542:ALA:HB3	1.78	0.47
1:E:2044:THR:HG22	1:E:2299:ASP:O	2.14	0.47
1:F:2521:ARG:NH1	1:F:2673:GLU:OE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2566:GLU:C	1:F:2568:MET:N	2.70	0.47
1:A:271:LEU:HD12	1:A:288:VAL:HG22	1.95	0.47
1:B:545:PRO:O	1:B:546:MET:C	2.54	0.47
1:B:552:PHE:O	1:B:553:ILE:C	2.57	0.47
1:B:723:GLN:HE21	1:B:753:PRO:HB3	1.76	0.47
1:C:1248:ILE:HG22	1:C:1282:VAL:HG12	1.97	0.47
1:D:1426:LYS:O	1:D:1430:GLU:HB2	2.13	0.47
1:D:1624:ALA:C	1:D:1626:GLY:N	2.70	0.47
1:D:1723:GLN:OE1	1:D:1755:LEU:HD23	2.14	0.47
1:E:2139:MET:O	1:F:2507:GLY:HA3	2.14	0.47
1:E:2224:ALA:C	1:E:2225:LEU:HD23	2.40	0.47
1:A:28:ILE:HG23	1:B:593:TYR:HB3	1.95	0.47
1:C:1020:VAL:HG23	1:C:1021:TYR:N	2.29	0.47
1:C:1180:LEU:HD23	1:C:1181:ILE:N	2.29	0.47
1:E:2208:VAL:HG13	1:E:2217:GLU:CB	2.45	0.47
1:F:2648:ILE:CG2	1:F:2682:VAL:HG12	2.44	0.47
1:C:1069:ILE:O	1:C:1071:VAL:N	2.40	0.47
1:F:2426:LYS:O	1:F:2430:GLU:HB2	2.13	0.47
1:F:2469:ILE:HA	1:F:2470:PRO:HD3	1.76	0.47
1:F:2636:THR:HB	1:F:2641:ARG:HG2	1.96	0.47
1:A:39:LEU:HD23	1:A:321:ARG:HB2	1.97	0.47
1:A:193:TYR:HB3	1:B:428:ILE:HG23	1.97	0.47
1:A:205:ILE:HA	1:A:231:ALA:O	2.14	0.47
1:A:326:ARG:HH12	1:A:381:GLN:NE2	2.12	0.47
1:B:549:ARG:NH1	1:B:553:ILE:HD11	2.24	0.47
1:B:566:GLU:C	1:B:568:MET:N	2.71	0.47
1:C:1043:THR:HG22	1:C:1087:PRO:HA	1.97	0.47
1:C:1208:VAL:HG13	1:C:1217:GLU:CB	2.44	0.47
1:C:1343:ARG:HG2	1:C:1343:ARG:HH11	1.79	0.47
1:C:1366:VAL:CG1	1:C:1367:GLU:N	2.78	0.47
1:E:2323:GLN:OE1	1:E:2355:LEU:HD23	2.14	0.47
1:E:2375:ARG:HE	1:E:2379:LEU:HD11	1.78	0.47
1:F:2518:ALA:O	1:F:2522:ILE:HD13	2.14	0.47
1:F:2605:ILE:HD12	1:F:2605:ILE:N	2.29	0.47
1:F:2608:VAL:HG13	1:F:2617:GLU:CB	2.45	0.47
1:F:2702:LEU:C	1:F:2702:LEU:HD13	2.40	0.47
1:A:44:THR:CG2	1:A:298:VAL:HG12	2.32	0.47
1:A:191:TRP:CE3	1:A:206:ALA:HB1	2.50	0.47
1:A:326:ARG:HH11	1:A:385:PHE:HZ	1.61	0.47
1:C:1024:ARG:O	1:C:1028:ILE:HG12	2.15	0.47
1:C:1321:ARG:O	1:C:1322:LYS:HD2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1424:ARG:O	1:D:1428:ILE:HG12	2.15	0.47
1:D:1652:ARG:HD2	1:D:1682:VAL:HG13	1.97	0.47
1:E:2219:VAL:HG11	1:E:2258:ARG:HD2	1.97	0.47
1:E:2271:LEU:HD12	1:E:2288:VAL:HG22	1.96	0.47
1:A:222:ALA:HB1	1:A:260:TYR:CD2	2.50	0.47
1:D:1440:ALA:HA	1:D:1704:ILE:HA	1.97	0.47
1:D:1653:TRP:HD1	1:D:1654:GLU:OE2	1.97	0.47
1:E:2322:LYS:HZ2	1:E:2336:PRO:CA	2.27	0.47
1:E:2343:ARG:HG2	1:E:2343:ARG:NH1	2.30	0.47
1:A:9:GLU:HG2	1:B:403:ARG:HE	1.80	0.47
1:A:330:GLY:O	1:A:332:TYR:HD1	1.98	0.47
1:B:440:ALA:HA	1:B:704:ILE:HA	1.96	0.47
1:E:2165:ALA:HB2	1:E:2172:ALA:HB2	1.95	0.47
1:F:2420:VAL:HG23	1:F:2421:TYR:N	2.30	0.47
1:F:2440:ALA:HA	1:F:2704:ILE:HA	1.96	0.47
1:A:228:LYS:HA	1:A:228:LYS:CE	2.40	0.46
1:C:1330:GLY:O	1:C:1332:TYR:HD1	1.98	0.46
1:E:2327:CYS:SG	1:E:2329:ASN:HB2	2.55	0.46
1:F:2611:PHE:HB2	1:F:2612:TYR:HD1	1.80	0.46
1:A:30:GLU:HG3	1:A:35:ARG:NH1	2.31	0.46
1:A:208:VAL:HG13	1:A:217:GLU:CB	2.45	0.46
1:B:469:ILE:HG23	1:B:470:PRO:HD2	1.95	0.46
1:C:1225:LEU:CB	1:C:1228:LYS:HB2	2.39	0.46
1:D:1648:ILE:CG2	1:D:1682:VAL:HG12	2.46	0.46
1:E:2188:VAL:HA	1:E:2191:TRP:HE1	1.77	0.46
1:E:2191:TRP:CE3	1:E:2206:ALA:HB1	2.50	0.46
1:E:2212:TYR:N	1:E:2212:TYR:HD1	2.13	0.46
1:E:2222:ALA:HB1	1:E:2260:TYR:CD2	2.50	0.46
1:F:2612:TYR:N	1:F:2612:TYR:HD1	2.13	0.46
1:A:247:ILE:HG12	1:C:1240:ARG:HE	1.80	0.46
1:B:420:VAL:HG23	1:B:421:TYR:N	2.30	0.46
1:B:634:LEU:HD23	1:B:665:ILE:HG23	1.97	0.46
1:C:1177:PRO:HG3	1:D:1421:TYR:CD1	2.50	0.46
1:E:2003:ARG:NH2	4:E:42:HOH:O	2.39	0.46
1:E:2020:VAL:HG23	1:E:2021:TYR:N	2.30	0.46
1:E:2024:ARG:O	1:E:2028:ILE:HG12	2.15	0.46
1:F:2438:VAL:CG1	1:F:2707:VAL:HG13	2.41	0.46
1:F:2600:GLU:OE1	1:F:2600:GLU:HA	2.14	0.46
1:F:2624:ALA:C	1:F:2625:LEU:HD23	2.41	0.46
1:F:2634:LEU:HD23	1:F:2665:ILE:HG23	1.97	0.46
1:A:43:THR:HG22	1:A:87:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASP:C	1:A:209:ASP:OD1	2.58	0.46
1:B:438:VAL:CG1	1:B:707:VAL:HG13	2.40	0.46
1:B:669:GLY:O	1:B:670:GLY:C	2.58	0.46
1:C:1044:THR:CG2	1:C:1298:VAL:HG12	2.32	0.46
1:C:1224:ALA:C	1:C:1226:GLY:N	2.68	0.46
1:C:1344:CYS:SG	1:C:1346:VAL:CG1	3.03	0.46
1:E:2065:LEU:HD22	1:E:2108:MET:HE1	1.96	0.46
1:E:2200:GLU:HA	1:E:2200:GLU:OE1	2.15	0.46
1:E:2323:GLN:HE21	1:E:2353:PRO:HB3	1.75	0.46
1:A:252:ARG:HD2	1:A:282:VAL:HG13	1.98	0.46
1:B:439:LEU:HD23	1:B:721:ARG:HB2	1.98	0.46
1:B:605:ILE:N	1:B:605:ILE:HD12	2.31	0.46
1:D:1591:TRP:CE3	1:D:1606:ALA:HB1	2.50	0.46
1:E:2005:TYR:CE1	1:F:2549:ARG:NH2	2.82	0.46
1:E:2040:ALA:HA	1:E:2304:ILE:HA	1.98	0.46
1:F:2565:ALA:HB2	1:F:2572:ALA:HB2	1.96	0.46
1:F:2594:PHE:CE1	1:F:2598:ILE:HG13	2.50	0.46
1:A:188:VAL:HA	1:A:191:TRP:HE1	1.78	0.46
1:B:457:VAL:CG1	1:B:512:ALA:HB1	2.46	0.46
1:B:521:ARG:NH1	1:B:673:GLU:OE2	2.48	0.46
1:C:1172:ALA:HB3	1:D:1420:VAL:CG1	2.46	0.46
1:C:1211:PHE:HB2	1:C:1212:TYR:HD1	1.80	0.46
1:D:1566:GLU:C	1:D:1568:MET:N	2.73	0.46
1:E:2304:ILE:H	1:E:2304:ILE:HG12	1.58	0.46
1:E:2322:LYS:HZ2	1:E:2336:PRO:HA	1.81	0.46
1:E:2344:CYS:O	1:E:2345:PRO:C	2.59	0.46
1:F:2628:LYS:HA	1:F:2628:LYS:CE	2.41	0.46
1:B:622:ALA:HB1	1:B:660:TYR:CD2	2.51	0.46
1:B:648:ILE:HG22	1:B:682:VAL:HG12	1.98	0.46
1:D:1608:VAL:HG13	1:D:1617:GLU:CB	2.46	0.46
1:F:2743:ARG:HG2	1:F:2743:ARG:NH1	2.31	0.46
1:A:164:GLY:O	1:A:168:MET:HG3	2.15	0.46
1:A:212:TYR:N	1:A:212:TYR:HD1	2.14	0.46
1:B:469:ILE:HA	1:B:470:PRO:HD3	1.78	0.46
1:B:611:PHE:HB2	1:B:612:TYR:HD1	1.81	0.46
1:B:744:CYS:O	1:B:745:PRO:C	2.59	0.46
1:C:1038:VAL:CG1	1:C:1307:VAL:HG13	2.40	0.46
1:C:1375:ARG:HE	1:C:1379:LEU:HD11	1.81	0.46
1:D:1580:LEU:HD23	1:D:1581:ILE:N	2.30	0.46
1:D:1622:ALA:HB1	1:D:1660:TYR:CD2	2.51	0.46
1:E:2211:PHE:HB2	1:E:2212:TYR:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2283:VAL:HG21	1:E:2286:PHE:CE2	2.51	0.46
1:F:2415:GLY:O	1:F:2418:THR:HG23	2.16	0.46
1:F:2605:ILE:HA	1:F:2631:ALA:O	2.15	0.46
1:B:591:TRP:CE3	1:B:606:ALA:HB1	2.50	0.46
1:C:1040:ALA:HA	1:C:1304:ILE:HA	1.98	0.46
1:C:1194:PHE:CE1	1:C:1198:ILE:HG13	2.51	0.46
1:C:1222:ALA:HB1	1:C:1260:TYR:CD2	2.51	0.46
1:E:2043:THR:HG22	1:E:2087:PRO:HA	1.98	0.46
1:E:2205:ILE:HA	1:E:2231:ALA:O	2.15	0.46
1:E:2366:VAL:CG1	1:E:2367:GLU:N	2.79	0.46
1:F:2505:LEU:HD12	1:F:2506:LEU:N	2.31	0.46
1:F:2744:CYS:O	1:F:2745:PRO:C	2.59	0.46
1:A:211:PHE:HB2	1:A:212:TYR:HD1	1.81	0.46
1:B:533:SER:O	1:B:534:PHE:HD1	1.98	0.46
1:B:652:ARG:HD2	1:B:682:VAL:HG13	1.96	0.46
1:B:723:GLN:OE1	1:B:755:LEU:HD23	2.14	0.46
1:C:1028:ILE:HD11	1:D:1598:ILE:HG12	1.98	0.46
1:C:1121:ARG:NH1	1:C:1273:GLU:OE2	2.49	0.46
1:D:1443:THR:HG22	1:D:1487:PRO:HA	1.98	0.46
1:D:1605:ILE:HA	1:D:1631:ALA:O	2.16	0.46
1:D:1721:ARG:O	1:D:1722:LYS:HD2	2.12	0.46
1:E:2121:ARG:HB3	1:E:2389:ILE:HD11	1.97	0.46
1:E:2177:PRO:HG3	1:F:2421:TYR:CD1	2.51	0.46
1:F:2465:LEU:HD22	1:F:2508:MET:HE1	1.96	0.46
1:F:2648:ILE:HG22	1:F:2682:VAL:HG12	1.98	0.46
1:F:2721:ARG:O	1:F:2722:LYS:NZ	2.35	0.46
1:A:115:ILE:HG23	1:A:292:ILE:O	2.16	0.45
1:A:200:GLU:OE1	1:A:200:GLU:HA	2.17	0.45
1:A:240:ARG:HE	1:C:1247:ILE:HG12	1.80	0.45
1:B:580:LEU:HD23	1:B:581:ILE:N	2.30	0.45
1:B:600:GLU:HA	1:B:600:GLU:OE1	2.16	0.45
1:C:1145:PRO:O	1:C:1146:MET:C	2.55	0.45
1:C:1164:GLY:O	1:C:1168:MET:HG3	2.15	0.45
1:E:2030:GLU:HG3	1:E:2035:ARG:NH1	2.31	0.45
1:F:2669:GLY:O	1:F:2670:GLY:C	2.59	0.45
1:A:219:VAL:HG11	1:A:258:ARG:HD2	1.97	0.45
1:A:250:GLU:OE2	1:D:1716:GLY:HA2	2.16	0.45
1:A:366:VAL:CG1	1:A:367:GLU:N	2.78	0.45
1:C:1071:VAL:HG11	1:C:1098:PHE:CD2	2.51	0.45
1:C:1107:GLY:HA3	1:D:1539:MET:O	2.16	0.45
1:C:1373:GLU:OE2	1:C:1376:GLU:OE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2279:ILE:O	1:E:2283:VAL:HG22	2.16	0.45
1:F:2746:VAL:CG2	1:F:2747:CYS:H	2.06	0.45
1:A:173:VAL:CG2	1:A:174:GLY:N	2.78	0.45
1:A:234:LEU:N	1:A:234:LEU:HD22	2.32	0.45
1:B:430:GLU:HG3	1:B:435:ARG:NH1	2.32	0.45
1:D:1505:LEU:HD12	1:D:1506:LEU:N	2.31	0.45
1:D:1605:ILE:N	1:D:1605:ILE:HD12	2.31	0.45
1:D:1648:ILE:HG22	1:D:1682:VAL:HG12	1.98	0.45
1:F:2671:LEU:HD12	1:F:2688:VAL:HG22	1.98	0.45
1:F:2683:VAL:HG21	1:F:2686:PHE:CE2	2.51	0.45
1:B:613:ASP:CG	1:E:2240:ARG:NH1	2.74	0.45
1:C:1346:VAL:CG2	1:C:1347:CYS:N	2.67	0.45
1:C:1368:PHE:HA	1:C:1369:PRO:HD2	1.83	0.45
1:D:1438:VAL:CG1	1:D:1707:VAL:HG13	2.41	0.45
1:D:1439:LEU:HD23	1:D:1721:ARG:HB2	1.98	0.45
1:D:1747:CYS:O	1:D:1747:CYS:SG	2.75	0.45
1:E:2205:ILE:N	1:E:2205:ILE:HD12	2.31	0.45
1:E:2234:LEU:HD23	1:E:2265:ILE:HG23	1.99	0.45
1:F:2443:THR:HG22	1:F:2487:PRO:HA	1.98	0.45
1:F:2730:GLY:O	1:F:2732:TYR:HD1	1.98	0.45
1:A:283:VAL:HG21	1:A:286:PHE:CZ	2.52	0.45
1:B:443:THR:HG22	1:B:487:PRO:HA	1.98	0.45
1:B:594:PHE:CE1	1:B:598:ILE:HG13	2.52	0.45
1:B:605:ILE:HA	1:B:631:ALA:O	2.16	0.45
1:B:726:ARG:HG3	1:B:732:TYR:CE1	2.51	0.45
1:E:2173:VAL:CG2	1:E:2174:GLY:N	2.80	0.45
1:E:2194:PHE:CE1	1:E:2198:ILE:HG13	2.51	0.45
1:F:2444:THR:HG22	1:F:2699:ASP:C	2.41	0.45
1:F:2622:ALA:HB1	1:F:2660:TYR:CD2	2.52	0.45
1:B:505:LEU:HD12	1:B:506:LEU:N	2.30	0.45
1:C:1030:GLU:HG3	1:C:1035:ARG:NH1	2.31	0.45
1:C:1173:VAL:CG2	1:C:1174:GLY:N	2.80	0.45
1:D:1726:ARG:HG3	1:D:1732:TYR:CE1	2.52	0.45
1:D:1773:GLU:OE2	1:D:1776:GLU:OE1	2.34	0.45
1:F:2564:GLY:O	1:F:2568:MET:HG3	2.17	0.45
1:B:608:VAL:HG13	1:B:617:GLU:CB	2.46	0.45
1:C:1144:ALA:N	1:C:1145:PRO:HD2	2.32	0.45
1:D:1552:PHE:O	1:D:1553:ILE:C	2.58	0.45
1:D:1611:PHE:HB2	1:D:1612:TYR:HD1	1.81	0.45
1:E:2016:LYS:O	1:F:2563:LEU:HB2	2.17	0.45
1:E:2039:LEU:HD23	1:E:2321:ARG:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:GLU:OE2	1:B:776:GLU:OE1	2.34	0.45
1:C:1003:ARG:HD3	4:C:36:HOH:O	2.17	0.45
1:C:1326:ARG:HG3	1:C:1332:TYR:CE1	2.52	0.45
1:D:1589:LYS:HG2	1:D:1593:TYR:CZ	2.52	0.45
1:D:1634:LEU:HD23	1:D:1665:ILE:HG23	1.98	0.45
1:D:1652:ARG:HD2	1:D:1682:VAL:CG1	2.47	0.45
1:E:2020:VAL:HG11	1:F:2572:ALA:HB3	1.99	0.45
1:E:2033:ASN:HD22	1:E:2033:ASN:HA	1.60	0.45
1:F:2537:ARG:CG	1:F:2537:ARG:NH1	2.71	0.45
1:F:2704:ILE:H	1:F:2704:ILE:HG12	1.58	0.45
1:A:40:ALA:HA	1:A:304:ILE:HA	1.98	0.45
1:A:44:THR:HG22	1:A:299:ASP:O	2.17	0.45
1:B:544:ALA:N	1:B:545:PRO:HD2	2.32	0.45
1:B:612:TYR:N	1:B:612:TYR:HD1	2.14	0.45
1:C:1100:ILE:O	1:C:1100:ILE:HG22	2.17	0.45
1:C:1200:GLU:OE1	1:C:1200:GLU:HA	2.16	0.45
1:D:1537:ARG:CG	1:D:1537:ARG:NH1	2.75	0.45
1:D:1613:ASP:CG	1:F:2640:ARG:NH1	2.75	0.45
1:E:2224:ALA:C	1:E:2226:GLY:N	2.70	0.45
1:E:2248:ILE:CG2	1:E:2282:VAL:HG12	2.47	0.45
1:F:2430:GLU:HG3	1:F:2435:ARG:NH1	2.31	0.45
1:B:573:VAL:CG2	1:B:574:GLY:N	2.80	0.45
1:B:619:VAL:HG11	1:B:658:ARG:HD2	1.99	0.45
1:C:1065:LEU:HD22	1:C:1108:MET:HE1	1.99	0.45
1:C:1176:MET:HB2	1:C:1207:LEU:HB2	1.99	0.45
1:C:1234:LEU:HD23	1:C:1265:ILE:HG23	1.97	0.45
1:C:1252:ARG:HD2	1:C:1282:VAL:HG13	1.98	0.45
1:D:1444:THR:CG2	1:D:1698:VAL:HG12	2.33	0.45
1:D:1594:PHE:CE1	1:D:1598:ILE:HG13	2.52	0.45
1:D:1722:LYS:HZ2	1:D:1736:PRO:HA	1.81	0.45
1:E:2003:ARG:CB	1:F:2464:LYS:HD3	2.47	0.45
1:A:53:TRP:HZ3	1:A:388:GLU:O	2.00	0.44
1:A:198:ILE:O	1:A:204:ARG:NH2	2.50	0.44
1:A:321:ARG:O	1:A:322:LYS:NZ	2.40	0.44
1:D:1518:ALA:O	1:D:1522:ILE:HD13	2.17	0.44
1:E:2188:VAL:HA	1:E:2191:TRP:CD1	2.52	0.44
1:F:2591:TRP:CE3	1:F:2606:ALA:HB1	2.52	0.44
1:B:730:GLY:O	1:B:732:TYR:HD1	2.00	0.44
1:C:1212:TYR:N	1:C:1212:TYR:HD1	2.13	0.44
1:D:1576:MET:HB2	1:D:1607:LEU:HB2	2.00	0.44
1:D:1600:GLU:HA	1:D:1600:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1612:TYR:N	1:D:1612:TYR:HD1	2.14	0.44
1:E:2044:THR:CG2	1:E:2298:VAL:HG12	2.31	0.44
1:E:2163:LEU:HB2	1:F:2416:LYS:O	2.17	0.44
1:F:2655:LEU:HD13	1:F:2663:VAL:HG23	1.97	0.44
1:F:2727:CYS:SG	1:F:2729:ASN:HB2	2.56	0.44
1:A:225:LEU:O	1:A:226:GLY:C	2.60	0.44
1:B:743:ARG:HG2	1:B:743:ARG:NH1	2.33	0.44
1:C:1044:THR:HG22	1:C:1299:ASP:O	2.17	0.44
1:C:1118:ALA:O	1:C:1122:ILE:CD1	2.66	0.44
1:C:1139:MET:O	1:D:1507:GLY:HA3	2.18	0.44
1:D:1430:GLU:HG3	1:D:1435:ARG:NH1	2.32	0.44
1:D:1576:MET:HE3	1:D:1580:LEU:HD22	1.98	0.44
1:E:2164:GLY:O	1:E:2168:MET:HG3	2.17	0.44
1:E:2180:LEU:HD23	1:E:2181:ILE:N	2.32	0.44
1:E:2225:LEU:CB	1:E:2228:LYS:HB2	2.41	0.44
1:E:2248:ILE:HG22	1:E:2282:VAL:HG12	1.99	0.44
1:F:2548:ASP:HB3	1:F:2559:VAL:HG21	2.00	0.44
1:A:152:PHE:C	1:A:154:GLY:N	2.75	0.44
1:A:344:CYS:O	1:A:345:PRO:C	2.60	0.44
1:C:1061:GLU:OE1	1:D:1540:HIS:HE1	2.01	0.44
1:C:1188:VAL:HA	1:C:1191:TRP:HE1	1.78	0.44
1:D:1598:ILE:O	1:D:1604:ARG:NH2	2.50	0.44
1:D:1669:GLY:O	1:D:1670:GLY:C	2.60	0.44
1:A:194:PHE:CE1	1:A:198:ILE:HG13	2.52	0.44
1:C:1191:TRP:CE3	1:C:1206:ALA:HB1	2.52	0.44
1:C:1205:ILE:HD12	1:C:1205:ILE:N	2.32	0.44
1:D:1420:VAL:HG23	1:D:1421:TYR:N	2.31	0.44
1:D:1444:THR:HG22	1:D:1699:ASP:C	2.42	0.44
1:E:2071:VAL:HG11	1:E:2098:PHE:CD2	2.53	0.44
1:E:2198:ILE:O	1:E:2204:ARG:NH2	2.50	0.44
1:F:2545:PRO:O	1:F:2546:MET:C	2.60	0.44
1:A:26:LYS:HD3	1:A:100:ILE:CD1	2.48	0.44
1:A:57:VAL:CG1	1:A:112:ALA:HB1	2.48	0.44
1:A:177:PRO:HG3	1:B:421:TYR:CD1	2.53	0.44
1:B:537:ARG:CG	1:B:537:ARG:NH1	2.76	0.44
1:C:1327:CYS:SG	1:C:1329:ASN:HB2	2.58	0.44
1:E:2252:ARG:HD2	1:E:2282:VAL:CG1	2.47	0.44
1:A:71:VAL:HG11	1:A:98:PHE:CD2	2.53	0.44
1:B:549:ARG:O	1:B:553:ILE:HG13	2.18	0.44
1:C:1283:VAL:HG21	1:C:1286:PHE:CE2	2.53	0.44
1:C:1352:GLU:HA	1:C:1353:PRO:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1545:PRO:O	1:D:1546:MET:C	2.59	0.44
1:D:1565:ALA:HB2	1:D:1572:ALA:HB2	2.00	0.44
1:D:1744:CYS:O	1:D:1745:PRO:C	2.60	0.44
1:E:2054:GLY:HA2	1:E:2117:THR:HG23	2.00	0.44
1:F:2652:ARG:HD2	1:F:2682:VAL:HG13	2.00	0.44
1:B:444:THR:HG22	1:B:699:ASP:C	2.43	0.44
1:B:598:ILE:O	1:B:604:ARG:NH2	2.51	0.44
1:B:747:CYS:O	1:B:747:CYS:SG	2.76	0.44
1:C:1039:LEU:HD23	1:C:1321:ARG:HB2	2.00	0.44
1:C:1222:ALA:O	1:C:1226:GLY:HA2	2.18	0.44
1:C:1269:GLY:O	1:C:1270:GLY:C	2.61	0.44
1:C:1344:CYS:O	1:C:1345:PRO:C	2.60	0.44
1:D:1471:VAL:HG11	1:D:1498:PHE:CD2	2.53	0.44
1:D:1544:ALA:N	1:D:1545:PRO:HD2	2.32	0.44
1:E:2175:THR:O	1:F:2421:TYR:HB2	2.18	0.44
1:F:2766:VAL:CG1	1:F:2767:GLU:N	2.80	0.44
1:A:145:PRO:O	1:A:146:MET:C	2.61	0.43
1:D:1521:ARG:NH1	1:D:1673:GLU:OE2	2.47	0.43
1:D:1607:LEU:HD22	1:D:1607:LEU:HA	1.86	0.43
1:F:2588:VAL:HA	1:F:2591:TRP:CD1	2.53	0.43
1:F:2653:TRP:HD1	1:F:2654:GLU:OE2	2.01	0.43
1:A:176:MET:HB2	1:A:207:LEU:HB2	1.99	0.43
1:B:431:VAL:O	1:B:433:ASN:N	2.51	0.43
1:B:576:MET:HB2	1:B:607:LEU:HB2	1.99	0.43
1:F:2722:LYS:HZ2	1:F:2736:PRO:CA	2.30	0.43
1:A:205:ILE:HD12	1:A:205:ILE:N	2.33	0.43
1:A:24:ARG:O	1:A:28:ILE:HG12	2.18	0.43
1:A:28:ILE:HD11	1:B:598:ILE:HG12	2.00	0.43
1:A:69:ILE:O	1:A:71:VAL:N	2.43	0.43
1:A:347:CYS:SG	1:A:347:CYS:O	2.76	0.43
1:C:1054:GLY:HA2	1:C:1117:THR:HG23	2.01	0.43
1:C:1148:ASP:CG	1:C:1159:VAL:HG13	2.42	0.43
1:C:1326:ARG:HH12	1:C:1381:GLN:NE2	2.11	0.43
1:D:1683:VAL:HG21	1:D:1686:PHE:CE2	2.53	0.43
1:E:2044:THR:HG22	1:E:2299:ASP:C	2.44	0.43
1:F:2625:LEU:O	1:F:2626:GLY:C	2.62	0.43
1:A:321:ARG:O	1:A:322:LYS:HD2	2.14	0.43
1:B:471:VAL:HG11	1:B:498:PHE:CD2	2.53	0.43
1:B:565:ALA:HB2	1:B:572:ALA:HB2	2.00	0.43
1:C:1062:VAL:HG11	1:C:1089:LEU:HD11	1.99	0.43
1:C:1198:ILE:O	1:C:1204:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1457:VAL:CG1	1:D:1512:ALA:HB1	2.48	0.43
1:D:1463:ALA:HB2	1:D:1758:ILE:HD12	2.00	0.43
1:D:1730:GLY:O	1:D:1732:TYR:HD1	2.01	0.43
1:E:2172:ALA:HB3	1:F:2420:VAL:HG11	1.99	0.43
1:E:2252:ARG:HD2	1:E:2282:VAL:HG13	2.00	0.43
1:F:2722:LYS:HZ2	1:F:2736:PRO:CB	2.31	0.43
1:F:2726:ARG:HG3	1:F:2732:TYR:CE1	2.53	0.43
1:A:107:GLY:HA3	1:B:539:MET:O	2.19	0.43
1:C:1057:VAL:CG1	1:C:1112:ALA:HB1	2.48	0.43
1:D:1743:ARG:HG2	1:D:1743:ARG:NH1	2.31	0.43
1:E:2152:PHE:C	1:E:2154:GLY:N	2.76	0.43
1:E:2321:ARG:O	1:E:2322:LYS:HD2	2.15	0.43
1:A:121:ARG:NH1	1:A:273:GLU:OE2	2.50	0.43
1:B:521:ARG:HA	1:B:789:ILE:HD11	2.00	0.43
1:B:576:MET:HE3	1:B:580:LEU:HD22	2.00	0.43
1:C:1224:ALA:C	1:C:1225:LEU:HD23	2.43	0.43
1:C:1346:VAL:HG13	1:C:1347:CYS:N	2.34	0.43
1:E:2176:MET:HB2	1:E:2207:LEU:HB2	2.01	0.43
1:F:2471:VAL:HG11	1:F:2498:PHE:CD2	2.53	0.43
1:F:2512:ALA:CA	1:F:2546:MET:HE1	2.41	0.43
1:A:224:ALA:C	1:A:225:LEU:HD23	2.44	0.43
1:B:652:ARG:HD2	1:B:682:VAL:CG1	2.48	0.43
1:B:746:VAL:HG13	1:B:747:CYS:N	2.34	0.43
1:C:1026:LYS:HD3	1:C:1100:ILE:CD1	2.48	0.43
1:C:1252:ARG:HD2	1:C:1282:VAL:CG1	2.49	0.43
1:C:1347:CYS:SG	1:C:1347:CYS:O	2.77	0.43
1:D:1573:VAL:CG2	1:D:1574:GLY:N	2.79	0.43
1:E:2064:LYS:HD3	1:F:2403:ARG:CB	2.49	0.43
1:C:1003:ARG:HE	1:D:1409:GLU:HG2	1.84	0.43
1:C:1020:VAL:CG1	1:D:1572:ALA:HB3	2.49	0.43
1:F:2426:LYS:HD3	1:F:2500:ILE:CD1	2.49	0.43
1:A:188:VAL:HA	1:A:191:TRP:CD1	2.54	0.43
1:A:222:ALA:O	1:A:226:GLY:HA2	2.19	0.43
1:B:725:TYR:HE2	1:B:753:PRO:HG3	1.82	0.43
1:E:2225:LEU:O	1:E:2226:GLY:C	2.61	0.43
1:E:2310:LYS:HA	1:E:2311:PRO:HD3	1.88	0.43
1:B:683:VAL:CG2	1:B:686:PHE:CZ	3.01	0.42
1:D:1426:LYS:HD3	1:D:1500:ILE:CD1	2.49	0.42
1:E:2069:ILE:HA	1:E:2070:PRO:HD3	1.76	0.42
1:E:2197:VAL:CB	1:F:2428:ILE:HD13	2.39	0.42
1:E:2344:CYS:SG	1:E:2346:VAL:CG1	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2420:VAL:O	1:F:2422:PHE:N	2.52	0.42
1:A:224:ALA:C	1:A:226:GLY:N	2.68	0.42
1:B:589:LYS:HG2	1:B:593:TYR:CZ	2.54	0.42
1:B:683:VAL:HG21	1:B:686:PHE:CE2	2.54	0.42
1:D:1476:MET:HE3	1:D:1487:PRO:O	2.19	0.42
1:D:1551:ALA:O	1:D:1556:CYS:HB2	2.19	0.42
1:D:1564:GLY:O	1:D:1568:MET:HG3	2.19	0.42
1:D:1634:LEU:N	1:D:1634:LEU:HD22	2.34	0.42
1:D:1746:VAL:HG13	1:D:1747:CYS:N	2.34	0.42
1:E:2069:ILE:O	1:E:2071:VAL:N	2.44	0.42
1:F:2454:GLY:HA2	1:F:2517:THR:HG23	2.01	0.42
1:D:1573:VAL:CG2	1:D:1574:GLY:H	2.31	0.42
1:D:1652:ARG:CD	1:D:1682:VAL:HG13	2.49	0.42
1:E:2028:ILE:HD13	1:F:2597:VAL:CB	2.39	0.42
1:E:2359:ILE:O	1:E:2359:ILE:HG22	2.19	0.42
1:F:2580:LEU:HD23	1:F:2581:ILE:N	2.35	0.42
1:F:2744:CYS:SG	1:F:2746:VAL:CG1	3.07	0.42
1:A:234:LEU:HD23	1:A:265:ILE:HG23	2.00	0.42
1:A:310:LYS:HA	1:A:311:PRO:HD3	1.89	0.42
1:F:2544:ALA:N	1:F:2545:PRO:HD2	2.35	0.42
1:C:1085:TYR:OH	1:F:2646:LYS:HD3	2.20	0.42
1:C:1130:PRO:HA	1:C:1157:ASP:OD1	2.19	0.42
1:C:1152:PHE:O	1:C:1153:ILE:C	2.61	0.42
1:C:1327:CYS:SG	1:C:1329:ASN:N	2.82	0.42
1:D:1588:VAL:HA	1:D:1591:TRP:CD1	2.54	0.42
1:E:2350:LYS:CE	1:E:2350:LYS:N	2.73	0.42
1:F:2457:VAL:CG1	1:F:2512:ALA:HB1	2.49	0.42
1:A:263:VAL:O	1:A:263:VAL:HG23	2.19	0.42
1:A:326:ARG:HG3	1:A:332:TYR:CE1	2.55	0.42
1:B:444:THR:CG2	1:B:698:VAL:HG12	2.32	0.42
1:B:576:MET:HA	1:B:577:PRO:HD3	1.83	0.42
1:C:1009:GLU:HG2	1:D:1403:ARG:HE	1.85	0.42
1:C:1225:LEU:O	1:C:1226:GLY:C	2.62	0.42
1:C:1283:VAL:CG2	1:C:1286:PHE:CZ	3.03	0.42
1:E:2057:VAL:CG1	1:E:2112:ALA:HB1	2.49	0.42
1:E:2118:ALA:O	1:E:2122:ILE:HD13	2.19	0.42
1:F:2752:GLU:HA	1:F:2753:PRO:HD3	1.88	0.42
1:A:152:PHE:O	1:A:153:ILE:C	2.61	0.42
1:A:327:CYS:SG	1:A:329:ASN:HB2	2.60	0.42
1:B:415:GLY:O	1:B:418:THR:HG23	2.19	0.42
1:B:564:GLY:O	1:B:568:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1053:TRP:HZ3	1:C:1388:GLU:O	2.01	0.42
1:C:1255:LEU:HD13	1:C:1263:VAL:HG23	2.00	0.42
1:D:1624:ALA:C	1:D:1625:LEU:HD23	2.45	0.42
1:D:1638:SER:O	1:F:2642:GLY:HA3	2.20	0.42
1:E:2020:VAL:HG13	1:F:2572:ALA:HB3	2.01	0.42
1:E:2189:LYS:HG2	1:E:2193:TYR:CZ	2.54	0.42
1:E:2207:LEU:HD21	1:E:2233:ARG:NH2	2.34	0.42
1:E:2269:GLY:O	1:E:2270:GLY:C	2.62	0.42
1:F:2486:GLU:HG2	1:F:2734:VAL:CG2	2.50	0.42
1:F:2489:LEU:HD23	1:F:2490:GLN:N	2.35	0.42
1:F:2500:ILE:O	1:F:2500:ILE:HG22	2.20	0.42
1:A:62:VAL:HG11	1:A:89:LEU:HD11	2.01	0.42
1:A:368:PHE:HA	1:A:369:PRO:HD2	1.84	0.42
1:B:462:VAL:HG11	1:B:489:LEU:HD11	2.01	0.42
1:B:640:ARG:NH1	1:E:2213:ASP:OD1	2.52	0.42
1:D:1696:LYS:HA	1:D:1697:PRO:HD3	1.94	0.42
1:E:2086:GLU:HG2	1:E:2334:VAL:CG2	2.50	0.42
1:F:2566:GLU:C	1:F:2568:MET:H	2.27	0.42
1:F:2721:ARG:O	1:F:2722:LYS:HD2	2.14	0.42
1:A:44:THR:HG22	1:A:299:ASP:C	2.45	0.42
1:A:61:GLU:OE1	1:B:540:HIS:HE1	2.03	0.42
1:A:176:MET:HA	1:A:177:PRO:HD3	1.85	0.42
1:B:552:PHE:C	1:B:554:GLY:N	2.76	0.42
1:B:588:VAL:HA	1:B:591:TRP:CD1	2.55	0.42
1:B:624:ALA:C	1:B:625:LEU:HD23	2.45	0.42
1:F:2529:LYS:HB3	1:F:2530:PRO:HD2	2.01	0.42
1:F:2652:ARG:HD2	1:F:2682:VAL:CG1	2.49	0.42
1:A:252:ARG:HD2	1:A:282:VAL:CG1	2.49	0.42
1:A:282:VAL:O	1:A:282:VAL:CG1	2.68	0.42
1:B:548:ASP:CG	1:B:559:VAL:HG13	2.44	0.42
1:C:1044:THR:HG22	1:C:1299:ASP:C	2.45	0.42
1:C:1166:GLU:O	1:C:1167:MET:C	2.63	0.42
1:D:1431:VAL:O	1:D:1433:ASN:N	2.52	0.42
1:D:1552:PHE:C	1:D:1554:GLY:N	2.75	0.42
1:D:1608:VAL:HG12	1:D:1614:GLU:HA	2.02	0.42
1:D:1655:LEU:HD13	1:D:1663:VAL:HG23	2.00	0.42
1:D:1768:PHE:HA	1:D:1769:PRO:HD2	1.84	0.42
1:E:2064:LYS:HB3	1:F:2403:ARG:HB2	2.02	0.42
1:E:2233:ARG:HG3	1:E:2266:PHE:HD1	1.85	0.42
1:F:2573:VAL:CG2	1:F:2574:GLY:N	2.82	0.42
1:C:1188:VAL:HA	1:C:1191:TRP:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1310:LYS:HA	1:C:1311:PRO:HD3	1.88	0.41
1:D:1625:LEU:O	1:D:1628:LYS:HB2	2.20	0.41
1:D:1663:VAL:HG23	1:D:1663:VAL:O	2.19	0.41
1:D:1750:LYS:CE	1:D:1750:LYS:N	2.73	0.41
1:E:2234:LEU:HD22	1:E:2234:LEU:N	2.34	0.41
1:F:2439:LEU:HD23	1:F:2721:ARG:HB2	2.01	0.41
1:F:2521:ARG:HA	1:F:2789:ILE:HD11	2.01	0.41
1:A:162:VAL:HG22	1:B:420:VAL:HG12	2.01	0.41
1:B:653:TRP:CD1	1:F:2718:LEU:HD22	2.55	0.41
1:D:1664:LYS:HB3	1:D:1684:ASP:CG	2.45	0.41
1:F:2454:GLY:HA2	1:F:2517:THR:CG2	2.50	0.41
1:F:2607:LEU:HD22	1:F:2607:LEU:HA	1.86	0.41
1:A:252:ARG:CD	1:A:282:VAL:HG13	2.51	0.41
1:C:1152:PHE:C	1:C:1154:GLY:N	2.77	0.41
1:C:1350:LYS:CE	1:C:1350:LYS:N	2.73	0.41
1:E:2208:VAL:HG12	1:E:2214:GLU:HA	2.03	0.41
1:E:2283:VAL:CG2	1:E:2286:PHE:CZ	3.04	0.41
1:F:2576:MET:HB2	1:F:2607:LEU:HB2	2.01	0.41
1:F:2602:VAL:O	1:F:2603:PRO:C	2.63	0.41
1:F:2628:LYS:HE2	1:F:2628:LYS:CA	2.44	0.41
1:F:2683:VAL:CG2	1:F:2686:PHE:CZ	3.03	0.41
1:A:20:VAL:CG1	1:B:572:ALA:HB3	2.50	0.41
1:A:92:GLU:CD	1:A:321:ARG:HH22	2.27	0.41
1:A:121:ARG:HA	1:A:389:ILE:HD11	2.02	0.41
1:A:144:ALA:N	1:A:145:PRO:HD2	2.35	0.41
1:A:212:TYR:HB2	1:A:217:GLU:CG	2.44	0.41
1:A:343:ARG:HG2	1:A:343:ARG:NH1	2.35	0.41
1:C:1189:LYS:HG2	1:C:1193:TYR:CZ	2.56	0.41
1:D:1619:VAL:HG11	1:D:1658:ARG:HD2	2.02	0.41
1:E:2253:TRP:HD1	1:E:2254:GLU:OE2	2.03	0.41
1:F:2420:VAL:C	1:F:2422:PHE:H	2.27	0.41
1:F:2462:VAL:HG11	1:F:2489:LEU:HD11	2.02	0.41
1:F:2576:MET:HE3	1:F:2580:LEU:HD22	2.03	0.41
1:F:2750:LYS:CE	1:F:2750:LYS:N	2.73	0.41
1:A:173:VAL:CG2	1:A:174:GLY:H	2.30	0.41
1:A:346:VAL:HG13	1:A:347:CYS:N	2.34	0.41
1:E:2021:TYR:HB2	1:F:2575:THR:O	2.19	0.41
1:E:2026:LYS:HD3	1:E:2100:ILE:CD1	2.50	0.41
1:E:2054:GLY:HA2	1:E:2117:THR:CG2	2.51	0.41
1:A:187:GLN:H	1:A:187:GLN:NE2	2.19	0.41
1:A:283:VAL:HG21	1:A:286:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:VAL:C	1:B:422:PHE:H	2.29	0.41
1:C:1089:LEU:C	1:C:1089:LEU:CD2	2.93	0.41
1:C:1264:LYS:HB3	1:C:1284:ASP:CG	2.46	0.41
1:D:1462:VAL:HG11	1:D:1489:LEU:HD11	2.03	0.41
1:D:1469:ILE:O	1:D:1471:VAL:N	2.46	0.41
1:D:1625:LEU:O	1:D:1626:GLY:C	2.62	0.41
1:D:1683:VAL:CG2	1:D:1686:PHE:CZ	3.04	0.41
1:E:2062:VAL:HG11	1:E:2089:LEU:HD11	2.02	0.41
1:A:208:VAL:HG21	1:A:232:VAL:CG1	2.51	0.41
1:A:304:ILE:H	1:A:304:ILE:HG12	1.57	0.41
1:B:521:ARG:CG	1:B:789:ILE:HD11	2.50	0.41
1:C:1208:VAL:HG12	1:C:1214:GLU:HA	2.03	0.41
1:D:1415:GLY:O	1:D:1418:THR:HG23	2.20	0.41
1:D:1537:ARG:CZ	3:D:1792:PCP:O2	2.69	0.41
1:D:1608:VAL:HG21	1:D:1632:VAL:CG1	2.51	0.41
1:D:1724:VAL:HG22	1:D:1755:LEU:CD2	2.50	0.41
1:E:2031:VAL:O	1:E:2033:ASN:N	2.54	0.41
1:E:2326:ARG:HG3	1:E:2332:TYR:CE1	2.56	0.41
1:F:2598:ILE:O	1:F:2604:ARG:NH2	2.53	0.41
1:F:2622:ALA:O	1:F:2626:GLY:HA2	2.21	0.41
1:F:2703:ASP:HB2	1:F:2717:LYS:HE3	2.03	0.41
1:A:346:VAL:CG2	1:A:347:CYS:N	2.68	0.41
1:B:664:LYS:HB3	1:B:684:ASP:CG	2.46	0.41
1:C:1202:VAL:O	1:C:1203:PRO:C	2.63	0.41
1:C:1343:ARG:HG2	1:C:1343:ARG:NH1	2.35	0.41
1:D:1521:ARG:CG	1:D:1789:ILE:HD11	2.50	0.41
1:D:1622:ALA:O	1:D:1626:GLY:HA2	2.21	0.41
1:D:1789:ILE:HD12	1:D:1789:ILE:HA	1.85	0.41
1:E:2121:ARG:CG	1:E:2389:ILE:HD11	2.51	0.41
1:E:2252:ARG:CD	1:E:2282:VAL:HG13	2.51	0.41
1:F:2489:LEU:C	1:F:2489:LEU:CD2	2.90	0.41
1:F:2549:ARG:O	1:F:2553:ILE:HG13	2.21	0.41
1:F:2624:ALA:O	1:F:2625:LEU:HG	2.21	0.41
1:F:2759:ILE:O	1:F:2759:ILE:HG22	2.20	0.41
1:A:20:VAL:HG12	1:B:562:VAL:HG22	2.02	0.41
1:A:54:GLY:HA2	1:A:117:THR:HG23	2.02	0.41
1:A:81:ILE:H	1:A:381:GLN:HE22	1.68	0.41
1:A:140:HIS:HE1	1:B:461:GLU:OE1	2.04	0.41
1:A:151:ALA:O	1:A:156:CYS:HB2	2.21	0.41
1:A:166:GLU:O	1:A:167:MET:C	2.64	0.41
1:A:225:LEU:O	1:A:228:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:ALA:HB2	1:B:758:ILE:HD12	2.02	0.41
1:B:682:VAL:O	1:B:682:VAL:CG1	2.68	0.41
1:B:704:ILE:H	1:B:704:ILE:HG12	1.57	0.41
1:B:724:VAL:HG22	1:B:755:LEU:CD2	2.51	0.41
1:C:1092:GLU:CD	1:C:1321:ARG:HH22	2.28	0.41
1:C:1303:ASP:HB2	1:C:1317:LYS:HE3	2.02	0.41
1:C:1324:VAL:HG22	1:C:1355:LEU:CD2	2.51	0.41
1:D:1703:ASP:HB2	1:D:1717:LYS:HE3	2.03	0.41
1:D:1722:LYS:HZ2	1:D:1736:PRO:CB	2.34	0.41
1:E:2003:ARG:HB2	1:F:2464:LYS:HB3	2.02	0.41
1:E:2172:ALA:HB3	1:F:2420:VAL:HG13	2.02	0.41
1:E:2222:ALA:O	1:E:2226:GLY:HA2	2.21	0.41
1:E:2255:LEU:HD13	1:E:2263:VAL:HG23	1.98	0.41
1:E:2346:VAL:HG13	1:E:2347:CYS:N	2.36	0.41
1:F:2431:VAL:O	1:F:2433:ASN:N	2.53	0.41
1:F:2548:ASP:CG	1:F:2559:VAL:HG13	2.45	0.41
1:A:26:LYS:CD	1:A:100:ILE:HD11	2.51	0.41
1:A:148:ASP:CG	1:A:159:VAL:HG13	2.46	0.41
1:A:208:VAL:HG12	1:A:214:GLU:HA	2.03	0.41
1:A:233:ARG:HG3	1:A:266:PHE:HD1	1.86	0.41
1:B:420:VAL:O	1:B:422:PHE:N	2.54	0.41
1:B:523:LYS:HE3	1:B:528:PHE:HA	2.03	0.41
1:B:624:ALA:O	1:B:625:LEU:HG	2.21	0.41
1:C:1028:ILE:HD11	1:D:1594:PHE:HA	2.03	0.41
1:C:1140:HIS:HE1	1:D:1461:GLU:OE1	2.04	0.41
1:C:1173:VAL:CG2	1:C:1174:GLY:H	2.33	0.41
1:D:1477:PRO:O	1:D:1478:GLU:C	2.64	0.41
1:D:1481:ILE:H	1:D:1781:GLN:HE22	1.69	0.41
1:D:1640:ARG:NH1	1:F:2613:ASP:OD1	2.53	0.41
1:A:100:ILE:O	1:A:100:ILE:HG22	2.21	0.40
1:A:236:THR:HB	1:A:241:ARG:CG	2.51	0.40
1:B:530:PRO:HA	1:B:557:ASP:OD1	2.21	0.40
1:B:625:LEU:O	1:B:626:GLY:C	2.64	0.40
1:B:652:ARG:CD	1:B:682:VAL:HG13	2.50	0.40
1:B:653:TRP:CZ2	1:F:2722:LYS:HG2	2.57	0.40
1:C:1191:TRP:HZ3	1:C:1207:LEU:O	2.04	0.40
1:C:1194:PHE:HA	1:D:1428:ILE:HD11	2.01	0.40
1:C:1208:VAL:CG1	1:C:1217:GLU:HB2	2.51	0.40
1:D:1521:ARG:HA	1:D:1789:ILE:HD11	2.03	0.40
1:D:1602:VAL:O	1:D:1603:PRO:C	2.64	0.40
1:E:2152:PHE:O	1:E:2153:ILE:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2176:MET:HE3	1:E:2180:LEU:HD22	2.03	0.40
1:F:2521:ARG:CG	1:F:2789:ILE:HD11	2.51	0.40
1:A:303:ASP:HB2	1:A:317:LYS:HE3	2.03	0.40
1:B:529:LYS:HB3	1:B:530:PRO:HD2	2.03	0.40
1:B:573:VAL:CG2	1:B:574:GLY:H	2.32	0.40
1:B:638:SER:O	1:E:2242:GLY:HA3	2.20	0.40
1:B:705:VAL:HA	1:B:713:ALA:HB2	2.04	0.40
1:D:1710:LYS:HA	1:D:1711:PRO:HD3	1.87	0.40
1:E:2060:GLU:O	1:E:2061:GLU:C	2.64	0.40
1:E:2173:VAL:CG2	1:E:2174:GLY:H	2.32	0.40
1:F:2419:ASP:HB2	1:F:2421:TYR:CE2	2.56	0.40
1:F:2492:GLU:CD	1:F:2721:ARG:HH22	2.28	0.40
1:F:2523:LYS:HE3	1:F:2528:PHE:HA	2.03	0.40
1:F:2576:MET:HE2	1:F:2576:MET:HB3	1.91	0.40
1:A:137:ARG:CZ	3:A:392:PCP:O2	2.69	0.40
1:A:189:LYS:HG2	1:A:193:TYR:CZ	2.55	0.40
1:B:426:LYS:HD3	1:B:500:ILE:CD1	2.51	0.40
1:C:1031:VAL:O	1:C:1033:ASN:N	2.54	0.40
1:C:1193:TYR:CE2	1:D:1432:LYS:HD3	2.56	0.40
1:D:1576:MET:HA	1:D:1577:PRO:HD3	1.82	0.40
1:D:1647:ILE:HG12	1:F:2640:ARG:HE	1.87	0.40
1:E:2208:VAL:HG21	1:E:2232:VAL:CG1	2.51	0.40
1:F:2581:ILE:HG23	1:F:2587:GLN:HA	2.04	0.40
1:F:2746:VAL:HG13	1:F:2747:CYS:N	2.36	0.40
1:A:315:ARG:HE	1:B:640:ARG:NH1	2.20	0.40
1:A:324:VAL:HG22	1:A:355:LEU:CD2	2.51	0.40
1:B:492:GLU:CD	1:B:721:ARG:HH22	2.28	0.40
1:B:625:LEU:O	1:B:628:LYS:HB2	2.21	0.40
1:C:1032:LYS:HD3	1:D:1593:TYR:CE2	2.56	0.40
1:C:1323:GLN:HE21	1:C:1353:PRO:HB3	1.75	0.40
1:D:1759:ILE:O	1:D:1759:ILE:HG22	2.20	0.40
1:E:2015:GLY:O	1:E:2018:THR:HG23	2.21	0.40
1:E:2072:ASN:HA	1:E:2359:ILE:O	2.21	0.40
1:E:2121:ARG:HA	1:E:2389:ILE:HD11	2.02	0.40
1:E:2305:VAL:HA	1:E:2313:ALA:HB2	2.03	0.40
1:E:2330:GLY:O	1:E:2332:TYR:CD1	2.75	0.40
1:F:2608:VAL:HG12	1:F:2614:GLU:HA	2.03	0.40
1:A:72:ASN:HA	1:A:359:ILE:O	2.22	0.40
1:B:608:VAL:HG12	1:B:614:GLU:HA	2.04	0.40
1:B:703:ASP:HB2	1:B:717:LYS:HE3	2.03	0.40
1:B:722:LYS:HG2	1:C:1253:TRP:HH2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1121:ARG:HA	1:C:1389:ILE:HD11	2.03	0.40
1:C:1166:GLU:C	1:C:1168:MET:H	2.29	0.40
1:C:1224:ALA:O	1:C:1225:LEU:HG	2.20	0.40
1:D:1484:PRO:O	1:D:1485:TYR:HB2	2.22	0.40
1:E:2053:TRP:HZ3	1:E:2388:GLU:O	2.05	0.40
1:E:2089:LEU:C	1:E:2089:LEU:CD2	2.92	0.40
1:E:2324:VAL:HG23	1:E:2354:LEU:HD12	2.03	0.40
1:E:2346:VAL:CG2	1:E:2347:CYS:H	2.06	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2376:GLU:OE1	1:F:2776:GLU:OE1[3_884]	1.90	0.30
1:C:1373:GLU:OE2	1:D:1780:GLU:OE1[2_865]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/395 (98%)	329 (85%)	44 (11%)	14 (4%)	2	11
1	B	387/395 (98%)	328 (85%)	40 (10%)	19 (5%)	1	6
1	C	387/395 (98%)	329 (85%)	45 (12%)	13 (3%)	3	12
1	D	387/395 (98%)	329 (85%)	41 (11%)	17 (4%)	2	8
1	E	387/395 (98%)	330 (85%)	40 (10%)	17 (4%)	2	8
1	F	387/395 (98%)	326 (84%)	42 (11%)	19 (5%)	1	6
All	All	2322/2370 (98%)	1971 (85%)	252 (11%)	99 (4%)	2	8

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	VAL
1	B	746	VAL
1	C	1346	VAL
1	D	1746	VAL
1	E	2346	VAL
1	F	2746	VAL
1	A	70	PRO
1	A	167	MET
1	A	208	VAL
1	A	225	LEU
1	A	226	GLY
1	A	299	ASP
1	A	347	CYS
1	B	470	PRO
1	B	567	MET
1	B	608	VAL
1	B	626	GLY
1	C	1070	PRO
1	C	1167	MET
1	C	1208	VAL
1	C	1225	LEU
1	C	1226	GLY
1	C	1299	ASP
1	C	1347	CYS
1	D	1470	PRO
1	D	1528	PHE
1	D	1567	MET
1	D	1608	VAL
1	D	1625	LEU
1	D	1626	GLY
1	D	1699	ASP
1	E	2070	PRO
1	E	2167	MET
1	E	2208	VAL
1	E	2225	LEU
1	E	2226	GLY
1	E	2270	GLY
1	E	2299	ASP
1	E	2347	CYS
1	F	2470	PRO
1	F	2567	MET
1	F	2608	VAL
1	F	2625	LEU

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Mol	Chain	Res	Type
1	F	2626	GLY
1	F	2670	GLY
1	F	2747	CYS
1	A	33	ASN
1	A	270	GLY
1	B	433	ASN
1	B	528	PHE
1	B	625	LEU
1	B	670	GLY
1	B	699	ASP
1	B	747	CYS
1	C	1033	ASN
1	C	1224	ALA
1	D	1433	ASN
1	D	1670	GLY
1	D	1747	CYS
1	E	2033	ASN
1	E	2128	PHE
1	E	2224	ALA
1	F	2433	ASN
1	F	2624	ALA
1	F	2699	ASP
1	A	224	ALA
1	B	624	ALA
1	B	679	ILE
1	C	1270	GLY
1	D	1624	ALA
1	D	1679	ILE
1	E	2281	ASP
1	F	2528	PHE
1	A	279	ILE
1	B	421	TYR
1	B	432	LYS
1	B	765	VAL
1	C	1279	ILE
1	C	1365	VAL
1	D	1681	ASP
1	F	2421	TYR
1	F	2432	LYS
1	F	2765	VAL
1	A	199	GLU
1	A	365	VAL

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Mol	Chain	Res	Type
1	B	599	GLU
1	B	681	ASP
1	D	1432	LYS
1	D	1765	VAL
1	E	2032	LYS
1	E	2279	ILE
1	E	2365	VAL
1	F	2681	ASP
1	F	2679	ILE
1	F	2562	VAL
1	E	2031	VAL
1	F	2431	VAL
1	B	431	VAL
1	D	1431	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/321 (100%)	284 (88%)	37 (12%)	5	18
1	B	321/321 (100%)	283 (88%)	38 (12%)	5	17
1	C	321/321 (100%)	283 (88%)	38 (12%)	5	17
1	D	321/321 (100%)	284 (88%)	37 (12%)	5	18
1	E	321/321 (100%)	283 (88%)	38 (12%)	5	17
1	F	321/321 (100%)	283 (88%)	38 (12%)	5	17
All	All	1926/1926 (100%)	1700 (88%)	226 (12%)	5	17

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ILE
1	A	10	ASP
1	A	13	LYS

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Mol	Chain	Res	Type
1	A	21	TYR
1	A	26	LYS
1	A	32	LYS
1	A	33	ASN
1	A	56	LEU
1	A	66	LEU
1	A	74	TYR
1	A	100	ILE
1	A	137	ARG
1	A	146	MET
1	A	149	ARG
1	A	159	VAL
1	A	187	GLN
1	A	207	LEU
1	A	212	TYR
1	A	225	LEU
1	A	232	VAL
1	A	254	GLU
1	A	271	LEU
1	A	279	ILE
1	A	280	VAL
1	A	304	ILE
1	A	308	GLU
1	A	314	LYS
1	A	322	LYS
1	A	323	GLN
1	A	326	ARG
1	A	333	HIS
1	A	350	LYS
1	A	359	ILE
1	A	363	GLU
1	A	388	GLU
1	A	389	ILE
1	B	401	MET
1	B	406	ILE
1	B	410	ASP
1	B	413	LYS
1	B	421	TYR
1	B	426	LYS
1	B	432	LYS
1	B	433	ASN
1	B	456	LEU

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Mol	Chain	Res	Type
1	B	466	LEU
1	B	474	TYR
1	B	500	ILE
1	B	537	ARG
1	B	546	MET
1	B	549	ARG
1	B	559	VAL
1	B	587	GLN
1	B	607	LEU
1	B	612	TYR
1	B	625	LEU
1	B	632	VAL
1	B	654	GLU
1	B	671	LEU
1	B	679	ILE
1	B	680	VAL
1	B	704	ILE
1	B	708	GLU
1	B	714	LYS
1	B	722	LYS
1	B	723	GLN
1	B	726	ARG
1	B	733	HIS
1	B	750	LYS
1	B	759	ILE
1	B	763	GLU
1	B	784	LYS
1	B	788	GLU
1	B	789	ILE
1	C	1001	MET
1	C	1006	ILE
1	C	1010	ASP
1	C	1013	LYS
1	C	1021	TYR
1	C	1026	LYS
1	C	1032	LYS
1	C	1033	ASN
1	C	1056	LEU
1	C	1066	LEU
1	C	1074	TYR
1	C	1100	ILE
1	C	1137	ARG

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Mol	Chain	Res	Type
1	C	1146	MET
1	C	1149	ARG
1	C	1159	VAL
1	C	1187	GLN
1	C	1207	LEU
1	C	1212	TYR
1	C	1225	LEU
1	C	1232	VAL
1	C	1254	GLU
1	C	1271	LEU
1	C	1279	ILE
1	C	1280	VAL
1	C	1304	ILE
1	C	1308	GLU
1	C	1314	LYS
1	C	1322	LYS
1	C	1323	GLN
1	C	1326	ARG
1	C	1333	HIS
1	C	1350	LYS
1	C	1359	ILE
1	C	1363	GLU
1	C	1384	LYS
1	C	1388	GLU
1	C	1389	ILE
1	D	1401	MET
1	D	1406	ILE
1	D	1410	ASP
1	D	1413	LYS
1	D	1421	TYR
1	D	1426	LYS
1	D	1432	LYS
1	D	1433	ASN
1	D	1456	LEU
1	D	1466	LEU
1	D	1474	TYR
1	D	1500	ILE
1	D	1537	ARG
1	D	1546	MET
1	D	1549	ARG
1	D	1559	VAL
1	D	1587	GLN

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Mol	Chain	Res	Type
1	D	1607	LEU
1	D	1612	TYR
1	D	1625	LEU
1	D	1632	VAL
1	D	1654	GLU
1	D	1671	LEU
1	D	1679	ILE
1	D	1680	VAL
1	D	1704	ILE
1	D	1708	GLU
1	D	1714	LYS
1	D	1722	LYS
1	D	1723	GLN
1	D	1726	ARG
1	D	1733	HIS
1	D	1750	LYS
1	D	1759	ILE
1	D	1763	GLU
1	D	1788	GLU
1	D	1789	ILE
1	E	2001	MET
1	E	2006	ILE
1	E	2010	ASP
1	E	2013	LYS
1	E	2021	TYR
1	E	2026	LYS
1	E	2032	LYS
1	E	2033	ASN
1	E	2056	LEU
1	E	2066	LEU
1	E	2074	TYR
1	E	2100	ILE
1	E	2137	ARG
1	E	2146	MET
1	E	2149	ARG
1	E	2159	VAL
1	E	2187	GLN
1	E	2207	LEU
1	E	2212	TYR
1	E	2225	LEU
1	E	2232	VAL
1	E	2254	GLU

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Mol	Chain	Res	Type
1	E	2271	LEU
1	E	2279	ILE
1	E	2280	VAL
1	E	2304	ILE
1	E	2308	GLU
1	E	2314	LYS
1	E	2322	LYS
1	E	2323	GLN
1	E	2326	ARG
1	E	2333	HIS
1	E	2350	LYS
1	E	2359	ILE
1	E	2363	GLU
1	E	2384	LYS
1	E	2388	GLU
1	E	2389	ILE
1	F	2401	MET
1	F	2406	ILE
1	F	2410	ASP
1	F	2413	LYS
1	F	2421	TYR
1	F	2426	LYS
1	F	2432	LYS
1	F	2433	ASN
1	F	2456	LEU
1	F	2466	LEU
1	F	2474	TYR
1	F	2500	ILE
1	F	2537	ARG
1	F	2546	MET
1	F	2549	ARG
1	F	2559	VAL
1	F	2587	GLN
1	F	2607	LEU
1	F	2612	TYR
1	F	2625	LEU
1	F	2632	VAL
1	F	2654	GLU
1	F	2671	LEU
1	F	2679	ILE
1	F	2680	VAL
1	F	2704	ILE

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Mol	Chain	Res	Type
1	F	2708	GLU
1	F	2714	LYS
1	F	2722	LYS
1	F	2723	GLN
1	F	2726	ARG
1	F	2733	HIS
1	F	2750	LYS
1	F	2759	ILE
1	F	2763	GLU
1	F	2784	LYS
1	F	2788	GLU
1	F	2789	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	33	ASN
1	A	50	ASN
1	A	83	HIS
1	A	111	GLN
1	A	140	HIS
1	A	178	HIS
1	A	187	GLN
1	A	333	HIS
1	A	381	GLN
1	A	386	ASN
1	B	408	ASN
1	B	433	ASN
1	B	450	ASN
1	B	483	HIS
1	B	511	GLN
1	B	540	HIS
1	B	578	HIS
1	B	587	GLN
1	B	729	ASN
1	B	733	HIS
1	B	781	GLN
1	B	786	ASN
1	C	1008	ASN
1	C	1033	ASN
1	C	1050	ASN

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Mol	Chain	Res	Type
1	C	1083	HIS
1	C	1111	GLN
1	C	1140	HIS
1	C	1178	HIS
1	C	1187	GLN
1	C	1333	HIS
1	C	1361	ASN
1	C	1381	GLN
1	C	1386	ASN
1	D	1408	ASN
1	D	1433	ASN
1	D	1450	ASN
1	D	1483	HIS
1	D	1511	GLN
1	D	1540	HIS
1	D	1578	HIS
1	D	1587	GLN
1	D	1729	ASN
1	D	1733	HIS
1	D	1781	GLN
1	D	1786	ASN
1	E	2008	ASN
1	E	2033	ASN
1	E	2050	ASN
1	E	2083	HIS
1	E	2111	GLN
1	E	2140	HIS
1	E	2178	HIS
1	E	2187	GLN
1	E	2329	ASN
1	E	2333	HIS
1	E	2381	GLN
1	E	2386	ASN
1	F	2408	ASN
1	F	2433	ASN
1	F	2450	ASN
1	F	2483	HIS
1	F	2511	GLN
1	F	2540	HIS
1	F	2578	HIS
1	F	2587	GLN
1	F	2729	ASN

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Mol	Chain	Res	Type
1	F	2733	HIS
1	F	2781	GLN
1	F	2786	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PCP	E	2392	-	21,22,22	1.34	3 (14%)	30,35,35	1.49	4 (13%)
3	PCP	B	792	-	21,22,22	1.38	4 (19%)	30,35,35	1.50	4 (13%)
3	PCP	A	392	-	21,22,22	1.40	4 (19%)	30,35,35	1.47	3 (10%)
3	PCP	D	1792	-	21,22,22	1.44	4 (19%)	30,35,35	1.51	4 (13%)
3	PCP	C	1392	-	21,22,22	1.41	4 (19%)	30,35,35	1.45	4 (13%)
3	PCP	F	2792	-	21,22,22	1.32	3 (14%)	30,35,35	1.51	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCP	E	2392	-	-	4/17/33/33	0/1/1/1
3	PCP	B	792	-	-	4/17/33/33	0/1/1/1
3	PCP	A	392	-	-	4/17/33/33	0/1/1/1
3	PCP	D	1792	-	-	4/17/33/33	0/1/1/1
3	PCP	C	1392	-	-	4/17/33/33	0/1/1/1
3	PCP	F	2792	-	-	4/17/33/33	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1792	PCP	O1-C1	2.87	1.53	1.46
3	A	392	PCP	O1-C1	2.80	1.53	1.46
3	B	792	PCP	O1-C1	2.73	1.52	1.46
3	D	1792	PCP	PA-O3A	-2.73	1.56	1.59
3	F	2792	PCP	O1-C1	2.70	1.52	1.46
3	C	1392	PCP	O1-C1	2.68	1.52	1.46
3	E	2392	PCP	O1-C1	2.64	1.52	1.46
3	C	1392	PCP	PA-O3A	-2.62	1.56	1.59
3	C	1392	PCP	CP-C4	2.62	1.56	1.51
3	E	2392	PCP	CP-C4	2.60	1.56	1.51
3	E	2392	PCP	PB-O2B	-2.59	1.45	1.54
3	B	792	PCP	CP-C4	2.59	1.56	1.51
3	D	1792	PCP	PB-O2B	-2.58	1.45	1.54
3	D	1792	PCP	CP-C4	2.57	1.56	1.51
3	A	392	PCP	PB-O2B	-2.54	1.45	1.54
3	A	392	PCP	PA-O3A	-2.53	1.56	1.59
3	F	2792	PCP	CP-C4	2.48	1.56	1.51
3	A	392	PCP	CP-C4	2.48	1.56	1.51
3	B	792	PCP	PB-O2B	-2.44	1.45	1.54
3	F	2792	PCP	PB-O2B	-2.43	1.45	1.54
3	C	1392	PCP	PB-O2B	-2.43	1.45	1.54
3	B	792	PCP	PA-O3A	-2.39	1.56	1.59

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2792	PCP	C4-C5-C1	5.90	113.24	103.73
3	D	1792	PCP	C4-C5-C1	5.83	113.11	103.73
3	B	792	PCP	C4-C5-C1	5.82	113.11	103.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2392	PCP	C4-C5-C1	5.77	113.02	103.73
3	A	392	PCP	C4-C5-C1	5.75	112.98	103.73
3	C	1392	PCP	C4-C5-C1	5.74	112.97	103.73
3	B	792	PCP	O2A-PA-O3A	2.67	114.50	107.27
3	D	1792	PCP	O2A-PA-O3A	2.67	114.50	107.27
3	F	2792	PCP	O2A-PA-O3A	2.60	114.31	107.27
3	E	2392	PCP	O2A-PA-O3A	2.57	114.21	107.27
3	A	392	PCP	O2A-PA-O3A	2.50	114.02	107.27
3	C	1392	PCP	O2A-PA-O3A	2.46	113.93	107.27
3	B	792	PCP	O3B-PB-O3A	2.20	112.02	104.64
3	A	392	PCP	O2B-PB-O3A	2.18	111.96	104.64
3	F	2792	PCP	O3B-PB-O3A	2.13	111.79	104.64
3	D	1792	PCP	O3B-PB-O3A	2.12	111.74	104.64
3	D	1792	PCP	O2B-PB-O3A	2.12	111.74	104.64
3	F	2792	PCP	O2B-PB-O3A	2.11	111.72	104.64
3	C	1392	PCP	O2B-PB-O3A	2.09	111.66	104.64
3	C	1392	PCP	O3B-PB-O3A	2.07	111.58	104.64
3	E	2392	PCP	O3B-PB-O3A	2.06	111.55	104.64
3	E	2392	PCP	O2B-PB-O3A	2.06	111.54	104.64
3	B	792	PCP	O2B-PB-O3A	2.05	111.51	104.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	392	PCP	CP-OP-P-O1P
3	A	392	PCP	CP-OP-P-O2P
3	A	392	PCP	CP-OP-P-O3P
3	B	792	PCP	CP-OP-P-O1P
3	B	792	PCP	CP-OP-P-O2P
3	B	792	PCP	CP-OP-P-O3P
3	C	1392	PCP	CP-OP-P-O1P
3	C	1392	PCP	CP-OP-P-O2P
3	C	1392	PCP	CP-OP-P-O3P
3	D	1792	PCP	CP-OP-P-O1P
3	D	1792	PCP	CP-OP-P-O2P
3	D	1792	PCP	CP-OP-P-O3P
3	E	2392	PCP	CP-OP-P-O1P
3	E	2392	PCP	CP-OP-P-O2P
3	E	2392	PCP	CP-OP-P-O3P
3	F	2792	PCP	CP-OP-P-O1P
3	F	2792	PCP	CP-OP-P-O2P

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Mol	Chain	Res	Type	Atoms
3	F	2792	PCP	CP-OP-P-O3P
3	A	392	PCP	PB-O3A-PA-O1
3	B	792	PCP	PB-O3A-PA-O1
3	C	1392	PCP	PB-O3A-PA-O1
3	D	1792	PCP	PB-O3A-PA-O1
3	E	2392	PCP	PB-O3A-PA-O1
3	F	2792	PCP	PB-O3A-PA-O1

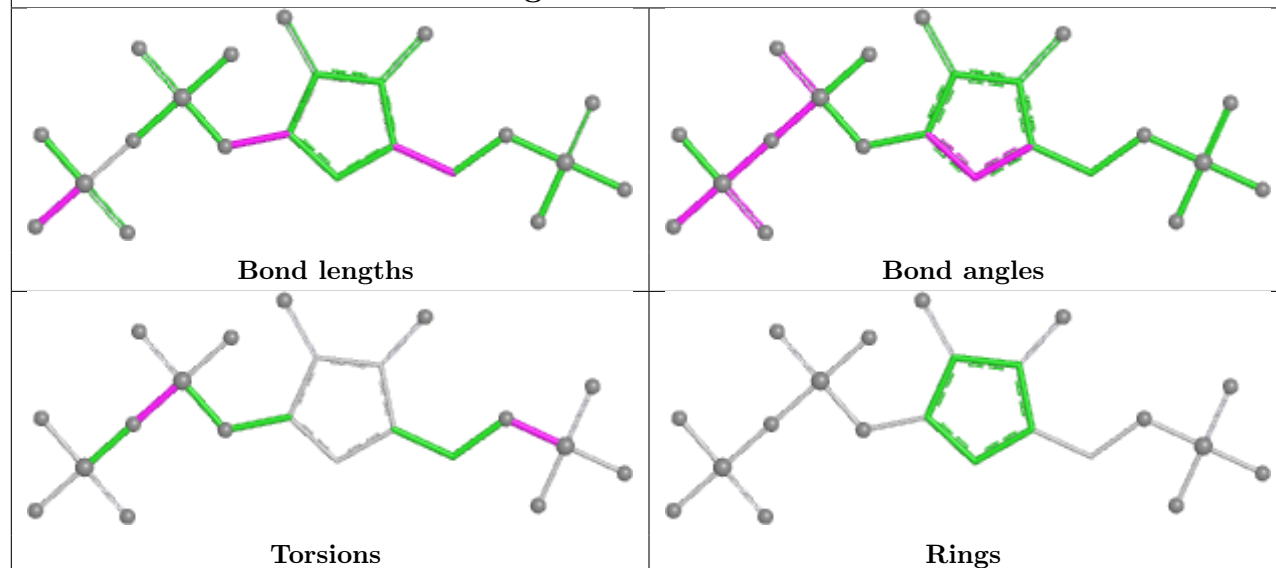
There are no ring outliers.

6 monomers are involved in 8 short contacts:

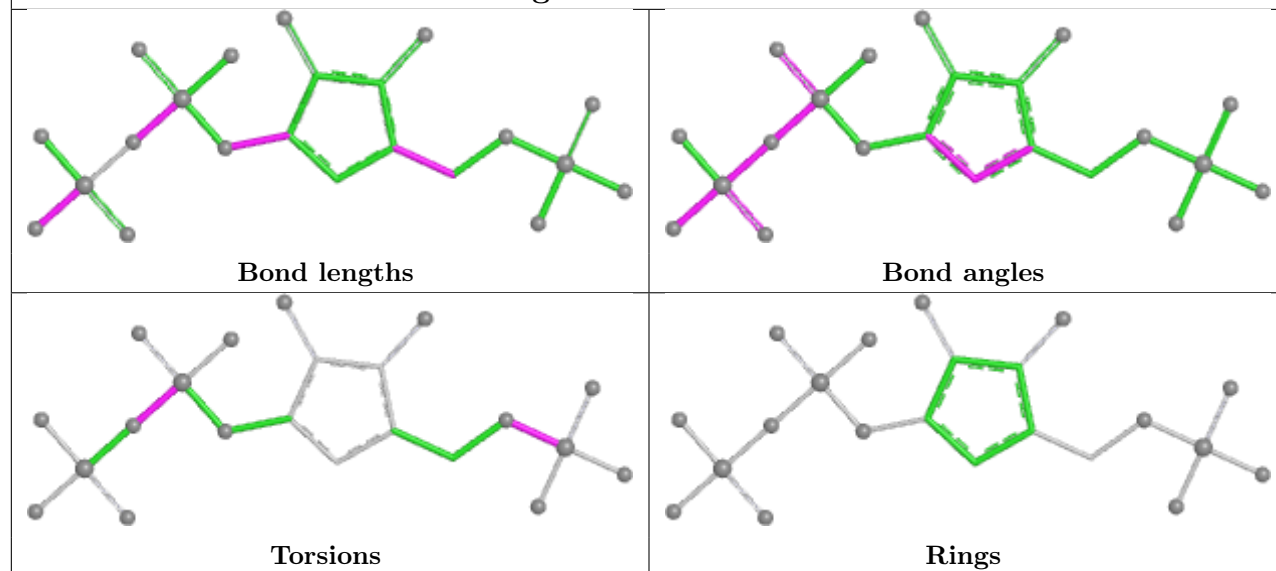
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2392	PCP	1	0
3	B	792	PCP	1	0
3	A	392	PCP	2	0
3	D	1792	PCP	2	0
3	C	1392	PCP	1	0
3	F	2792	PCP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

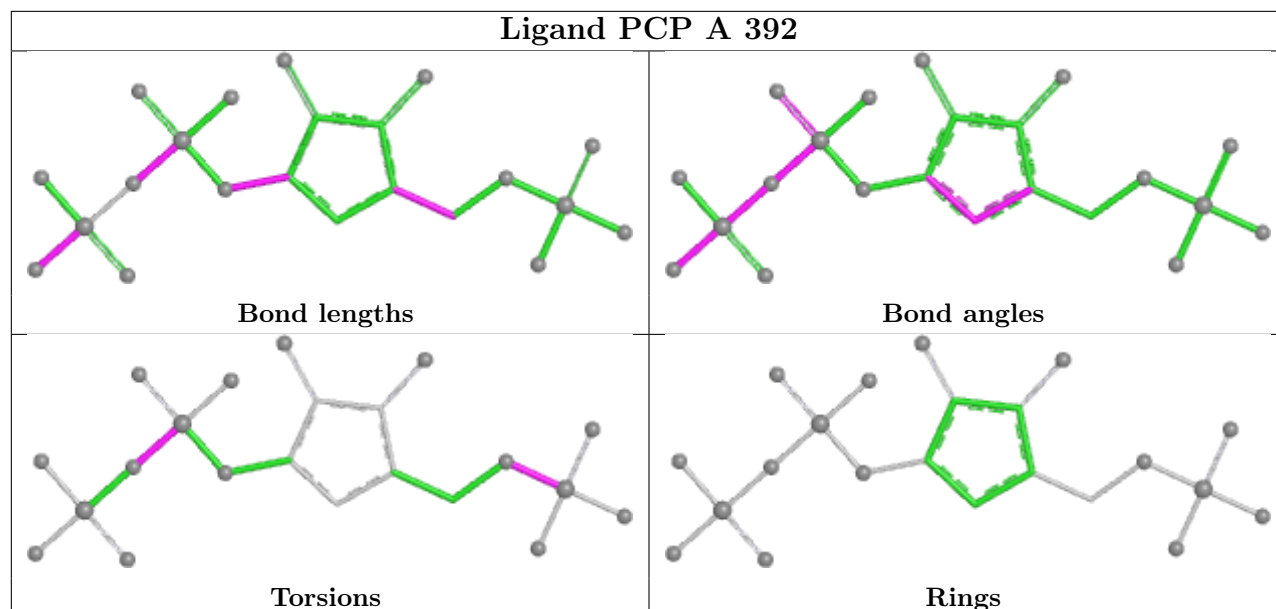
Ligand PCP E 2392



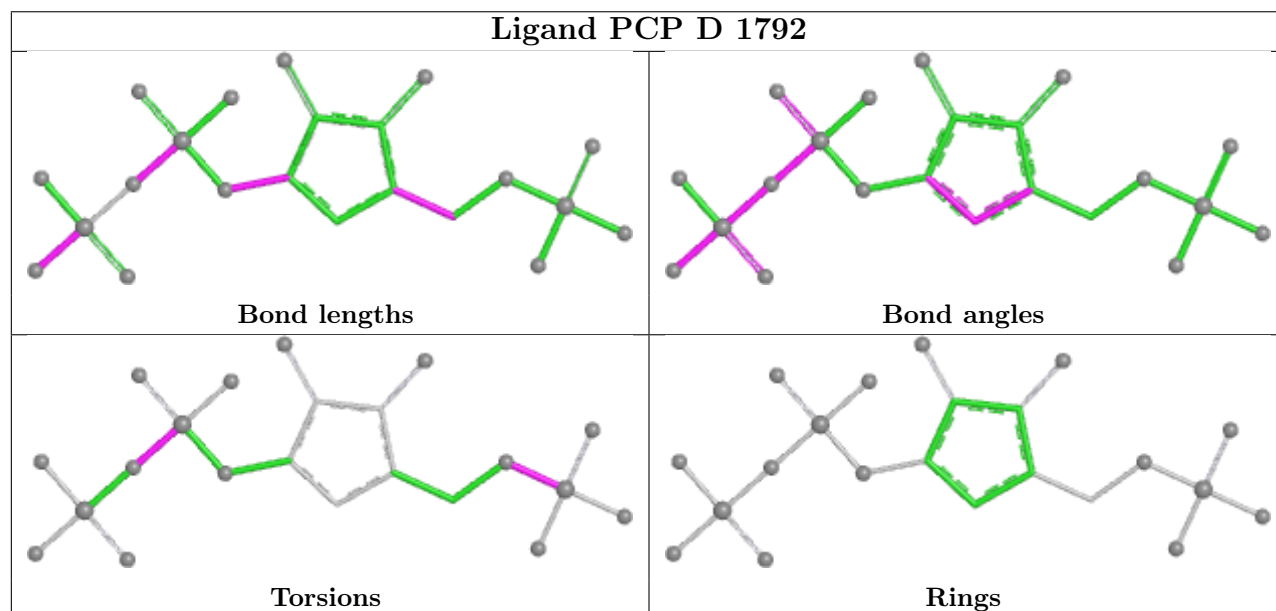
Ligand PCP B 792

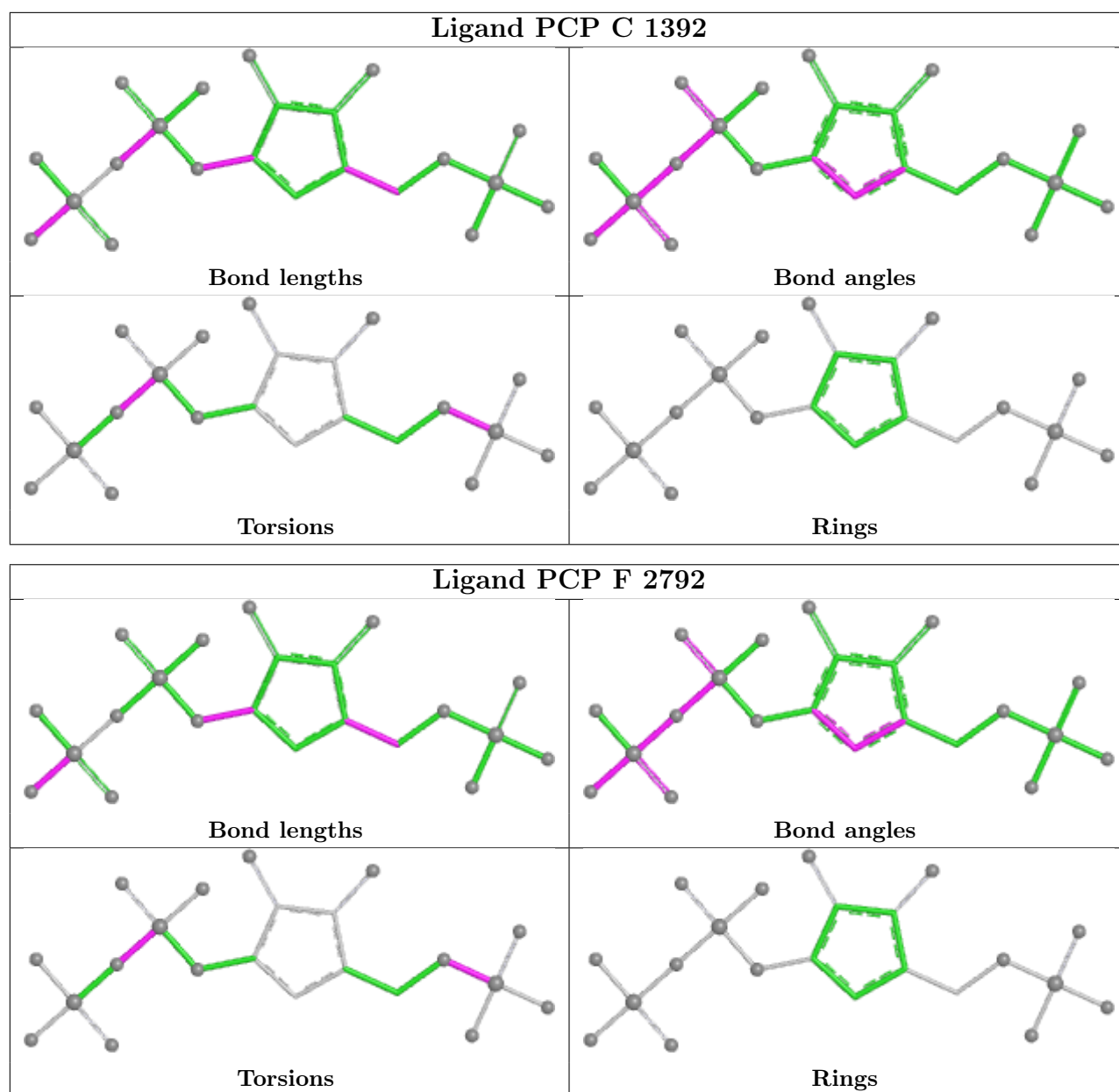


Ligand PCP A 392



Ligand PCP D 1792





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	389/395 (98%)	-0.98	0 100 100	32, 65, 86, 105	0
1	B	389/395 (98%)	-0.94	0 100 100	34, 66, 86, 106	0
1	C	389/395 (98%)	-0.97	0 100 100	31, 65, 85, 105	0
1	D	389/395 (98%)	-0.96	0 100 100	35, 66, 86, 106	0
1	E	389/395 (98%)	-0.96	0 100 100	32, 65, 86, 106	0
1	F	389/395 (98%)	-0.95	0 100 100	32, 65, 86, 106	0
All	All	2334/2370 (98%)	-0.96	0 100 100	31, 65, 87, 106	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PCP	B	792	22/22	0.97	0.07	103,109,112,112	0

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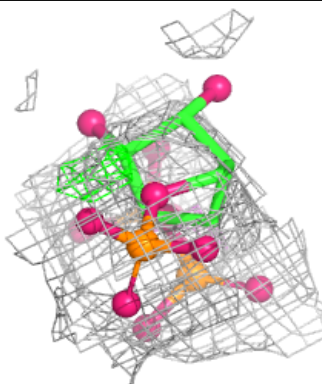
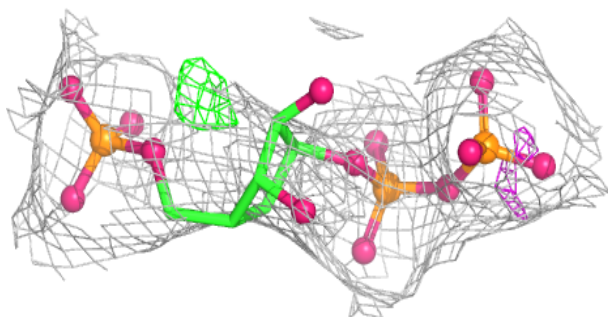
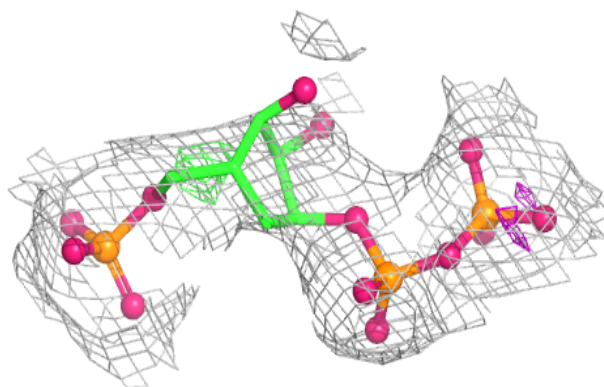
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PCP	A	392	22/22	0.98	0.06	103,109,112,112	0
3	PCP	C	1392	22/22	0.98	0.06	104,110,112,113	0
3	PCP	D	1792	22/22	0.98	0.06	102,109,112,113	0
3	PCP	E	2392	22/22	0.98	0.07	103,109,112,112	0
3	PCP	F	2792	22/22	0.98	0.06	103,109,112,112	0
2	ZN	B	793	1/1	0.99	0.02	85,85,85,85	0
2	ZN	C	1391	1/1	0.99	0.02	62,62,62,62	0
2	ZN	E	2391	1/1	0.99	0.02	82,82,82,82	0
2	ZN	E	2393	1/1	0.99	0.02	77,77,77,77	0
2	ZN	F	2791	1/1	0.99	0.02	83,83,83,83	0
2	ZN	F	2793	1/1	0.99	0.02	77,77,77,77	0
2	ZN	D	1791	1/1	1.00	0.02	77,77,77,77	0
2	ZN	D	1793	1/1	1.00	0.02	84,84,84,84	0
2	ZN	B	791	1/1	1.00	0.01	78,78,78,78	0
2	ZN	A	391	1/1	1.00	0.02	57,57,57,57	0
2	ZN	A	393	1/1	1.00	0.02	76,76,76,76	0
2	ZN	C	1393	1/1	1.00	0.01	85,85,85,85	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

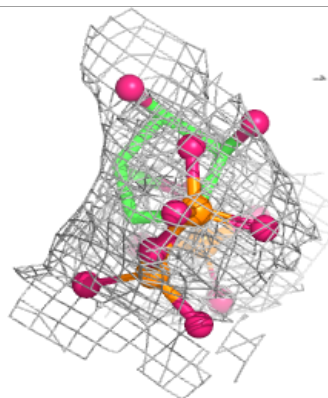
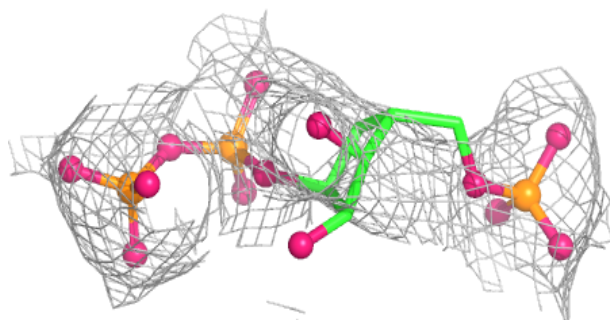
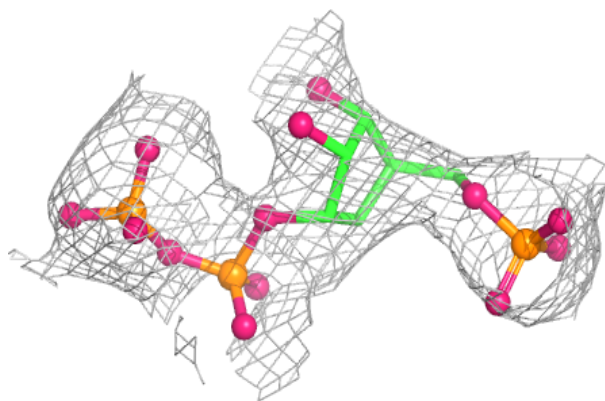
Electron density around PCP B 792:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

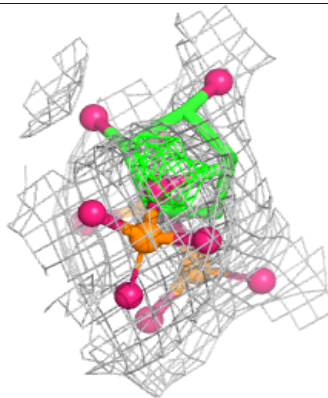
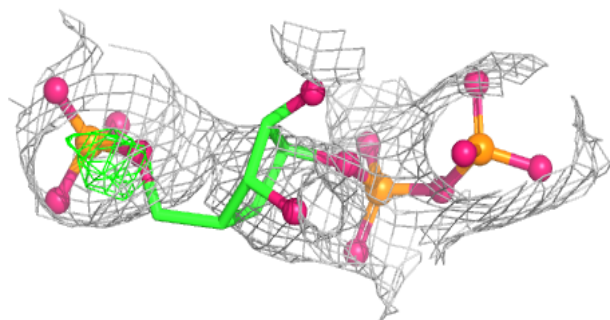
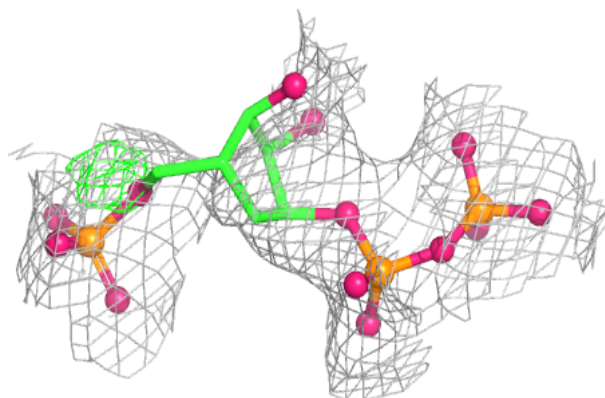


Electron density around PCP A 392:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

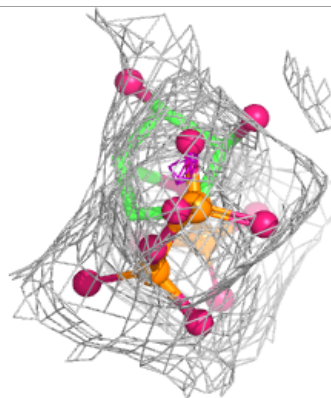
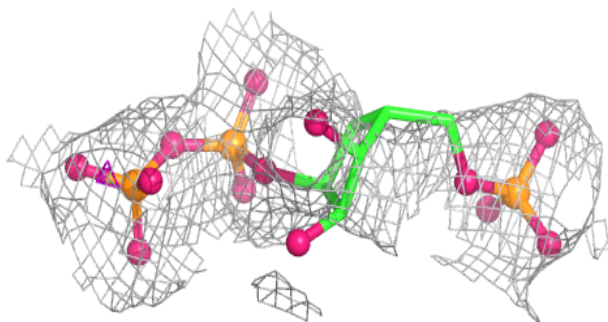
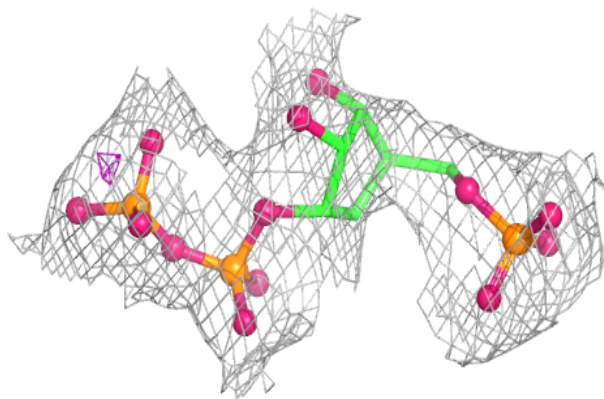
**Electron density around PCP C 1392:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

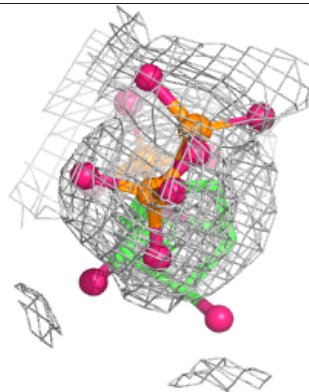
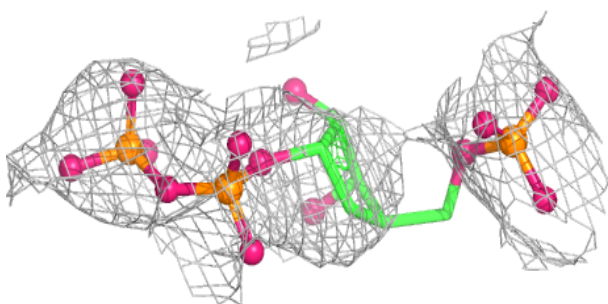
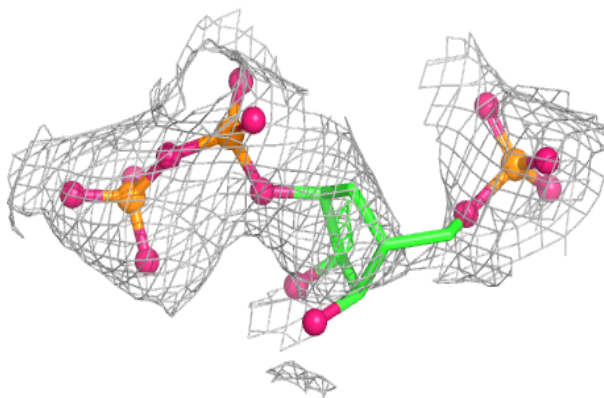


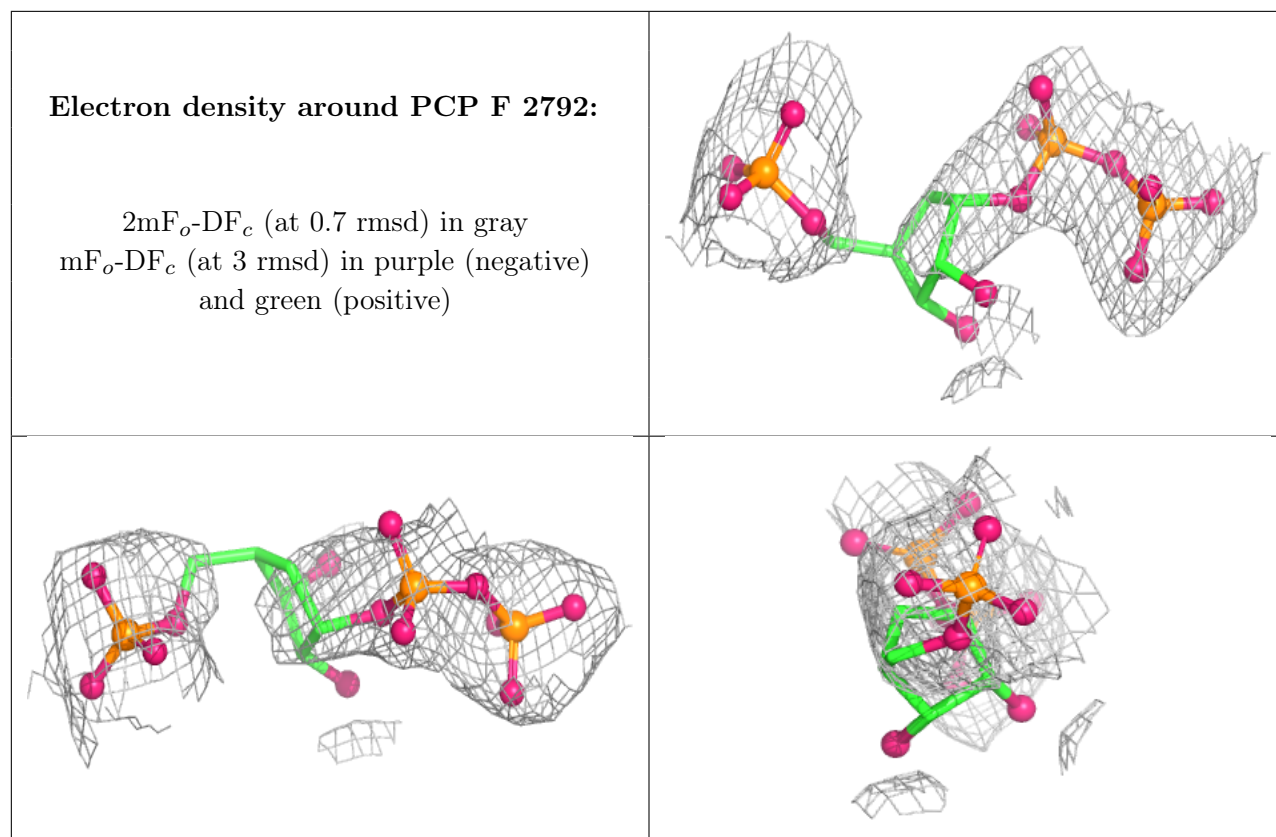
Electron density around PCP D 1792:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PCP E 2392:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.