



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:00 PM UTC

PDB ID : 1BMF / pdb_00001bmf
Title : BOVINE MITOCHONDRIAL F1-ATPASE
Authors : Abrahams, J.P.; Leslie, A.G.W.; Lutter, R.; Walker, J.E.
Deposited on : 1996-03-13
Resolution : 2.85 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

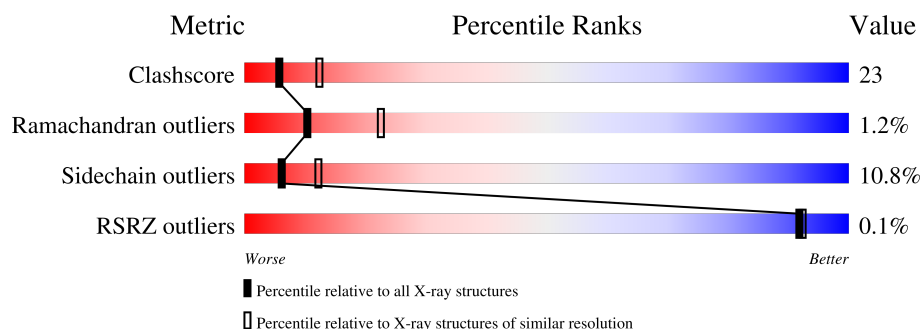
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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))
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	272	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23481 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 BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	487	Total	C	N	O	S	59	0	0
			3715	2341	656	706	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	engineered mutation	UNP P19483
B	481	GLY	SER	engineered mutation	UNP P19483
C	481	GLY	SER	engineered mutation	UNP P19483

- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

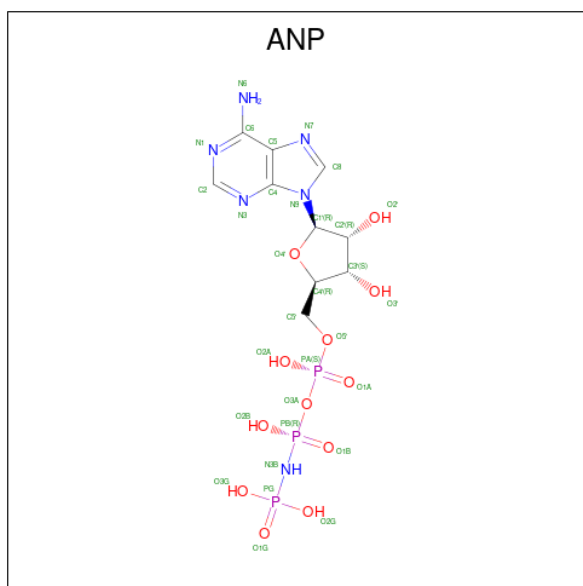
- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	122	Total	C	N	O	S	0	0	0
			945	591	171	176	7			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

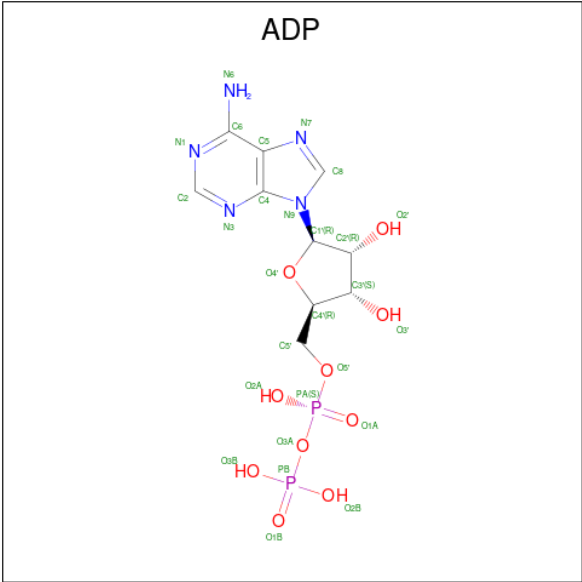
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 10 6 12 3	0	0
5	B	1	Total C N O P 31 10 6 12 3	0	0
5	C	1	Total C N O P 31 10 6 12 3	0	0
5	F	1	Total C N O P 31 10 6 12 3	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

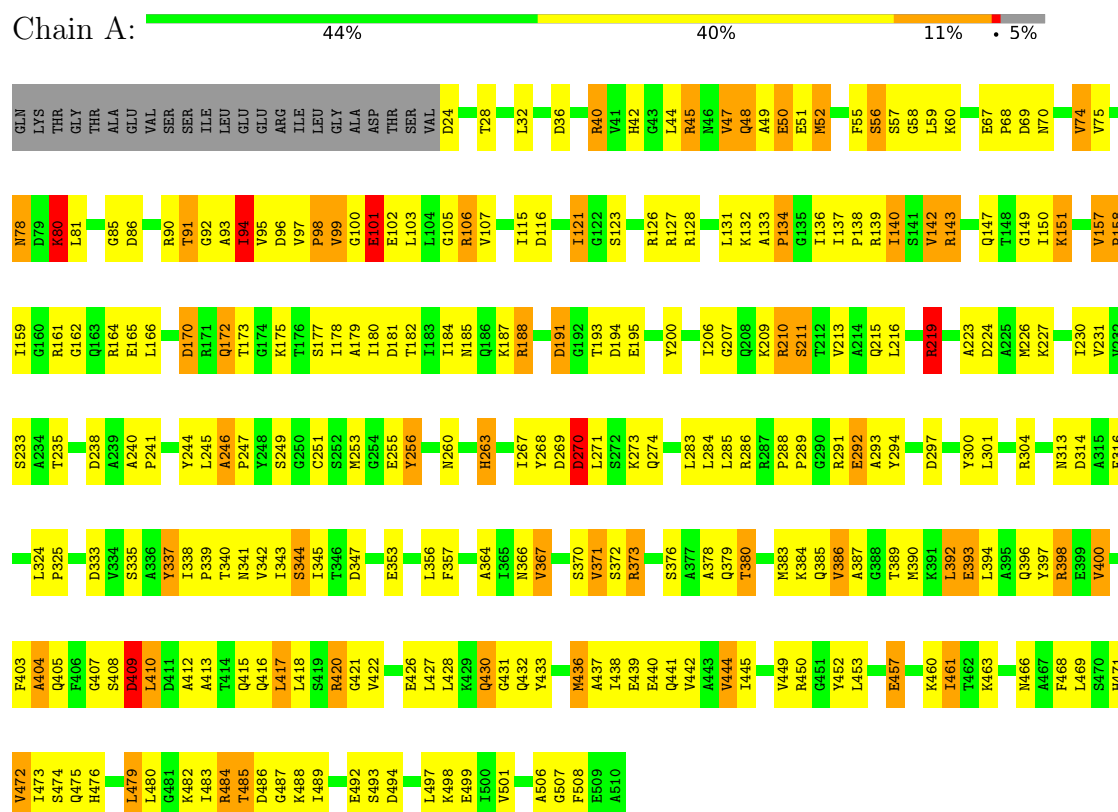
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	92	Total	O	0	0
			92	92		
7	B	96	Total	O	0	0
			96	96		
7	C	123	Total	O	0	0
			123	123		
7	D	105	Total	O	0	0
			105	105		
7	E	49	Total	O	0	0
			49	49		
7	F	104	Total	O	0	0
			104	104		
7	G	34	Total	O	0	0
			34	34		

3 Residue-property plots

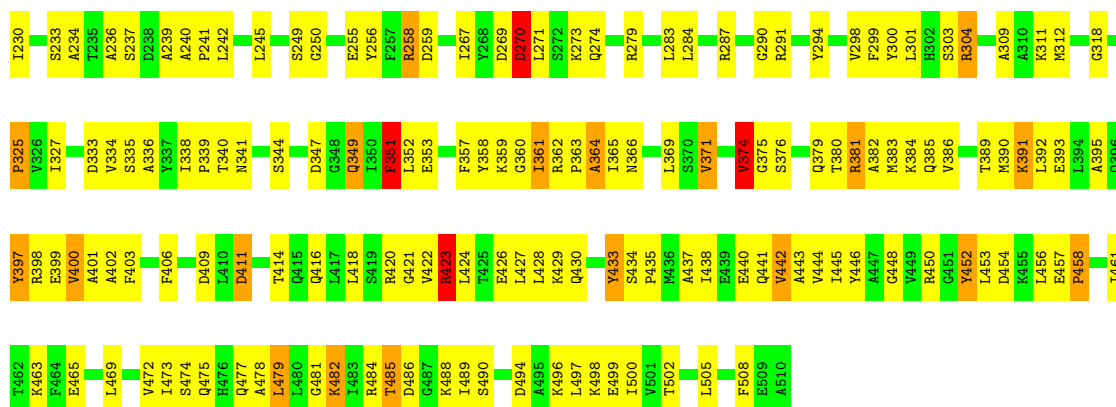
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BOVINE MITOCHONDRIAL F1-ATPASE



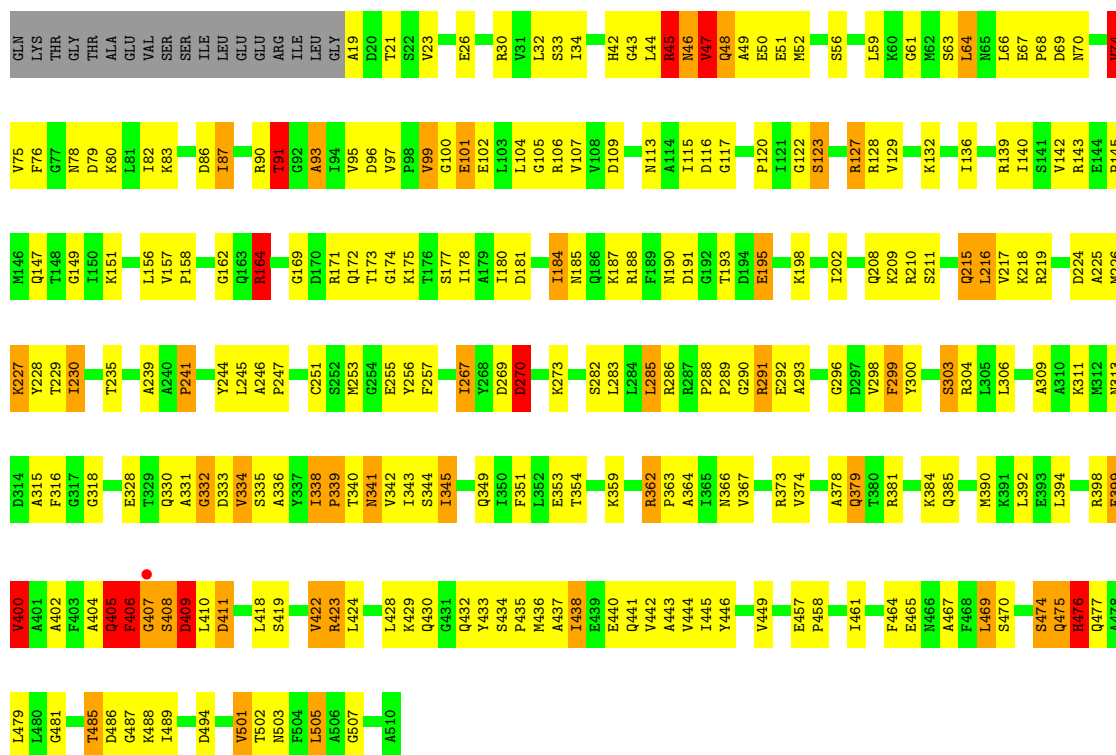
• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE





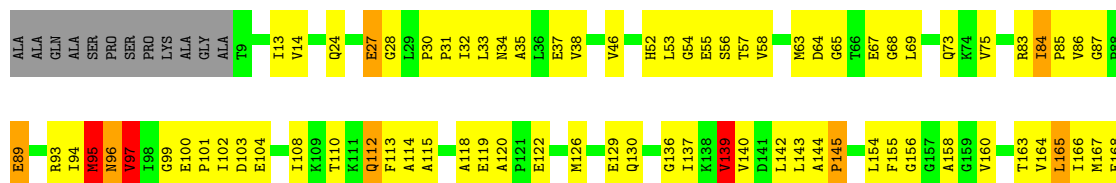
• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

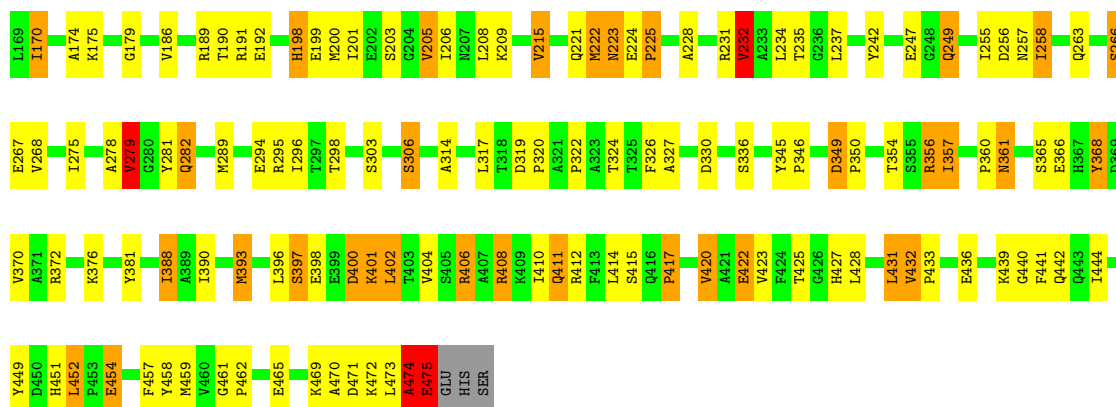
Chain C: 47% 39% 8%



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

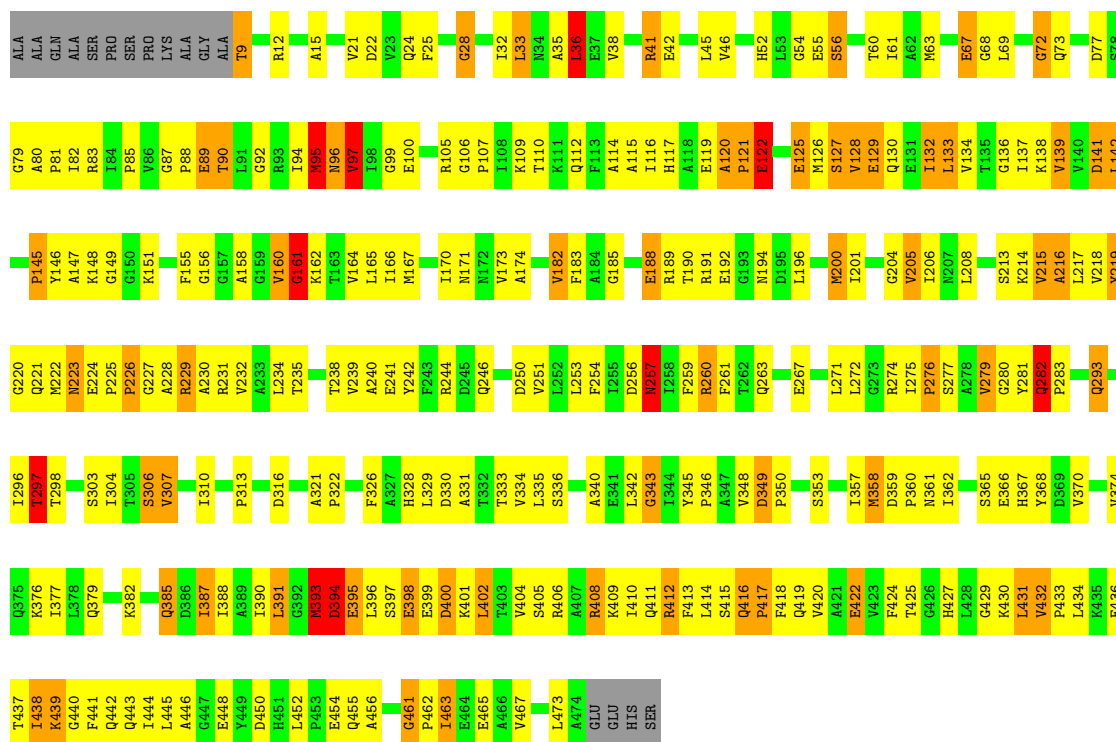
Chain D: 54% 33% 8%





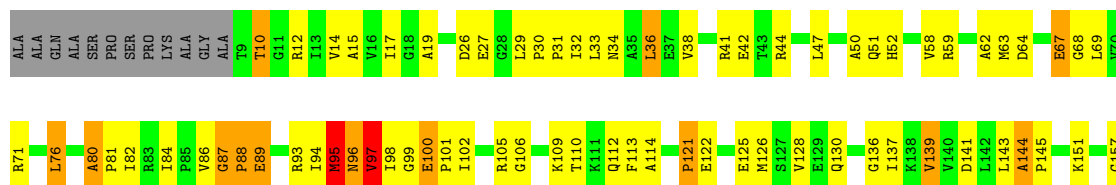
• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

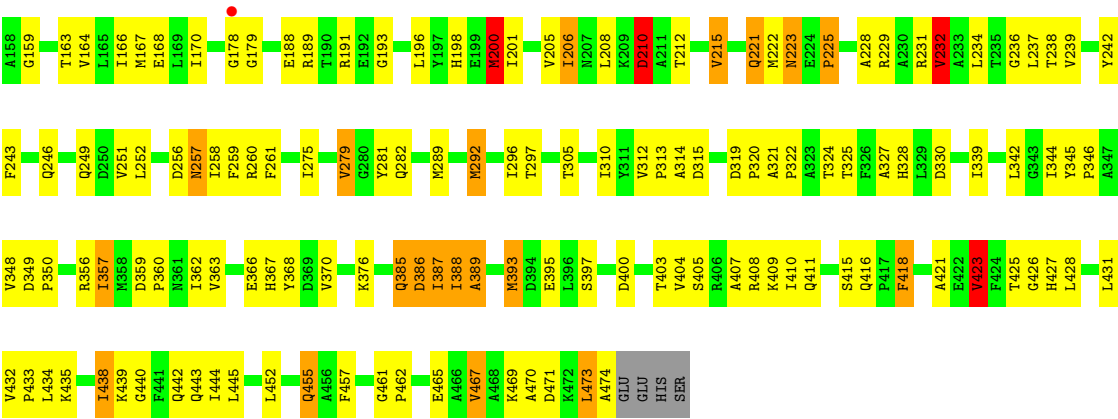
Chain E: 40% 42% 12% . .



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

Chain F: 52% 36% 7% . .





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	284.22Å 107.76Å 139.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.85 6.00 – 2.87	Depositor EDS
% Data completeness (in resolution range)	95.0 (6.00-2.85) 86.6 (6.00-2.87)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.86Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available) 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 82.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23481	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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: ANP, ADP, MG

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	0.76	0/3766	1.74	64/5080 (1.3%)
1	B	0.81	2/3766 (0.1%)	1.78	77/5080 (1.5%)
1	C	0.80	0/3799	1.80	72/5126 (1.4%)
2	D	0.81	1/3596 (0.0%)	1.78	67/4879 (1.4%)
2	E	0.77	0/3587	1.78	87/4867 (1.8%)
2	F	0.80	1/3587 (0.0%)	1.79	90/4867 (1.8%)
3	G	0.67	0/949	1.55	12/1266 (0.9%)
All	All	0.79	4/23050 (0.0%)	1.77	469/31165 (1.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	ALA	C-N	-12.91	1.16	1.33
1	B	409	ASP	C-N	-11.01	1.18	1.33
2	F	96	ASN	CA-CB	5.40	1.61	1.53
2	D	96	ASN	CA-CB	5.28	1.61	1.53

All (469) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	22.80	156.31	124.40
2	F	282	GLN	CB-CG-CD	15.17	138.39	112.60
2	E	408	ARG	CD-NE-CZ	13.43	143.20	124.40
1	B	409	ASP	CA-C-N	11.21	141.66	122.82
1	B	409	ASP	C-N-CA	11.21	141.66	122.82
1	B	351	PHE	CA-CB-CG	11.08	124.88	113.80
1	A	270	ASP	CA-CB-CG	10.93	123.53	112.60
2	F	139	VAL	CB-CA-C	-10.83	98.02	111.88
1	B	270	ASP	CA-CB-CG	10.46	123.06	112.60
1	B	375	GLY	N-CA-C	9.78	125.43	114.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ARG	CD-NE-CZ	9.34	137.47	124.40
3	G	15	ASN	CA-CB-CG	-9.25	103.35	112.60
2	F	97	VAL	CB-CA-C	-9.15	99.78	112.14
2	D	96	ASN	CA-CB-CG	-8.68	103.92	112.60
2	D	95	MET	CA-C-N	8.64	138.35	122.02
2	D	95	MET	C-N-CA	8.64	138.35	122.02
2	D	139	VAL	CB-CA-C	-8.64	100.64	111.70
1	C	503	ASN	CA-CB-CG	-8.48	104.11	112.60
2	E	307	VAL	N-CA-CB	8.43	121.95	111.41
1	C	113	ASN	CA-CB-CG	-8.41	104.19	112.60
2	F	96	ASN	CB-CA-C	-8.27	93.29	110.40
1	A	269	ASP	CA-C-N	8.16	136.38	121.70
1	A	269	ASP	C-N-CA	8.16	136.38	121.70
2	F	427	HIS	CA-CB-CG	8.14	121.94	113.80
1	C	74	VAL	N-CA-CB	-8.05	101.94	110.72
2	F	95	MET	CA-C-N	8.01	138.58	121.45
2	F	95	MET	C-N-CA	8.01	138.58	121.45
1	C	476	HIS	N-CA-C	7.91	127.64	110.80
2	D	349	ASP	CA-C-N	7.86	127.58	119.56
2	D	349	ASP	C-N-CA	7.86	127.58	119.56
1	A	123	SER	N-CA-C	7.85	121.26	109.25
2	D	474	ALA	CA-C-N	7.80	135.74	121.70
2	D	474	ALA	C-N-CA	7.80	135.74	121.70
1	B	309	ALA	N-CA-C	-7.72	99.62	110.50
1	B	401	ALA	O-C-N	-7.69	113.30	122.46
1	C	409	ASP	CA-CB-CG	7.66	120.26	112.60
1	B	270	ASP	CB-CA-C	-7.61	95.63	110.10
2	E	349	ASP	CA-C-O	7.53	124.19	119.29
2	E	95	MET	CA-C-O	7.53	129.92	121.11
2	F	221	GLN	N-CA-C	7.51	120.71	110.35
1	A	91	THR	N-CA-C	-7.47	104.69	113.88
1	B	475	GLN	N-CA-C	7.47	119.50	111.36
2	F	95	MET	CA-CB-CG	7.42	128.94	114.10
2	E	276	PRO	CA-C-O	-7.35	112.67	122.08
1	A	270	ASP	CB-CA-C	-7.33	96.17	110.10
2	D	417	PRO	N-CA-CB	7.27	106.99	102.92
1	A	170	ASP	CA-CB-CG	7.27	119.87	112.60
1	C	429	LYS	CA-C-O	-7.26	113.45	121.87
1	A	392	LEU	N-CA-C	7.24	119.25	111.36
2	E	395	GLU	N-CA-C	-7.21	104.61	113.19
1	B	53	VAL	CA-C-O	-7.21	114.32	121.67
1	C	501	VAL	N-CA-CB	7.16	118.43	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	129	GLU	N-CA-C	7.13	120.29	109.23
2	D	393	MET	N-CA-C	7.10	122.11	113.38
2	F	256	ASP	CA-CB-CG	7.08	119.68	112.60
2	E	343	GLY	N-CA-C	-7.06	106.67	115.08
1	A	210	ARG	CA-C-O	-7.06	112.12	120.10
2	D	97	VAL	CB-CA-C	-7.06	102.48	112.22
2	D	249	GLN	N-CA-C	7.05	119.62	110.53
2	F	232	VAL	CB-CA-C	-7.02	101.80	112.05
1	A	260	ASN	CA-CB-CG	-7.02	105.58	112.60
1	A	431	GLY	N-CA-C	-7.00	101.58	112.85
1	B	219	ARG	NE-CZ-NH2	6.97	125.47	119.20
2	D	406	ARG	NE-CZ-NH1	-6.96	114.54	121.50
2	E	160	VAL	N-CA-C	-6.95	98.57	108.58
1	B	349	GLN	CA-CB-CG	6.95	127.99	114.10
1	A	149	GLY	N-CA-C	-6.90	105.54	115.27
2	F	59	ARG	NE-CZ-NH1	-6.90	114.60	121.50
1	C	476	HIS	CA-CB-CG	-6.88	106.92	113.80
2	F	179	GLY	N-CA-C	-6.87	103.73	111.63
2	E	261	PHE	CA-C-N	6.87	129.37	120.44
2	E	261	PHE	C-N-CA	6.87	129.37	120.44
2	F	312	VAL	CA-C-N	6.85	127.23	119.83
2	F	312	VAL	C-N-CA	6.85	127.23	119.83
2	E	95	MET	CA-CB-CG	6.84	127.79	114.10
1	A	476	HIS	N-CA-C	6.81	121.51	112.25
2	E	306	SER	N-CA-C	6.79	120.00	109.07
2	E	22	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	314	ASP	CA-CB-CG	-6.76	105.84	112.60
1	A	285	LEU	CA-C-O	6.70	127.39	119.28
2	D	96	ASN	CB-CA-C	-6.68	97.09	111.78
1	C	149	GLY	N-CA-C	-6.67	105.39	115.00
2	E	342	LEU	N-CA-C	-6.65	105.15	113.20
2	D	101	PRO	N-CA-CB	6.64	109.12	103.35
1	B	403	PHE	N-CA-C	-6.63	104.13	111.36
2	D	400	ASP	CA-CB-CG	6.62	119.22	112.60
2	F	385	GLN	N-CA-C	6.62	120.22	111.75
2	F	349	ASP	CA-C-N	6.61	126.23	119.56
2	F	349	ASP	C-N-CA	6.61	126.23	119.56
1	B	209	LYS	CA-C-O	-6.61	113.47	120.80
2	E	87	GLY	CA-C-N	6.60	126.37	119.05
2	E	87	GLY	C-N-CA	6.60	126.37	119.05
1	C	215	GLN	OE1-CD-NE2	6.59	129.19	122.60
1	C	328	GLU	CB-CG-CD	-6.58	101.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ARG	CD-NE-CZ	-6.58	115.19	124.40
2	E	41	ARG	CD-NE-CZ	6.56	133.58	124.40
2	E	156	GLY	N-CA-C	-6.55	104.55	112.48
1	C	235	THR	N-CA-C	6.55	118.98	110.53
1	A	80	LYS	N-CA-C	-6.55	104.32	112.90
1	B	119	GLY	CA-C-N	6.54	126.56	119.89
1	B	119	GLY	C-N-CA	6.54	126.56	119.89
1	B	258	ARG	CD-NE-CZ	6.53	133.54	124.40
2	E	432	VAL	CA-C-N	6.53	127.06	120.14
2	E	432	VAL	C-N-CA	6.53	127.06	120.14
2	E	141	ASP	CA-CB-CG	6.53	119.12	112.60
1	C	47	VAL	CB-CA-C	-6.52	104.15	111.45
2	E	394	ASP	CA-CB-CG	-6.50	106.10	112.60
2	F	313	PRO	N-CA-CB	6.49	109.11	103.27
2	E	394	ASP	N-CA-C	6.47	123.77	114.39
1	A	172	GLN	N-CA-CB	-6.46	102.39	111.62
2	F	143	LEU	N-CA-C	6.45	121.35	112.90
2	E	125	GLU	N-CA-C	-6.44	105.73	113.97
1	A	230	ILE	CA-C-N	-6.43	114.55	123.10
1	A	230	ILE	C-N-CA	-6.43	114.55	123.10
2	D	420	VAL	N-CA-CB	-6.42	103.97	112.26
3	G	221	THR	N-CA-CB	6.42	119.12	110.59
1	A	78	ASN	CA-CB-CG	6.41	119.01	112.60
2	F	193	GLY	N-CA-C	-6.41	105.07	112.50
2	F	225	PRO	CA-C-N	6.41	127.85	119.84
2	F	225	PRO	C-N-CA	6.41	127.85	119.84
3	G	32	ALA	N-CA-C	-6.39	103.94	111.03
2	D	113	PHE	CA-CB-CG	-6.38	107.42	113.80
2	D	84	ILE	N-CA-C	6.37	114.91	107.84
1	B	279	ARG	CD-NE-CZ	6.37	133.32	124.40
2	F	275	ILE	N-CA-C	-6.36	102.72	108.95
1	B	299	PHE	N-CA-C	-6.36	104.43	111.36
2	D	144	ALA	CA-C-N	6.36	126.38	119.90
2	D	144	ALA	C-N-CA	6.36	126.38	119.90
2	D	221	GLN	N-CA-C	6.33	118.20	110.41
1	B	406	PHE	CA-CB-CG	-6.31	107.49	113.80
2	F	64	ASP	CA-C-O	-6.29	114.72	121.45
1	A	231	VAL	CA-C-N	-6.29	115.01	122.93
1	A	231	VAL	C-N-CA	-6.29	115.01	122.93
1	A	371	VAL	CB-CA-C	-6.26	99.20	110.48
1	B	409	ASP	O-C-N	-6.26	115.02	123.10
2	F	59	ARG	NE-CZ-NH2	6.26	124.83	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	416	GLN	CA-C-N	6.25	127.20	120.13
2	E	416	GLN	C-N-CA	6.25	127.20	120.13
1	A	337	TYR	CA-C-N	6.25	124.18	120.24
1	A	337	TYR	C-N-CA	6.25	124.18	120.24
1	A	157	VAL	CA-C-N	6.25	126.61	119.93
1	A	157	VAL	C-N-CA	6.25	126.61	119.93
2	F	403	THR	N-CA-C	-6.25	104.39	111.14
1	C	288	PRO	N-CA-CB	6.21	109.10	103.08
1	B	93	ALA	N-CA-C	6.20	118.51	108.41
2	E	145	PRO	N-CA-CB	6.19	108.76	103.19
1	A	158	PRO	N-CA-CB	6.18	108.75	103.19
1	B	142	VAL	N-CA-CB	6.18	118.41	110.13
1	C	70	ASN	CA-C-O	-6.17	114.83	121.38
1	C	291	ARG	NE-CZ-NH2	-6.17	113.64	119.20
2	F	26	ASP	CA-CB-CG	-6.16	106.44	112.60
1	A	292	GLU	CB-CG-CD	6.13	123.03	112.60
2	E	94	ILE	N-CA-CB	6.12	119.57	111.25
2	E	225	PRO	N-CA-CB	6.12	109.02	103.08
2	E	106	GLY	CA-C-N	6.11	126.06	119.76
2	E	106	GLY	C-N-CA	6.11	126.06	119.76
2	D	422	GLU	N-CA-C	-6.11	104.73	111.82
1	C	164	ARG	NE-CZ-NH1	-6.11	115.39	121.50
2	D	120	ALA	CA-C-N	6.10	126.12	119.90
2	D	120	ALA	C-N-CA	6.10	126.12	119.90
1	B	374	VAL	N-CA-C	6.09	120.06	113.43
2	E	422	GLU	N-CA-C	-6.08	105.89	113.55
2	E	90	THR	N-CA-C	-6.08	106.00	113.41
1	A	94	ILE	CB-CA-C	6.06	119.86	111.38
1	B	287	ARG	CB-CA-C	6.06	118.17	109.26
1	C	157	VAL	CA-C-N	6.06	126.08	119.90
1	C	157	VAL	C-N-CA	6.06	126.08	119.90
2	F	80	ALA	CA-C-N	6.06	126.25	120.31
2	F	80	ALA	C-N-CA	6.06	126.25	120.31
1	B	210	ARG	N-CA-CB	6.05	118.79	110.01
2	F	261	PHE	CA-C-O	6.05	126.96	120.55
2	F	144	ALA	CA-C-N	6.04	126.06	119.90
2	F	144	ALA	C-N-CA	6.04	126.06	119.90
2	D	139	VAL	N-CA-CB	6.03	116.95	110.62
2	F	432	VAL	CB-CA-C	-6.02	104.15	110.53
1	C	341	ASN	CA-C-O	-6.01	114.47	120.90
1	A	162	GLY	N-CA-C	-6.01	106.80	114.37
1	C	405	GLN	CA-C-N	6.01	133.01	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	405	GLN	C-N-CA	6.01	133.01	121.54
2	F	206	ILE	N-CA-CB	6.00	119.03	111.46
2	F	342	LEU	N-CA-C	-6.00	105.92	113.18
1	C	400	VAL	N-CA-CB	6.00	117.97	110.47
2	D	402	LEU	N-CA-C	-6.00	105.04	112.90
1	C	507	GLY	N-CA-C	-6.00	105.54	112.73
2	F	229	ARG	NE-CZ-NH1	-5.99	115.51	121.50
1	C	45	ARG	N-CA-C	5.99	118.59	111.71
1	B	401	ALA	CA-C-N	5.97	132.29	121.06
1	B	401	ALA	C-N-CA	5.97	132.29	121.06
3	G	39	LYS	CA-C-N	5.97	125.67	119.05
3	G	39	LYS	C-N-CA	5.97	125.67	119.05
1	C	406	PHE	CA-CB-CG	5.96	119.76	113.80
1	B	167	ILE	N-CA-CB	5.95	118.17	111.21
1	C	162	GLY	N-CA-C	-5.95	107.18	114.92
1	B	91	THR	N-CA-C	-5.94	105.37	114.16
1	B	371	VAL	CB-CA-C	-5.94	99.79	110.48
1	C	336	ALA	O-C-N	-5.94	115.99	123.12
1	B	162	GLY	N-CA-C	-5.94	106.78	115.63
1	B	423	ARG	CD-NE-CZ	5.94	132.71	124.40
2	F	370	VAL	N-CA-C	-5.93	104.96	110.53
2	F	96	ASN	N-CA-CB	-5.93	101.96	110.44
1	A	67	GLU	CA-C-N	5.92	125.40	119.24
1	A	67	GLU	C-N-CA	5.92	125.40	119.24
3	G	221	THR	N-CA-C	-5.92	106.59	113.88
2	F	461	GLY	CA-C-N	5.92	126.25	119.92
2	F	461	GLY	C-N-CA	5.92	126.25	119.92
1	A	98	PRO	N-CA-CB	5.92	108.95	103.39
2	D	143	LEU	N-CA-C	5.92	120.63	113.41
1	A	106	ARG	CD-NE-CZ	5.91	132.68	124.40
1	A	75	VAL	N-CA-C	5.91	116.68	109.30
1	C	109	ASP	CA-CB-CG	5.90	118.50	112.60
2	D	247	GLU	N-CA-C	-5.90	106.72	114.04
1	C	46	ASN	CA-CB-CG	5.89	118.49	112.60
1	C	422	VAL	CB-CA-C	-5.89	104.19	112.14
1	C	69	ASP	CA-CB-CG	-5.89	106.71	112.60
2	F	426	GLY	N-CA-C	-5.88	107.13	115.30
2	F	221	GLN	CA-C-N	5.88	130.09	120.63
2	F	221	GLN	C-N-CA	5.88	130.09	120.63
2	E	461	GLY	CA-C-N	5.87	125.78	119.85
2	E	461	GLY	C-N-CA	5.87	125.78	119.85
2	F	388	ILE	CB-CA-C	-5.87	104.36	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	477	GLN	CA-C-N	5.86	128.13	120.28
1	B	477	GLN	C-N-CA	5.86	128.13	120.28
3	G	258	ILE	CB-CA-C	-5.85	104.24	112.14
1	C	379	GLN	N-CA-C	5.85	119.01	109.59
2	F	236	GLY	N-CA-C	-5.85	105.71	112.73
2	E	229	ARG	N-CA-C	-5.85	105.99	113.01
1	B	45	ARG	CB-CG-CD	-5.84	97.86	111.30
1	C	91	THR	N-CA-C	-5.84	107.14	114.56
1	C	345	ILE	N-CA-C	-5.83	107.01	111.62
1	B	109	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	373	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	B	351	PHE	N-CA-CB	5.82	119.90	110.42
2	F	210	ASP	CB-CA-C	-5.82	100.37	111.48
1	C	93	ALA	N-CA-C	5.81	118.43	109.07
1	C	241	PRO	N-CA-CB	5.81	109.67	103.39
1	C	100	GLY	N-CA-C	5.80	117.94	112.08
2	E	349	ASP	CA-C-N	5.79	125.89	119.87
2	E	349	ASP	C-N-CA	5.79	125.89	119.87
1	B	136	ILE	CA-C-N	5.79	124.96	120.33
1	B	136	ILE	C-N-CA	5.79	124.96	120.33
1	B	79	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	341	ASN	O-C-N	5.76	128.08	122.09
2	D	454	GLU	CA-CB-CG	5.76	125.61	114.10
1	A	370	SER	CA-C-O	-5.75	115.02	121.81
2	D	225	PRO	N-CA-CB	5.73	106.20	103.22
2	D	96	ASN	N-CA-CB	-5.73	101.73	110.49
1	B	304	ARG	NE-CZ-NH1	-5.72	115.78	121.50
2	D	368	TYR	N-CA-C	5.72	117.52	111.28
2	F	157	GLY	CA-C-O	-5.71	115.50	122.75
1	C	303	SER	CA-C-N	5.70	129.38	120.82
1	C	303	SER	C-N-CA	5.70	129.38	120.82
2	D	145	PRO	CA-C-O	-5.70	114.92	121.36
2	E	36	LEU	CA-C-O	-5.69	114.73	121.16
2	E	97	VAL	CB-CA-C	-5.69	102.88	112.16
2	F	389	ALA	N-CA-C	5.68	118.24	111.71
2	F	229	ARG	NE-CZ-NH2	5.68	124.31	119.20
2	D	145	PRO	N-CA-CB	5.67	108.24	103.25
1	C	230	ILE	CA-C-N	-5.67	115.28	123.11
1	C	230	ILE	C-N-CA	-5.67	115.28	123.11
1	C	120	PRO	N-CA-CB	5.67	108.72	103.39
2	D	163	THR	N-CA-C	5.67	117.45	111.28
2	E	133	LEU	CA-C-O	-5.65	114.31	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	356	ARG	CD-NE-CZ	-5.65	116.49	124.40
3	G	237	LYS	CB-CA-C	5.65	121.52	110.67
2	F	113	PHE	CA-CB-CG	-5.65	108.15	113.80
1	C	381	ARG	CD-NE-CZ	5.65	132.31	124.40
1	A	335	SER	CB-CA-C	-5.64	99.86	110.01
1	A	194	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	420	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	B	245	LEU	N-CA-C	5.63	117.10	111.07
1	B	433	TYR	CA-C-N	-5.63	116.34	122.59
1	B	433	TYR	C-N-CA	-5.63	116.34	122.59
1	A	164	ARG	CA-C-O	-5.62	113.48	120.57
1	C	362	ARG	NE-CZ-NH2	5.62	124.25	119.20
2	D	225	PRO	CA-C-N	5.62	126.86	119.84
2	D	225	PRO	C-N-CA	5.62	126.86	119.84
1	B	127	ARG	CD-NE-CZ	5.60	132.24	124.40
1	B	304	ARG	NE-CZ-NH2	5.59	124.24	119.20
2	F	84	ILE	N-CA-C	5.59	113.78	109.19
2	D	164	VAL	N-CA-C	-5.59	105.05	110.42
1	B	402	ALA	N-CA-C	5.59	117.28	110.41
2	E	96	ASN	CA-CB-CG	5.59	118.19	112.60
1	B	103	LEU	N-CA-C	-5.58	106.60	113.41
1	A	200	TYR	CA-CB-CG	-5.58	103.86	113.90
2	E	120	ALA	CA-C-N	5.56	126.79	119.84
2	E	120	ALA	C-N-CA	5.56	126.79	119.84
2	E	336	SER	N-CA-C	5.55	117.95	108.90
1	B	151	LYS	N-CA-C	5.55	117.77	111.11
2	D	30	PRO	N-CA-CB	5.55	108.46	103.08
2	D	215	VAL	CA-C-O	-5.54	113.85	120.78
2	F	96	ASN	N-CA-C	5.54	117.68	110.53
2	E	95	MET	CA-C-N	5.54	132.13	121.54
2	E	95	MET	C-N-CA	5.54	132.13	121.54
2	E	219	TYR	N-CA-C	5.54	118.43	109.40
2	F	473	LEU	N-CA-C	-5.54	106.03	112.89
2	F	95	MET	O-C-N	-5.53	116.48	123.17
1	A	92	GLY	N-CA-C	-5.53	108.40	115.42
1	C	74	VAL	CB-CA-C	5.53	117.76	110.91
2	E	216	ALA	CA-C-N	-5.52	115.38	123.00
2	E	216	ALA	C-N-CA	-5.52	115.38	123.00
1	A	466	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	A	235	THR	N-CA-C	5.52	118.59	110.59
1	A	367	VAL	CB-CA-C	5.51	119.58	112.14
2	D	179	GLY	CA-C-O	-5.49	116.23	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	272	LEU	N-CA-C	-5.49	106.89	113.21
1	C	366	ASN	CA-C-O	5.48	126.62	120.92
2	F	282	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	B	141	SER	CA-C-O	-5.47	115.00	120.96
1	C	423	ARG	CD-NE-CZ	5.46	132.05	124.40
2	F	215	VAL	N-CA-C	5.46	115.98	108.12
1	A	233	SER	N-CA-CB	-5.46	102.20	110.77
1	C	285	LEU	N-CA-C	-5.45	106.40	113.16
2	E	83	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	A	271	LEU	CA-C-O	5.45	125.64	119.27
2	E	239	VAL	N-CA-CB	-5.45	104.90	110.62
1	A	74	VAL	N-CA-CB	-5.44	105.46	111.66
1	A	263	HIS	CA-CB-CG	-5.44	108.36	113.80
2	E	127	SER	N-CA-C	-5.44	101.67	110.32
2	E	257	ASN	CA-CB-CG	5.43	118.03	112.60
2	F	88	PRO	N-CA-CB	5.42	108.72	103.51
2	F	12	ARG	CD-NE-CZ	-5.42	116.82	124.40
1	A	172	GLN	N-CA-C	5.41	118.66	111.30
2	E	196	LEU	N-CA-C	-5.41	105.03	111.69
2	E	260	ARG	NE-CZ-NH1	-5.41	116.09	121.50
2	D	232	VAL	N-CA-CB	5.41	120.15	111.23
1	C	106	ARG	CA-CB-CG	-5.40	103.30	114.10
2	D	119	GLU	CA-C-O	-5.39	115.68	121.56
2	D	198	HIS	CA-CB-CG	-5.39	108.41	113.80
1	A	93	ALA	CA-C-N	-5.38	114.86	122.34
1	A	93	ALA	C-N-CA	-5.38	114.86	122.34
2	E	83	ARG	CD-NE-CZ	-5.38	116.87	124.40
2	F	121	PRO	N-CA-CB	5.37	107.97	103.25
2	E	200	MET	N-CA-C	-5.37	105.09	111.69
2	E	331	ALA	CA-C-O	5.37	128.18	120.51
2	E	297	THR	CB-CA-C	-5.36	101.16	111.78
1	C	304	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	E	137	ILE	CA-C-O	5.36	126.95	120.74
3	G	222	THR	N-CA-C	-5.36	105.52	111.36
1	B	478	ALA	N-CA-C	5.35	117.11	111.28
1	C	123	SER	N-CA-C	5.35	117.98	109.96
1	C	309	ALA	N-CA-C	-5.34	101.94	109.96
2	D	155	PHE	CA-CB-CG	5.34	119.14	113.80
2	D	222	MET	CB-CA-C	-5.34	98.52	110.21
2	F	408	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	398	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	B	287	ARG	CA-C-N	5.33	125.87	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	ARG	C-N-CA	5.33	125.87	120.38
1	C	33	SER	CA-C-O	-5.33	115.53	121.23
2	E	96	ASN	N-CA-CB	-5.33	101.48	110.49
2	F	366	GLU	N-CA-C	-5.33	105.37	111.07
2	F	41	ARG	CG-CD-NE	5.32	123.71	112.00
2	E	393	MET	N-CA-C	5.32	122.12	110.80
1	B	259	ASP	CA-CB-CG	-5.31	107.29	112.60
2	E	417	PRO	CB-CA-C	-5.31	104.89	111.11
2	F	393	MET	N-CA-C	5.31	119.81	113.23
1	B	40	ARG	NE-CZ-NH1	5.29	126.79	121.50
1	C	48	GLN	CA-C-O	-5.29	115.18	121.16
2	F	76	LEU	N-CA-C	5.29	117.15	108.52
1	B	148	THR	N-CA-C	-5.29	106.95	113.41
2	F	423	VAL	CB-CA-C	-5.29	101.68	111.79
2	F	387	ILE	CB-CA-C	-5.29	105.09	112.02
1	A	134	PRO	N-CA-C	-5.29	102.89	111.14
1	B	116	ASP	N-CA-C	-5.28	106.61	113.16
1	A	372	SER	N-CA-CB	5.28	120.08	110.95
2	E	398	GLU	N-CA-C	-5.28	105.48	112.34
1	C	75	VAL	N-CA-C	5.28	115.69	107.99
1	A	52	MET	CA-C-N	-5.26	115.34	122.92
1	A	52	MET	C-N-CA	-5.26	115.34	122.92
2	D	327	ALA	CA-C-O	-5.26	113.12	119.49
2	E	122	GLU	CA-CB-CG	5.26	124.62	114.10
2	F	330	ASP	CA-CB-CG	-5.26	107.34	112.60
1	C	127	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	C	411	ASP	CA-CB-CG	5.25	117.85	112.60
2	D	118	ALA	CA-C-O	-5.25	115.62	121.23
2	E	282	GLN	CA-C-N	5.25	125.05	119.28
2	E	282	GLN	C-N-CA	5.25	125.05	119.28
1	C	405	GLN	CA-C-O	5.24	128.01	120.51
1	B	279	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	C	299	PHE	N-CA-C	-5.24	105.26	110.97
2	D	322	PRO	N-CA-C	-5.23	105.98	113.47
2	F	225	PRO	N-CA-C	-5.23	104.32	110.70
2	F	87	GLY	CA-C-N	5.23	124.84	119.56
2	F	87	GLY	C-N-CA	5.23	124.84	119.56
1	B	318	GLY	N-CA-C	-5.22	108.63	115.47
2	D	432	VAL	CA-C-N	5.22	125.12	119.85
2	D	432	VAL	C-N-CA	5.22	125.12	119.85
1	C	336	ALA	CA-C-O	5.22	126.71	121.07
2	D	411	GLN	CA-C-O	5.22	126.27	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	GLY	N-CA-C	-5.21	108.43	115.21
2	D	160	VAL	N-CA-CB	5.21	117.94	112.21
1	C	136	ILE	CA-C-N	5.20	124.49	120.33
1	C	136	ILE	C-N-CA	5.20	124.49	120.33
2	D	268	VAL	CA-C-O	5.20	123.48	118.90
2	F	19	ALA	CA-C-N	-5.20	116.04	123.11
2	F	19	ALA	C-N-CA	-5.20	116.04	123.11
1	B	130	GLY	O-C-N	-5.20	115.94	122.70
1	B	309	ALA	CA-C-O	-5.20	115.90	121.56
2	E	171	ASN	OD1-CG-ND2	5.19	127.79	122.60
2	E	72	GLY	N-CA-C	-5.19	108.52	114.69
1	C	336	ALA	N-CA-C	5.18	117.61	110.35
2	E	358	MET	N-CA-CB	5.18	116.85	110.53
3	G	237	LYS	N-CA-C	-5.18	105.81	111.82
1	B	230	ILE	CA-C-O	-5.18	115.86	121.92
2	D	354	THR	CA-C-O	-5.18	115.55	121.40
1	C	296	GLY	N-CA-C	-5.17	108.98	114.67
2	F	416	GLN	CA-C-N	5.17	125.97	120.13
2	F	416	GLN	C-N-CA	5.17	125.97	120.13
2	E	400	ASP	CA-CB-CG	-5.16	107.44	112.60
2	F	200	MET	CA-C-O	5.16	125.89	120.42
3	G	250	PHE	CA-CB-CG	-5.16	108.64	113.80
2	F	257	ASN	OD1-CG-ND2	5.16	127.76	122.60
2	E	330	ASP	CA-CB-CG	-5.15	107.45	112.60
2	F	178	GLY	CA-C-N	-5.15	114.37	122.92
2	F	178	GLY	C-N-CA	-5.15	114.37	122.92
2	F	418	PHE	CA-CB-CG	5.15	118.95	113.80
2	F	59	ARG	CD-NE-CZ	-5.15	117.19	124.40
2	E	173	VAL	N-CA-C	-5.14	105.39	111.00
2	E	250	ASP	CA-CB-CG	-5.13	107.47	112.60
2	D	175	LYS	N-CA-C	5.13	116.87	111.28
2	D	475	GLU	N-CA-CB	5.13	119.22	110.50
1	B	397	TYR	N-CA-C	-5.12	107.58	113.88
1	A	219	ARG	CD-NE-CZ	5.12	131.57	124.40
2	D	165	LEU	N-CA-CB	5.12	117.65	110.12
2	F	200	MET	N-CA-CB	-5.12	102.58	110.16
2	E	439	LYS	O-C-N	5.12	127.34	122.07
2	D	224	GLU	CA-C-N	5.11	123.34	119.66
2	D	224	GLU	C-N-CA	5.11	123.34	119.66
2	D	361	ASN	CA-CB-CG	-5.11	107.49	112.60
2	F	281	TYR	CA-C-N	5.11	127.75	120.49
2	F	281	TYR	C-N-CA	5.11	127.75	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	251	VAL	CB-CA-C	-5.11	105.97	111.59
2	E	415	SER	CA-C-O	-5.11	115.91	121.89
2	F	388	ILE	N-CA-CB	5.11	116.85	110.47
2	D	454	GLU	CB-CA-C	-5.10	102.81	110.92
2	D	170	ILE	N-CA-C	-5.09	105.57	110.72
2	E	107	PRO	N-CA-CB	5.09	107.84	103.31
1	B	219	ARG	NE-CZ-NH1	-5.09	116.41	121.50
2	F	100	GLU	CA-C-O	-5.09	115.91	120.19
1	C	270	ASP	CA-CB-CG	5.09	117.69	112.60
2	F	170	ILE	N-CA-C	-5.07	105.45	110.62
2	F	101	PRO	N-CA-CB	5.07	107.76	103.35
1	A	400	VAL	N-CA-C	5.07	119.49	112.35
2	E	125	GLU	CA-C-O	5.06	124.39	118.97
1	B	374	VAL	CB-CA-C	-5.06	104.52	110.84
1	C	145	PRO	N-CA-CB	5.06	108.15	103.39
3	G	44	TYR	CA-CB-CG	5.06	123.01	113.90
1	B	274	GLN	N-CA-C	-5.06	105.85	111.36
2	D	357	ILE	N-CA-CB	5.06	119.58	112.15
1	A	101	GLU	N-CA-C	5.05	118.91	112.34
2	E	56	SER	CA-C-N	-5.05	115.36	122.94
2	E	56	SER	C-N-CA	-5.05	115.36	122.94
2	E	226	PRO	CA-C-N	5.05	125.69	120.03
2	E	226	PRO	C-N-CA	5.05	125.69	120.03
1	B	391	LYS	N-CA-C	-5.05	105.96	111.82
2	F	330	ASP	N-CA-C	-5.05	107.25	113.41
2	F	433	PRO	N-CA-CB	5.04	108.03	103.34
1	B	94	ILE	N-CA-C	-5.04	102.57	109.37
1	A	178	ILE	CB-CA-C	-5.04	105.43	111.88
1	A	191	ASP	N-CA-C	-5.03	107.19	113.38
2	E	161	GLY	N-CA-C	5.03	125.11	113.18
1	B	349	GLN	N-CA-CB	5.03	120.44	111.69
1	B	141	SER	CB-CA-C	-5.03	102.30	109.84
1	B	222	ASP	CA-C-N	-5.02	114.26	122.54
1	B	222	ASP	C-N-CA	-5.02	114.26	122.54
1	C	132	LYS	CA-CB-CG	5.02	124.14	114.10
1	C	438	ILE	N-CA-C	5.02	115.63	110.36
1	B	325	PRO	CA-C-N	-5.01	116.64	123.10
1	B	325	PRO	C-N-CA	-5.01	116.64	123.10
1	C	136	ILE	N-CA-C	5.00	115.23	110.53

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	3715	0	3815	182	0
1	B	3715	0	3812	176	0
1	C	3748	0	3844	187	0
2	D	3539	0	3592	166	0
2	E	3530	0	3587	223	0
2	F	3530	0	3586	137	0
3	G	945	0	1019	59	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	31	0	13	2	0
5	B	31	0	13	5	0
5	C	31	0	13	4	0
5	F	31	0	13	4	0
6	D	27	0	12	2	0
7	A	92	0	0	9	0
7	B	96	0	0	14	0
7	C	123	0	0	11	0
7	D	105	0	0	6	0
7	E	49	0	0	6	0
7	F	104	0	0	5	0
7	G	34	0	0	1	0
All	All	23481	0	23319	1070	0

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 23.

All (1070) 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:C:127:ARG:HH12	1:C:255:GLU:HB2	1.00	1.15
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.12	1.12
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.73	1.02
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.40	1.02
2:F:223:ASN:HD22	2:F:223:ASN:H	1.08	1.02
1:C:404:ALA:C	1:C:406:PHE:H	1.64	0.97
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.30	0.95
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.48	0.93
2:E:223:ASN:HD22	2:E:223:ASN:H	1.00	0.92
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.84	0.91
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.52	0.91
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.37	0.89
1:C:215:GLN:HG3	2:F:356:ARG:NH2	1.89	0.88
1:C:398:ARG:HG2	7:C:627:HOH:O	1.72	0.88
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.55	0.87
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.57	0.86
1:B:456:LEU:HD12	1:B:457:GLU:H	1.42	0.84
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.60	0.84
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.61	0.79
2:D:282:GLN:H	2:D:282:GLN:HE21	1.30	0.79
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.65	0.79
1:B:141:SER:O	1:B:143:ARG:HD2	1.83	0.79
1:B:211:SER:HB2	7:B:674:HOH:O	1.82	0.79
2:E:223:ASN:H	2:E:223:ASN:ND2	1.72	0.78
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.65	0.78
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.50	0.77
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.66	0.77
2:E:394:ASP:C	2:E:396:LEU:H	1.93	0.76
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.65	0.76
2:D:404:VAL:O	2:D:408:ARG:HG3	1.84	0.76
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.66	0.76
1:B:172:GLN:HA	5:B:600:ANP:HNB1	1.51	0.75
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.67	0.75
2:E:96:ASN:HB3	2:E:100:GLU:H	1.52	0.75
1:B:379:GLN:HB3	1:B:384:LYS:HE2	1.68	0.74
2:E:89:GLU:HG3	2:E:109:LYS:O	1.87	0.74
3:G:2:THR:HG22	3:G:4:LYS:H	1.51	0.74
2:E:275:ILE:HG23	3:G:266:ILE:HD13	1.68	0.74
2:F:159:GLY:HA2	5:F:600:ANP:HNB1	1.52	0.74
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.68	0.74
1:C:101:GLU:HB2	7:C:723:HOH:O	1.88	0.73
2:E:345:TYR:HA	2:E:346:PRO:C	2.13	0.73
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.70	0.72
2:D:223:ASN:H	2:D:223:ASN:HD22	1.35	0.72
1:A:297:ASP:HA	7:A:628:HOH:O	1.89	0.72
2:F:89:GLU:HG3	2:F:109:LYS:O	1.89	0.72
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.71	0.72
2:D:156:GLY:HA2	7:D:659:HOH:O	1.90	0.71
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.71	0.71
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.72	0.71
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.71	0.71
1:A:291:ARG:HA	3:G:262:LEU:HD13	1.72	0.70
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.71	0.70
1:C:211:SER:O	1:C:215:GLN:HG2	1.91	0.70
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.56	0.70
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.73	0.70
1:A:407:GLY:HA2	1:A:410:LEU:HD21	1.73	0.70
1:B:218:LYS:HB2	2:E:128:VAL:HG12	1.74	0.69
2:E:388:ILE:HG23	2:E:393:MET:HG3	1.73	0.69
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.75	0.69
2:D:200:MET:HE3	2:D:215:VAL:HG21	1.74	0.69
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.92	0.69
2:D:96:ASN:HB2	2:D:100:GLU:H	1.56	0.69
2:E:105:ARG:CZ	2:E:208:LEU:HD23	2.23	0.69
2:F:252:LEU:HD23	2:F:305:THR:HB	1.75	0.69
2:D:223:ASN:HD22	2:D:223:ASN:N	1.89	0.69
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.73	0.68
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.74	0.68
1:B:283:LEU:CD1	2:E:277:SER:HB3	2.22	0.68
1:A:440:GLU:O	1:A:444:VAL:HG13	1.94	0.67
2:E:425:THR:O	2:E:427:HIS:ND1	2.20	0.67
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.76	0.67
2:F:409:LYS:HD3	2:F:457:PHE:CE2	2.30	0.67
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.75	0.67
1:A:134:PRO:O	1:A:139:ARG:NH2	2.27	0.67
1:A:44:LEU:O	1:A:47:VAL:HG22	1.94	0.67
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.76	0.67
1:C:418:LEU:O	1:C:422:VAL:HG23	1.94	0.67
1:C:173:THR:HG22	1:C:354:THR:HG22	1.77	0.67
3:G:23:MET:SD	3:G:232:MET:HE2	2.35	0.67
1:A:383:MET:HE2	1:A:438:ILE:HD11	1.77	0.66
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.93	0.66
1:B:363:PRO:O	7:B:609:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:HD23	1:C:82:ILE:HD11	1.77	0.66
2:F:223:ASN:HD22	2:F:223:ASN:N	1.85	0.66
1:C:99:VAL:HG22	1:C:253:MET:HA	1.78	0.66
2:E:224:GLU:HG2	7:E:501:HOH:O	1.96	0.66
2:D:223:ASN:H	2:D:223:ASN:ND2	1.93	0.66
2:F:223:ASN:H	2:F:223:ASN:ND2	1.85	0.66
3:G:20:THR:HA	3:G:232:MET:HE3	1.77	0.66
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.78	0.65
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.78	0.65
2:F:314:ALA:O	2:F:315:ASP:HB2	1.95	0.65
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.77	0.65
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.26	0.65
2:D:54:GLY:O	2:D:55:GLU:HB2	1.96	0.65
1:A:376:SER:C	1:A:378:ALA:H	2.03	0.65
1:B:283:LEU:HD12	2:E:277:SER:HB3	1.78	0.65
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.96	0.65
3:G:24:LYS:HE3	3:G:233:ASP:HB2	1.78	0.65
1:A:403:PHE:CZ	3:G:22:SER:HB2	2.32	0.65
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.77	0.65
2:E:223:ASN:HD22	2:E:223:ASN:N	1.84	0.65
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.26	0.65
1:B:215:GLN:NE2	2:E:130:GLN:NE2	2.45	0.65
2:D:225:PRO:HB2	7:D:649:HOH:O	1.95	0.65
1:B:437:ALA:O	1:B:440:GLU:N	2.30	0.65
2:E:394:ASP:C	2:E:396:LEU:N	2.54	0.65
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.62	0.64
1:C:44:LEU:O	1:C:47:VAL:HG22	1.96	0.64
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.79	0.64
1:B:362:ARG:HA	1:B:363:PRO:C	2.22	0.64
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.77	0.64
2:F:200:MET:HG3	2:F:205:VAL:CG2	2.27	0.64
2:E:400:ASP:O	2:E:404:VAL:HG23	1.98	0.64
1:C:436:MET:HE3	1:C:469:LEU:HD21	1.79	0.64
1:C:404:ALA:C	1:C:406:PHE:N	2.44	0.64
1:C:488:LYS:HG2	1:C:489:ILE:H	1.63	0.64
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.33	0.64
1:B:390:MET:HE1	1:B:428:LEU:HD21	1.80	0.64
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.28	0.64
1:C:215:GLN:CG	2:F:356:ARG:HH22	2.02	0.63
1:C:419:SER:O	1:C:423:ARG:HG2	1.98	0.63
2:D:200:MET:HB3	2:D:206:ILE:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:200:MET:HG3	2:F:205:VAL:HG23	1.80	0.63
1:C:362:ARG:HA	1:C:363:PRO:C	2.21	0.63
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.98	0.63
1:A:211:SER:N	2:D:126:MET:HE2	2.14	0.63
1:A:376:SER:C	1:A:378:ALA:N	2.55	0.63
1:C:52:MET:O	1:C:91:THR:HB	1.98	0.63
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.33	0.63
1:C:52:MET:HE2	1:C:76:PHE:HE2	1.62	0.63
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.62	0.63
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.63	0.63
2:E:138:LYS:HE2	2:E:432:VAL:HG21	1.81	0.63
1:A:48:GLN:HB3	2:E:68:GLY:O	1.99	0.62
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.80	0.62
1:C:211:SER:HB3	2:F:126:MET:HE2	1.79	0.62
2:E:204:GLY:O	2:E:206:ILE:N	2.32	0.62
1:A:341:ASN:O	1:A:345:ILE:HG13	1.99	0.62
2:E:422:GLU:HG2	2:E:427:HIS:O	1.99	0.62
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.80	0.62
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.82	0.62
1:B:389:THR:HA	1:B:392:LEU:CD1	2.28	0.62
1:B:422:VAL:O	1:B:426:GLU:HG2	2.00	0.61
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.30	0.61
1:B:389:THR:HA	1:B:392:LEU:HD12	1.81	0.61
1:C:218:LYS:HD2	2:F:128:VAL:HG21	1.81	0.61
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.34	0.61
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.83	0.61
2:E:158:ALA:C	2:E:160:VAL:H	2.08	0.61
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.82	0.61
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.34	0.61
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.80	0.61
1:C:362:ARG:NH1	7:C:689:HOH:O	2.34	0.61
1:B:68:PRO:HD3	2:F:15:ALA:HB2	1.81	0.61
1:A:121:ILE:HD13	1:A:121:ILE:H	1.66	0.61
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.81	0.61
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.01	0.61
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.82	0.61
2:E:298:THR:HG23	2:E:303:SER:HB3	1.81	0.61
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.15	0.61
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.81	0.61
1:B:102:GLU:HG3	1:B:122:GLY:O	2.00	0.60
2:D:93:ARG:HG3	2:D:93:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MET:O	1:A:91:THR:HG23	2.01	0.60
2:E:92:GLY:N	2:E:215:VAL:O	2.30	0.60
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.82	0.60
1:C:292:GLU:O	1:C:293:ALA:HB3	2.00	0.60
1:C:344:SER:O	2:D:222:MET:HE1	2.00	0.60
2:D:473:LEU:C	2:D:475:GLU:H	2.08	0.60
2:E:223:ASN:ND2	2:E:223:ASN:N	2.46	0.60
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.83	0.60
1:C:408:SER:O	1:C:409:ASP:C	2.44	0.60
1:C:433:TYR:C	1:C:435:PRO:HD3	2.26	0.60
2:D:63:MET:HE3	2:D:228:ALA:HA	1.83	0.60
1:C:373:ARG:HA	6:D:600:ADP:O3'	2.02	0.60
2:E:419:GLN:HG3	2:E:429:GLY:HA3	1.84	0.60
2:F:63:MET:HE1	2:F:97:VAL:HG11	1.82	0.60
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.34	0.60
1:B:51:GLU:HA	1:B:94:ILE:HA	1.83	0.60
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.67	0.60
1:A:432:GLN:HB3	1:A:433:TYR:CD2	2.37	0.60
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.83	0.60
2:E:149:GLY:HA2	2:E:304:ILE:O	2.02	0.60
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.83	0.60
3:G:13:ILE:HG22	3:G:243:ILE:HG12	1.84	0.60
1:B:237:SER:HB3	7:B:687:HOH:O	2.02	0.59
1:C:175:LYS:HE3	5:C:600:ANP:O1B	2.02	0.59
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.83	0.59
2:E:263:GLN:HB3	7:E:490:HOH:O	2.00	0.59
1:A:132:LYS:HA	7:A:643:HOH:O	2.01	0.59
2:E:224:GLU:O	2:E:229:ARG:NH1	2.32	0.59
2:E:316:ASP:OD2	3:G:254:ARG:NH1	2.35	0.59
1:A:457:GLU:CB	1:A:460:LYS:HD3	2.32	0.59
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.85	0.59
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.84	0.59
3:G:239:ALA:O	3:G:243:ILE:HG13	2.02	0.59
1:A:157:VAL:N	1:A:158:PRO:CD	2.65	0.59
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.59
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.66	0.59
1:A:403:PHE:CE1	3:G:22:SER:HB2	2.38	0.59
2:E:397:SER:H	2:E:400:ASP:HB2	1.66	0.59
1:B:215:GLN:HE22	2:E:130:GLN:NE2	1.99	0.59
1:C:140:ILE:HD11	1:C:143:ARG:NH2	2.18	0.59
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:O	1:B:175:LYS:HE2	2.03	0.59
1:B:499:GLU:O	1:B:502:THR:HB	2.03	0.59
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.03	0.59
1:B:452:TYR:O	1:B:453:LEU:HD23	2.03	0.59
1:A:68:PRO:HD3	2:E:15:ALA:HB2	1.85	0.58
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.37	0.58
2:D:263:GLN:O	2:D:267:GLU:HG3	2.03	0.58
2:E:200:MET:HB3	2:E:205:VAL:HG23	1.84	0.58
7:B:617:HOH:O	2:F:67:GLU:HG3	2.02	0.58
2:D:393:MET:HE3	2:D:404:VAL:HG21	1.83	0.58
2:E:408:ARG:O	2:E:412:ARG:HG3	2.02	0.58
1:C:406:PHE:O	1:C:408:SER:N	2.36	0.58
2:E:32:ILE:O	2:E:33:LEU:HB2	2.02	0.58
1:B:391:LYS:O	1:B:395:ALA:N	2.36	0.58
2:E:122:GLU:N	2:E:125:GLU:OE2	2.37	0.58
2:E:246:GLN:HA	2:E:246:GLN:NE2	2.19	0.58
2:F:105:ARG:NH1	2:F:208:LEU:HD23	2.18	0.58
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.85	0.58
1:C:405:GLN:C	1:C:406:PHE:HD1	2.11	0.58
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.85	0.58
2:E:397:SER:C	2:E:399:GLU:N	2.57	0.58
1:B:434:SER:N	1:B:435:PRO:HD3	2.18	0.58
1:C:102:GLU:OE2	1:C:123:SER:HA	2.03	0.58
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.84	0.58
2:E:85:PRO:HD2	2:E:95:MET:HE2	1.86	0.58
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.39	0.58
2:E:433:PRO:HG2	2:E:436:GLU:HG2	1.86	0.58
3:G:17:GLN:HB2	3:G:239:ALA:HB1	1.85	0.58
1:C:156:LEU:HD13	1:C:367:VAL:HG22	1.86	0.58
1:C:210:ARG:NH1	2:F:121:PRO:O	2.37	0.58
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.84	0.58
2:F:440:GLY:O	2:F:444:ILE:HG13	2.04	0.58
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.86	0.58
1:B:400:VAL:HB	1:B:418:LEU:HD21	1.85	0.58
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.58
2:E:95:MET:CG	2:E:99:GLY:HA2	2.34	0.58
1:C:107:VAL:HG12	1:C:115:ILE:HD11	1.86	0.57
1:C:399:GLU:OE2	2:D:408:ARG:NH2	2.37	0.57
1:B:62:MET:HE3	1:B:64:LEU:HD13	1.87	0.57
1:A:333:ASP:HB3	7:A:632:HOH:O	2.04	0.57
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:431:LEU:C	2:D:431:LEU:HD12	2.29	0.57
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.87	0.57
2:E:267:GLU:O	2:E:271:LEU:HG	2.05	0.57
1:B:358:TYR:C	1:B:360:GLY:H	2.12	0.57
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.85	0.57
1:B:352:LEU:HA	1:B:364:ALA:O	2.04	0.57
2:D:473:LEU:C	2:D:475:GLU:N	2.62	0.57
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.68	0.57
1:A:185:ASN:O	1:A:188:ARG:HG3	2.05	0.57
2:D:282:GLN:H	2:D:282:GLN:NE2	2.01	0.57
2:E:138:LYS:O	2:E:142:LEU:HB3	2.03	0.57
2:F:14:VAL:O	2:F:71:ARG:HG2	2.05	0.57
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.05	0.56
1:A:286:ARG:HH22	3:G:272:LEU:HD13	1.68	0.56
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.38	0.56
1:B:351:PHE:CE1	1:B:369:LEU:HB3	2.40	0.56
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.40	0.56
1:C:184:ILE:HG22	1:C:435:PRO:HG2	1.87	0.56
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.20	0.56
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.87	0.56
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.19	0.56
1:C:404:ALA:O	1:C:406:PHE:N	2.37	0.56
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.71	0.56
2:F:10:THR:HG23	2:F:76:LEU:HD12	1.88	0.56
1:C:219:ARG:HD3	1:C:433:TYR:CE1	2.41	0.56
3:G:20:THR:HG21	3:G:236:SER:N	2.21	0.56
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.05	0.56
2:E:155:PHE:CE1	2:E:310:ILE:HD12	2.40	0.56
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.36	0.56
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.71	0.56
1:B:218:LYS:NZ	2:E:129:GLU:OE2	2.39	0.56
1:C:187:LYS:HE2	1:C:191:ASP:OD2	2.05	0.56
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.88	0.56
1:C:52:MET:HE2	1:C:76:PHE:CE2	2.41	0.56
1:C:173:THR:CG2	1:C:354:THR:HG22	2.35	0.56
2:E:126:MET:HE1	2:E:297:THR:HG21	1.86	0.56
1:A:224:ASP:CG	1:A:227:LYS:HE3	2.31	0.55
1:B:70:ASN:OD1	7:B:632:HOH:O	2.18	0.55
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.72	0.55
1:C:102:GLU:HG2	1:C:122:GLY:O	2.06	0.55
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:MET:CE	2:F:97:VAL:HG11	2.37	0.55
1:A:99:VAL:CG2	1:A:253:MET:HA	2.36	0.55
2:D:278:ALA:HB1	3:G:261:GLU:OE2	2.06	0.55
2:D:471:ASP:O	2:D:474:ALA:N	2.39	0.55
2:E:138:LYS:HG3	2:E:416:GLN:OE1	2.06	0.55
2:E:396:LEU:HB3	2:E:401:LYS:HG2	1.88	0.55
1:B:175:LYS:HE3	5:B:600:ANP:O1B	2.06	0.55
1:B:180:ILE:O	1:B:181:ASP:C	2.47	0.55
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.88	0.55
2:F:324:THR:O	2:F:324:THR:HG22	2.05	0.55
2:E:77:ASP:OD1	2:E:79:GLY:N	2.34	0.55
2:F:32:ILE:O	2:F:33:LEU:HB2	2.05	0.55
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.88	0.55
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.42	0.55
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.89	0.55
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.71	0.55
1:B:482:LYS:O	1:B:486:ASP:N	2.37	0.55
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.42	0.55
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.72	0.55
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.88	0.54
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.89	0.54
2:D:451:HIS:CD2	2:D:452:LEU:HD23	2.42	0.54
2:D:473:LEU:O	2:D:475:GLU:N	2.40	0.54
1:B:172:GLN:HA	5:B:600:ANP:N3B	2.21	0.54
1:B:195:GLU:HB3	7:B:691:HOH:O	2.08	0.54
1:B:270:ASP:OD1	1:B:273:LYS:HG3	2.07	0.54
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.54
2:D:83:ARG:HA	2:D:114:ALA:O	2.07	0.54
3:G:81:ILE:HG22	3:G:82:HIS:HD2	1.73	0.54
1:A:161:ARG:HH11	1:A:263:HIS:CG	2.25	0.54
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.88	0.54
1:C:91:THR:HG22	1:C:93:ALA:H	1.72	0.54
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.54
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	0.54
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.43	0.54
1:B:446:TYR:CD2	1:B:497:LEU:HD23	2.43	0.54
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.42	0.54
1:A:172:GLN:HA	5:A:600:ANP:N3B	2.23	0.54
1:A:463:LYS:HD3	1:A:508:PHE:HZ	1.73	0.54
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.90	0.54
2:D:388:ILE:HD12	2:D:393:MET:SD	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:ILE:CD1	2:E:208:LEU:HD11	2.37	0.54
2:E:397:SER:O	2:E:401:LYS:HG3	2.08	0.54
2:F:395:GLU:OE2	3:G:77:LEU:HA	2.08	0.54
1:C:83:LYS:HB3	2:F:52:HIS:CE1	2.42	0.54
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.89	0.54
1:B:33:SER:HB2	2:E:52:HIS:O	2.08	0.54
7:B:624:HOH:O	2:F:198:HIS:CE1	2.60	0.54
2:D:122:GLU:OE1	2:D:122:GLU:HA	2.07	0.54
2:D:167:MET:CB	2:D:420:VAL:HG11	2.38	0.54
2:F:225:PRO:HB2	7:F:630:HOH:O	2.07	0.54
1:A:245:LEU:O	1:A:246:ALA:C	2.51	0.53
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.89	0.53
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.08	0.53
1:C:140:ILE:HD11	1:C:143:ARG:HH22	1.74	0.53
1:B:44:LEU:O	1:B:47:VAL:HG22	2.08	0.53
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.91	0.53
2:D:412:ARG:HH11	2:D:412:ARG:HG3	1.73	0.53
2:F:96:ASN:HB2	2:F:100:GLU:H	1.74	0.53
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.91	0.53
3:G:17:GLN:HB2	3:G:239:ALA:CB	2.39	0.53
1:A:150:ILE:HA	1:A:430:GLN:OE1	2.08	0.53
1:B:69:ASP:O	1:B:70:ASN:HB3	2.09	0.53
2:D:381:TYR:HE2	2:D:411:GLN:HE22	1.56	0.53
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.89	0.53
1:B:171:ARG:HD2	7:E:496:HOH:O	2.08	0.53
1:C:174:GLY:HA2	5:C:600:ANP:PA	2.49	0.53
2:F:210:ASP:HB2	2:F:212:THR:HG23	1.91	0.53
1:A:170:ASP:O	1:A:175:LYS:HE2	2.08	0.53
1:C:335:SER:O	2:D:314:ALA:HA	2.09	0.53
2:D:84:ILE:CD1	2:D:95:MET:HE1	2.34	0.53
2:F:292:MET:CE	2:F:296:ILE:HD11	2.38	0.53
1:C:390:MET:HE3	1:C:424:LEU:HD22	1.89	0.53
2:E:174:ALA:HB2	2:E:214:LYS:HD3	1.89	0.53
2:E:218:VAL:HG11	2:E:235:THR:CG2	2.38	0.53
3:G:14:LYS:HG2	3:G:243:ILE:HD13	1.91	0.53
1:C:338:ILE:O	1:C:339:PRO:C	2.51	0.53
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.89	0.53
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.73	0.53
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.90	0.53
2:D:96:ASN:CB	2:D:100:GLU:H	2.22	0.52
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:GLN:O	1:B:445:ILE:HG12	2.08	0.52
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.24	0.52
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.91	0.52
2:E:279:VAL:HG12	2:E:279:VAL:O	2.10	0.52
2:D:356:ARG:O	2:D:356:ARG:HG2	2.09	0.52
1:B:157:VAL:N	1:B:158:PRO:CD	2.73	0.52
1:B:386:VAL:HG22	1:B:442:VAL:HG12	1.91	0.52
1:C:172:GLN:HA	5:C:600:ANP:HNB1	1.75	0.52
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.09	0.52
2:E:97:VAL:HG13	2:E:232:VAL:CG1	2.39	0.52
2:E:334:VAL:HG23	2:E:353:SER:HA	1.92	0.52
1:B:284:LEU:CD2	2:E:274:ARG:HD3	2.39	0.52
2:E:216:ALA:HB1	7:E:487:HOH:O	2.09	0.52
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.45	0.52
3:G:209:LEU:O	3:G:210:ALA:C	2.52	0.52
1:B:333:ASP:HB2	3:G:252:ARG:HH21	1.74	0.52
1:C:267:ILE:N	1:C:267:ILE:HD12	2.25	0.52
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.75	0.52
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.91	0.52
1:A:313:ASN:O	1:A:316:PHE:N	2.37	0.52
2:E:25:PHE:O	2:E:56:SER:HB3	2.10	0.52
2:E:9:THR:HG21	2:E:28:GLY:O	2.09	0.52
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.91	0.52
3:G:214:TYR:CZ	3:G:218:LYS:HG3	2.45	0.52
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.91	0.52
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.91	0.52
2:D:390:ILE:HD13	3:G:16:ILE:CD1	2.40	0.52
1:C:354:THR:HG23	7:C:664:HOH:O	2.10	0.51
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.23	0.51
2:E:204:GLY:C	2:E:206:ILE:N	2.68	0.51
2:F:360:PRO:HD3	2:F:368:TYR:CD2	2.45	0.51
1:A:140:ILE:HG21	1:A:313:ASN:HA	1.92	0.51
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.40	0.51
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.11	0.51
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.92	0.51
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.91	0.51
2:D:422:GLU:HG2	2:D:427:HIS:O	2.09	0.51
2:E:293:GLN:HG3	2:E:328:HIS:CG	2.46	0.51
1:B:303:SER:HB2	2:F:222:MET:HB3	1.92	0.51
1:B:386:VAL:CG2	1:B:442:VAL:HG12	2.41	0.51
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LEU:HD23	1:C:74:VAL:HG21	1.91	0.51
1:C:102:GLU:HG2	1:C:122:GLY:C	2.36	0.51
2:F:289:MET:HE2	7:F:635:HOH:O	2.09	0.51
1:B:489:ILE:HG22	1:B:494:ASP:HB2	1.93	0.51
1:C:164:ARG:HD2	1:C:306:LEU:O	2.11	0.51
3:G:37:GLU:OE1	3:G:218:LYS:HE3	2.10	0.51
1:B:383:MET:O	1:B:384:LYS:C	2.52	0.51
1:C:443:ALA:O	1:C:446:TYR:HB3	2.10	0.51
2:E:218:VAL:HG11	2:E:235:THR:HG22	1.92	0.51
2:E:443:GLN:O	2:E:446:ALA:HB3	2.10	0.51
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.93	0.51
2:F:455:GLN:H	2:F:455:GLN:CD	2.18	0.51
3:G:6:ILE:HG23	3:G:246:LEU:HD22	1.93	0.51
2:E:82:ILE:HB	2:E:116:ILE:HD13	1.92	0.51
3:G:38:LEU:HD11	3:G:42:ARG:NE	2.26	0.51
1:A:85:GLY:O	1:A:86:ASP:C	2.53	0.51
1:A:140:ILE:HD11	1:A:143:ARG:NE	2.25	0.51
1:B:210:ARG:O	1:B:211:SER:C	2.54	0.51
7:B:621:HOH:O	2:F:189:ARG:HG2	2.09	0.51
1:C:83:LYS:HB3	2:F:52:HIS:HE1	1.76	0.51
3:G:1:ALA:HB1	3:G:6:ILE:HD11	1.92	0.51
2:E:142:LEU:HD21	2:E:374:VAL:HG21	1.93	0.51
2:E:242:TYR:C	2:E:244:ARG:H	2.18	0.51
1:C:406:PHE:N	1:C:406:PHE:CD1	2.79	0.50
1:A:177:SER:OG	5:A:600:ANP:H8	2.11	0.50
1:B:157:VAL:N	1:B:158:PRO:HD3	2.25	0.50
1:B:358:TYR:C	1:B:360:GLY:N	2.69	0.50
1:C:344:SER:HA	7:D:664:HOH:O	2.10	0.50
2:D:136:GLY:CA	2:D:431:LEU:HD13	2.37	0.50
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.93	0.50
1:A:137:ILE:N	1:A:138:PRO:CD	2.75	0.50
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.93	0.50
2:E:275:ILE:O	2:E:283:PRO:HG3	2.12	0.50
2:F:421:ALA:O	2:F:425:THR:HG23	2.11	0.50
1:A:240:ALA:N	1:A:241:PRO:HD2	2.27	0.50
1:B:151:LYS:NZ	1:B:429:LYS:O	2.45	0.50
1:B:174:GLY:HA2	5:B:600:ANP:PA	2.52	0.50
1:C:105:GLY:HA2	1:C:226:MET:HE3	1.93	0.50
1:C:331:ALA:O	1:C:333:ASP:N	2.44	0.50
2:E:221:GLN:N	2:E:224:GLU:OE1	2.44	0.50
1:A:175:LYS:NZ	7:A:625:HOH:O	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:C	1:A:247:PRO:HD2	2.36	0.50
1:C:362:ARG:NH1	1:C:362:ARG:HG3	2.27	0.50
1:C:436:MET:CE	1:C:469:LEU:HD21	2.41	0.50
3:G:39:LYS:HB2	3:G:40:PRO:CD	2.24	0.50
1:B:390:MET:CE	1:B:428:LEU:HD21	2.42	0.50
2:E:155:PHE:HE1	2:E:310:ILE:HD12	1.77	0.50
2:F:234:LEU:O	2:F:237:LEU:HB3	2.10	0.50
2:F:386:ASP:O	2:F:389:ALA:HB3	2.12	0.50
1:A:457:GLU:HB2	1:A:460:LYS:HD3	1.92	0.50
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.39	0.50
1:C:45:ARG:NH2	1:C:68:PRO:O	2.44	0.50
2:F:242:TYR:CD1	2:F:246:GLN:HG3	2.46	0.50
2:F:345:TYR:HA	2:F:346:PRO:C	2.36	0.50
1:C:402:ALA:O	1:C:405:GLN:HG3	2.12	0.50
2:E:204:GLY:O	2:E:205:VAL:C	2.54	0.50
3:G:39:LYS:CB	3:G:40:PRO:HD3	2.15	0.50
1:B:27:GLU:O	1:B:90:ARG:HG3	2.12	0.50
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.94	0.50
1:C:434:SER:N	1:C:435:PRO:HD3	2.27	0.50
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.92	0.50
1:C:171:ARG:NH2	7:C:707:HOH:O	2.27	0.49
1:C:244:TYR:O	1:C:247:PRO:HD2	2.11	0.49
2:D:154:LEU:HD22	2:D:165:LEU:HD23	1.92	0.49
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.40	0.49
2:E:382:LYS:O	2:E:385:GLN:HB2	2.11	0.49
2:F:297:THR:HA	7:F:675:HOH:O	2.12	0.49
1:C:23:VAL:HG12	1:C:23:VAL:O	2.11	0.49
2:D:136:GLY:HA2	2:D:432:VAL:O	2.12	0.49
2:D:319:ASP:O	2:D:320:PRO:C	2.55	0.49
2:D:406:ARG:O	2:D:410:ILE:HG13	2.11	0.49
2:E:41:ARG:O	2:E:42:GLU:C	2.53	0.49
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.94	0.49
2:F:168:GLU:OE1	2:F:418:PHE:HB3	2.12	0.49
3:G:30:LYS:HA	3:G:33:ARG:HE	1.77	0.49
3:G:210:ALA:HA	3:G:213:ILE:HB	1.93	0.49
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.76	0.49
2:D:168:GLU:HG3	2:D:168:GLU:O	2.11	0.49
2:E:444:ILE:HD11	2:E:463:ILE:HD11	1.93	0.49
1:A:417:LEU:HD23	1:A:417:LEU:H	1.77	0.49
1:C:225:ALA:HA	1:C:228:TYR:CE1	2.47	0.49
1:A:380:THR:O	1:A:384:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:462:PRO:HD2	2:E:465:GLU:HG3	1.94	0.49
2:F:164:VAL:HG23	5:F:600:ANP:O1A	2.13	0.49
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.95	0.49
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.95	0.49
2:D:93:ARG:HG3	2:D:93:ARG:NH1	2.27	0.49
2:D:306:SER:HB2	7:D:629:HOH:O	2.12	0.49
2:E:393:MET:HE3	2:E:396:LEU:HD12	1.95	0.49
2:E:463:ILE:O	2:E:467:VAL:HG23	2.12	0.49
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.26	0.49
2:F:163:THR:O	2:F:167:MET:HG2	2.12	0.49
1:B:437:ALA:O	1:B:438:ILE:C	2.54	0.49
1:C:343:ILE:HG22	2:D:158:ALA:HB1	1.94	0.49
3:G:82:HIS:H	3:G:82:HIS:CD2	2.29	0.49
1:B:49:ALA:O	1:B:50:GLU:HB2	2.12	0.49
2:D:376:LYS:HB2	7:D:631:HOH:O	2.11	0.49
2:F:86:VAL:HG11	2:F:114:ALA:HB3	1.94	0.49
1:B:24:ASP:O	1:B:28:THR:HB	2.12	0.49
1:B:456:LEU:HD12	1:B:457:GLU:N	2.20	0.49
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.48	0.49
1:C:30:ARG:HA	1:C:86:ASP:O	2.13	0.49
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.48	0.49
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.49
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.78	0.49
1:B:107:VAL:HG12	1:B:115:ILE:CG1	2.43	0.49
1:B:211:SER:O	1:B:215:GLN:HG3	2.13	0.49
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.49
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.13	0.49
3:G:20:THR:HG22	3:G:236:SER:HB3	1.94	0.49
1:A:49:ALA:O	1:A:50:GLU:HB2	2.13	0.48
2:E:227:GLY:O	2:E:230:ALA:HB3	2.13	0.48
1:A:94:ILE:HG12	1:A:95:VAL:N	2.27	0.48
1:A:389:THR:O	1:A:393:GLU:HG2	2.13	0.48
1:B:423:ARG:HE	1:B:458:PRO:CD	2.25	0.48
2:F:360:PRO:HD3	2:F:368:TYR:CE2	2.48	0.48
1:B:96:ASP:HB2	1:B:127:ARG:O	2.12	0.48
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.95	0.48
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.48	0.48
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.95	0.48
1:C:286:ARG:NH1	7:C:639:HOH:O	2.46	0.48
2:E:444:ILE:HD11	2:E:463:ILE:CD1	2.43	0.48
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:TYR:O	1:A:304:ARG:HG2	2.13	0.48
1:A:373:ARG:HG3	1:A:373:ARG:NH1	2.28	0.48
1:C:96:ASP:O	1:C:97:VAL:HG13	2.12	0.48
2:E:397:SER:C	2:E:399:GLU:H	2.20	0.48
1:A:166:LEU:HD13	1:A:342:VAL:HG12	1.95	0.48
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.78	0.48
1:C:245:LEU:O	1:C:246:ALA:C	2.56	0.48
2:E:253:LEU:O	2:E:306:SER:HA	2.14	0.48
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.49	0.48
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.48
1:A:444:VAL:CG1	1:A:469:LEU:HD13	2.44	0.48
1:B:40:ARG:NH1	7:B:632:HOH:O	2.27	0.48
1:B:351:PHE:HE1	1:B:369:LEU:O	1.96	0.48
1:B:481:GLY:O	1:B:485:THR:HB	2.14	0.48
2:D:83:ARG:HA	2:D:115:ALA:HA	1.95	0.48
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.44	0.48
2:E:326:PHE:HB3	7:E:496:HOH:O	2.13	0.48
2:E:374:VAL:O	2:E:377:ILE:HG22	2.14	0.48
2:E:404:VAL:O	2:E:408:ARG:HG3	2.14	0.48
2:F:467:VAL:O	2:F:470:ALA:HB3	2.14	0.48
1:B:311:LYS:HD2	1:B:312:MET:O	2.13	0.48
3:G:39:LYS:CB	3:G:40:PRO:CD	2.89	0.48
1:B:300:TYR:O	1:B:304:ARG:HG2	2.13	0.48
2:E:161:GLY:O	2:E:162:LYS:C	2.57	0.48
2:E:158:ALA:C	2:E:160:VAL:N	2.72	0.47
1:A:209:LYS:HE3	1:A:211:SER:CB	2.45	0.47
1:A:485:THR:HG22	1:A:486:ASP:N	2.29	0.47
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.14	0.47
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.79	0.47
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.34	0.47
1:C:481:GLY:O	1:C:485:THR:HB	2.14	0.47
2:D:32:ILE:O	2:D:33:LEU:HB2	2.14	0.47
2:E:54:GLY:O	2:E:55:GLU:HB2	2.13	0.47
2:F:36:LEU:N	2:F:36:LEU:HD23	2.30	0.47
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.79	0.47
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.96	0.47
2:D:14:VAL:HG11	2:D:24:GLN:HB2	1.95	0.47
2:F:44:ARG:NH2	7:F:653:HOH:O	2.39	0.47
1:B:389:THR:HA	1:B:392:LEU:HG	1.97	0.47
1:B:443:ALA:O	1:B:446:TYR:HB3	2.14	0.47
1:C:34:ILE:HD11	1:C:79:ASP:CB	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:GLN:O	1:C:445:ILE:HG12	2.15	0.47
2:D:129:GLU:OE1	2:D:129:GLU:HA	2.15	0.47
2:E:116:ILE:HA	2:E:238:THR:OG1	2.15	0.47
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.96	0.47
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.80	0.47
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.96	0.47
1:B:485:THR:O	1:B:486:ASP:C	2.58	0.47
1:C:292:GLU:O	1:C:293:ALA:CB	2.63	0.47
1:C:445:ILE:HG22	1:C:449:VAL:CG2	2.44	0.47
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.27	0.47
1:A:344:SER:O	2:E:222:MET:HE1	2.15	0.47
1:B:151:LYS:NZ	1:B:427:LEU:O	2.47	0.47
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.49	0.47
1:B:237:SER:CB	7:B:687:HOH:O	2.62	0.47
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.18	0.47
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.96	0.47
2:E:61:ILE:HG13	2:E:61:ILE:O	2.14	0.47
2:E:416:GLN:HG3	2:E:417:PRO:HD2	1.96	0.47
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.27	0.47
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.95	0.47
1:B:496:LYS:O	1:B:500:ILE:HG13	2.15	0.47
1:C:359:LYS:O	2:F:376:LYS:HE2	2.15	0.47
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.96	0.47
2:D:417:PRO:HA	2:D:459:MET:HE1	1.96	0.47
2:D:425:THR:HB	2:D:459:MET:HE2	1.96	0.47
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.45	0.47
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.47
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.47
2:F:409:LYS:HD3	2:F:457:PHE:HE2	1.78	0.47
1:B:83:LYS:HG2	7:B:631:HOH:O	2.15	0.47
2:D:368:TYR:CE1	2:D:372:ARG:HG3	2.50	0.47
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.50	0.47
2:F:93:ARG:NH2	2:F:106:GLY:O	2.48	0.47
3:G:210:ALA:O	3:G:213:ILE:N	2.47	0.47
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.27	0.47
1:B:269:ASP:HA	1:B:270:ASP:HA	1.78	0.47
2:D:393:MET:HE1	2:D:404:VAL:HG11	1.96	0.47
2:F:151:LYS:HD3	2:F:328:HIS:O	2.15	0.47
2:F:159:GLY:HA2	5:F:600:ANP:N3B	2.24	0.47
2:F:205:VAL:HG23	2:F:215:VAL:HG21	1.96	0.47
3:G:2:THR:O	3:G:3:LEU:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:22:SER:HA	3:G:25:MET:HE3	1.97	0.47
1:B:240:ALA:N	1:B:241:PRO:CD	2.77	0.46
1:C:485:THR:O	1:C:486:ASP:C	2.57	0.46
3:G:254:ARG:NH2	7:G:273:HOH:O	2.49	0.46
1:A:139:ARG:C	1:A:140:ILE:HG22	2.40	0.46
1:B:433:TYR:C	1:B:435:PRO:HD3	2.40	0.46
1:C:251:CYS:O	1:C:255:GLU:HG3	2.16	0.46
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.30	0.46
2:E:431:LEU:HD12	2:E:431:LEU:O	2.15	0.46
2:D:397:SER:O	2:D:398:GLU:C	2.58	0.46
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.98	0.46
2:F:319:ASP:O	2:F:322:PRO:HD2	2.14	0.46
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.45	0.46
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.14	0.46
2:F:81:PRO:O	2:F:82:ILE:C	2.58	0.46
2:F:200:MET:CG	2:F:206:ILE:HG12	2.45	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.98	0.46
1:A:51:GLU:OE2	1:A:90:ARG:HB3	2.16	0.46
1:A:485:THR:C	1:A:487:GLY:H	2.23	0.46
1:B:27:GLU:OE1	1:B:90:ARG:HD3	2.16	0.46
1:C:59:LEU:HD23	1:C:82:ILE:CD1	2.44	0.46
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.96	0.46
2:D:412:ARG:O	2:D:415:SER:OG	2.33	0.46
2:D:469:LYS:O	2:D:473:LEU:HG	2.15	0.46
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.46	0.46
1:A:52:MET:HE1	1:A:60:LYS:HD3	1.97	0.46
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.98	0.46
1:A:485:THR:C	1:A:487:GLY:N	2.73	0.46
1:B:179:ALA:O	1:B:182:THR:HB	2.14	0.46
1:C:91:THR:HG22	1:C:93:ALA:HB3	1.97	0.46
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.97	0.46
2:E:63:MET:CE	2:E:228:ALA:HA	2.45	0.46
2:E:120:ALA:HB1	2:E:121:PRO:HD2	1.98	0.46
1:A:376:SER:O	1:A:378:ALA:N	2.48	0.46
1:B:381:ARG:HG2	1:B:488:LYS:HG3	1.98	0.46
1:C:219:ARG:HD3	1:C:433:TYR:HE1	1.81	0.46
3:G:259:THR:O	3:G:263:ILE:HG13	2.16	0.46
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.97	0.46
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.98	0.46
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.31	0.46
2:E:77:ASP:C	2:E:79:GLY:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.50	0.46
2:F:243:PHE:O	2:F:249:GLN:HB2	2.16	0.46
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.98	0.46
1:A:403:PHE:O	1:A:404:ALA:C	2.59	0.46
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.31	0.46
2:E:425:THR:C	2:E:427:HIS:N	2.72	0.46
1:A:36:ASP:O	1:A:284:LEU:HD13	2.16	0.45
1:A:339:PRO:O	1:A:343:ILE:HG13	2.16	0.45
1:B:34:ILE:HD12	1:B:35:GLY:H	1.81	0.45
1:C:476:HIS:ND1	1:C:476:HIS:N	2.64	0.45
2:D:84:ILE:N	2:D:114:ALA:O	2.42	0.45
2:E:189:ARG:O	2:E:190:THR:C	2.58	0.45
2:E:340:ALA:O	2:E:343:GLY:N	2.42	0.45
3:G:210:ALA:O	3:G:211:ASN:C	2.59	0.45
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.45
1:B:284:LEU:HD21	2:E:274:ARG:HD3	1.97	0.45
2:E:343:GLY:O	2:E:345:TYR:HD1	1.99	0.45
2:E:432:VAL:HA	2:E:433:PRO:HD3	1.81	0.45
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.44	0.45
2:F:469:LYS:O	2:F:473:LEU:HG	2.16	0.45
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.45
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.98	0.45
1:C:400:VAL:HG22	7:C:698:HOH:O	2.15	0.45
1:C:432:GLN:O	1:C:433:TYR:HB2	2.16	0.45
7:C:687:HOH:O	2:D:198:HIS:HE1	1.99	0.45
2:D:397:SER:O	2:D:400:ASP:N	2.45	0.45
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.99	0.45
2:E:95:MET:HE2	2:E:99:GLY:CA	2.45	0.45
2:E:260:ARG:NH1	7:E:495:HOH:O	2.49	0.45
2:F:105:ARG:CZ	2:F:208:LEU:HD23	2.47	0.45
1:C:156:LEU:HD11	1:C:428:LEU:CD1	2.46	0.45
1:C:158:PRO:HB3	1:C:379:GLN:HG3	1.99	0.45
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.45
2:E:321:ALA:N	2:E:322:PRO:HD2	2.32	0.45
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.66	0.45
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.15	0.45
1:A:101:GLU:OE2	7:A:641:HOH:O	2.20	0.45
2:D:471:ASP:O	2:D:472:LYS:C	2.57	0.45
2:F:96:ASN:HB2	2:F:100:GLU:N	2.31	0.45
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.23	0.45
1:B:420:ARG:O	1:B:423:ARG:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.97	0.45
2:D:440:GLY:O	2:D:444:ILE:HG13	2.16	0.45
2:F:252:LEU:HD23	2:F:252:LEU:HA	1.81	0.45
3:G:234:ASN:HA	3:G:237:LYS:HB2	1.98	0.45
1:A:179:ALA:O	1:A:182:THR:HB	2.17	0.45
1:A:385:GLN:OE1	1:A:488:LYS:HB2	2.17	0.45
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.32	0.45
1:B:400:VAL:CG1	1:B:418:LEU:HD11	2.47	0.45
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.98	0.45
1:C:116:ASP:O	1:C:117:GLY:C	2.60	0.45
2:D:452:LEU:HD12	2:D:457:PHE:CZ	2.52	0.45
1:B:48:GLN:HB3	2:F:68:GLY:HA2	1.97	0.45
1:B:271:LEU:HD12	1:B:325:PRO:HB2	1.98	0.45
1:C:177:SER:O	1:C:178:ILE:C	2.60	0.45
2:D:461:GLY:HA3	2:D:462:PRO:HD3	1.74	0.45
2:E:35:ALA:HB2	2:E:82:ILE:HG13	1.99	0.45
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.31	0.45
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.98	0.45
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.52	0.45
1:A:142:VAL:HG22	1:A:161:ARG:O	2.16	0.45
1:A:270:ASP:OD2	7:A:625:HOH:O	2.20	0.45
1:A:413:ALA:O	1:A:416:GLN:HB3	2.17	0.45
1:C:489:ILE:HG22	1:C:494:ASP:HB2	1.99	0.45
2:D:130:GLN:HE22	2:D:356:ARG:HD3	1.81	0.45
2:E:146:TYR:O	2:E:357:ILE:HD11	2.16	0.45
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.98	0.45
1:A:24:ASP:OD1	1:A:24:ASP:C	2.60	0.45
1:B:212:THR:O	1:B:216:LEU:HB2	2.18	0.45
2:D:35:ALA:HB1	2:D:46:VAL:CG1	2.47	0.45
2:D:170:ILE:O	2:D:174:ALA:HB3	2.17	0.45
2:D:298:THR:HG23	2:D:303:SER:HA	1.98	0.45
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.45
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.17	0.45
1:B:423:ARG:HE	1:B:458:PRO:CG	2.31	0.44
1:B:465:GLU:O	1:B:469:LEU:HB2	2.17	0.44
2:D:231:ARG:O	2:D:232:VAL:C	2.60	0.44
2:E:422:GLU:C	2:E:424:PHE:N	2.74	0.44
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.73	0.44
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.99	0.44
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.99	0.44
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:HIS:ND1	1:A:475:GLN:HG3	2.33	0.44
2:E:388:ILE:HG23	2:E:393:MET:CG	2.43	0.44
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.99	0.44
1:A:251:CYS:O	1:A:255:GLU:HG3	2.18	0.44
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.00	0.44
1:C:474:SER:OG	1:C:475:GLN:N	2.49	0.44
2:D:63:MET:HE1	2:D:231:ARG:HB2	1.99	0.44
2:D:289:MET:SD	2:D:324:THR:HG22	2.56	0.44
2:D:470:ALA:O	2:D:474:ALA:N	2.51	0.44
2:E:402:LEU:O	2:E:406:ARG:HG3	2.16	0.44
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.17	0.44
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.44
2:D:190:THR:O	2:D:191:ARG:C	2.60	0.44
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.52	0.44
2:F:319:ASP:O	2:F:320:PRO:C	2.60	0.44
3:G:82:HIS:CD2	3:G:82:HIS:N	2.85	0.44
1:A:151:LYS:H	1:A:151:LYS:HG2	1.67	0.44
1:A:180:ILE:O	1:A:181:ASP:C	2.56	0.44
1:A:482:LYS:O	1:A:483:ILE:C	2.61	0.44
1:B:45:ARG:HH11	1:B:45:ARG:HD3	1.53	0.44
1:B:300:TYR:HA	1:B:303:SER:OG	2.17	0.44
2:D:209:LYS:HA	2:D:209:LYS:HD3	1.83	0.44
2:D:366:GLU:O	2:D:370:VAL:HG23	2.17	0.44
2:E:114:ALA:HB3	2:E:238:THR:CG2	2.47	0.44
2:E:433:PRO:HG2	2:E:436:GLU:CG	2.48	0.44
2:F:188:GLU:H	2:F:221:GLN:NE2	2.15	0.44
1:A:166:LEU:HD13	1:A:342:VAL:CG1	2.47	0.44
7:B:624:HOH:O	2:F:198:HIS:HE1	1.99	0.44
1:C:193:THR:O	1:C:195:GLU:OE1	2.36	0.44
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.99	0.44
2:D:425:THR:HG21	2:D:459:MET:HE1	1.99	0.44
2:E:405:SER:OG	2:E:406:ARG:N	2.49	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.18	0.44
1:A:492:GLU:C	1:A:494:ASP:N	2.73	0.44
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.99	0.44
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.44
2:D:93:ARG:NH1	2:D:108:ILE:HG12	2.33	0.44
2:E:105:ARG:NE	2:E:208:LEU:HD23	2.33	0.44
2:E:231:ARG:O	2:E:232:VAL:C	2.60	0.44
2:E:77:ASP:CG	2:E:79:GLY:H	2.24	0.44
2:E:443:GLN:HA	2:E:446:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:50:ALA:O	2:F:51:GLN:HB3	2.17	0.44
2:F:407:ALA:O	2:F:411:GLN:HB2	2.18	0.44
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.99	0.44
1:B:213:VAL:O	1:B:217:VAL:HG13	2.18	0.44
1:C:45:ARG:HD3	1:C:45:ARG:HA	1.29	0.44
1:C:172:GLN:HA	5:C:600:ANP:N3B	2.32	0.44
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.99	0.44
2:D:108:ILE:HG22	2:D:110:THR:HG23	2.00	0.44
1:A:460:LYS:N	1:A:460:LYS:HD2	2.32	0.43
1:C:390:MET:HE1	1:C:428:LEU:HD21	1.99	0.43
2:E:72:GLY:O	2:E:73:GLN:C	2.60	0.43
2:F:126:MET:HE3	7:F:638:HOH:O	2.17	0.43
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.83	0.43
1:A:379:GLN:HB2	1:A:384:LYS:HE3	2.00	0.43
1:B:434:SER:N	1:B:435:PRO:CD	2.82	0.43
1:C:180:ILE:O	1:C:181:ASP:C	2.62	0.43
1:C:353:GLU:O	1:C:364:ALA:HB1	2.19	0.43
2:D:38:VAL:HG11	2:D:69:LEU:CD2	2.48	0.43
2:D:462:PRO:HD2	2:D:465:GLU:HG3	2.00	0.43
1:A:209:LYS:HZ1	2:D:330:ASP:CG	2.26	0.43
1:B:294:TYR:CE2	1:B:338:ILE:HD13	2.53	0.43
1:C:457:GLU:O	1:C:458:PRO:C	2.62	0.43
2:D:103:ASP:O	2:D:104:GLU:HB2	2.18	0.43
2:D:189:ARG:O	2:D:192:GLU:HB2	2.18	0.43
2:E:67:GLU:H	2:E:67:GLU:HG3	1.16	0.43
2:F:31:PRO:O	2:F:34:ASN:HB2	2.18	0.43
1:A:55:PHE:O	1:A:56:SER:C	2.61	0.43
1:A:136:ILE:HG22	7:A:608:HOH:O	2.19	0.43
1:A:151:LYS:HE2	1:A:427:LEU:O	2.17	0.43
1:C:269:ASP:HA	1:C:270:ASP:HA	1.79	0.43
1:C:311:LYS:HE3	1:C:318:GLY:O	2.17	0.43
2:E:85:PRO:HD2	2:E:95:MET:CE	2.46	0.43
2:E:397:SER:O	2:E:398:GLU:C	2.62	0.43
2:F:136:GLY:HA3	2:F:431:LEU:HD11	1.99	0.43
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.47	0.43
1:C:32:LEU:HD21	1:C:42:HIS:HB2	2.00	0.43
1:C:49:ALA:O	1:C:50:GLU:HB2	2.19	0.43
1:C:107:VAL:O	1:C:115:ILE:HG12	2.18	0.43
1:C:209:LYS:HE3	1:C:211:SER:OG	2.18	0.43
1:C:303:SER:HB2	2:D:222:MET:HB3	1.99	0.43
1:C:340:THR:O	1:C:341:ASN:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.48	0.43
1:A:224:ASP:HA	7:A:616:HOH:O	2.19	0.43
1:B:400:VAL:HG12	1:B:418:LEU:HD11	2.00	0.43
1:B:438:ILE:HD12	1:B:438:ILE:HA	1.87	0.43
1:C:128:ARG:NH1	7:C:694:HOH:O	2.50	0.43
2:D:231:ARG:O	2:D:234:LEU:N	2.50	0.43
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.33	0.43
2:E:21:VAL:O	2:E:60:THR:OG1	2.35	0.43
1:A:48:GLN:HA	2:E:69:LEU:O	2.18	0.43
1:B:389:THR:HA	1:B:392:LEU:CG	2.48	0.43
1:C:285:LEU:C	1:C:286:ARG:HG2	2.43	0.43
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.49	0.43
2:D:400:ASP:O	2:D:404:VAL:HG23	2.18	0.43
1:A:52:MET:CG	1:A:95:VAL:HG22	2.48	0.43
1:C:90:ARG:HE	1:C:90:ARG:HB3	1.61	0.43
2:E:242:TYR:C	2:E:242:TYR:CD1	2.97	0.43
2:E:376:LYS:O	2:E:379:GLN:HB2	2.19	0.43
2:E:409:LYS:HZ2	2:E:450:ASP:HA	1.83	0.43
2:F:385:GLN:HA	2:F:388:ILE:HG12	2.01	0.43
1:A:99:VAL:HG23	1:A:253:MET:HA	2.01	0.43
1:B:55:PHE:O	1:B:56:SER:C	2.61	0.43
1:C:51:GLU:HG2	1:C:52:MET:N	2.33	0.43
1:C:164:ARG:HD2	1:C:164:ARG:HH11	1.41	0.43
2:F:95:MET:HG3	2:F:99:GLY:HA2	2.00	0.43
2:F:439:LYS:HG2	2:F:443:GLN:NE2	2.33	0.43
3:G:209:LEU:O	3:G:212:ILE:N	2.51	0.43
1:B:385:GLN:NE2	1:B:489:ILE:HB	2.34	0.42
1:C:185:ASN:HB2	1:C:435:PRO:HB3	2.00	0.42
1:C:187:LYS:O	1:C:188:ARG:C	2.62	0.42
2:E:89:GLU:HG2	2:E:110:THR:CG2	2.39	0.42
1:B:65:ASN:HD22	2:F:17:ILE:CG1	2.33	0.42
1:B:389:THR:HG22	1:B:392:LEU:HD12	2.00	0.42
1:C:139:ARG:HB3	1:C:311:LYS:O	2.19	0.42
2:D:266:SER:CB	2:D:282:GLN:NE2	2.82	0.42
2:E:95:MET:HE2	2:E:99:GLY:HA2	2.01	0.42
2:E:136:GLY:HA2	2:E:432:VAL:O	2.18	0.42
2:E:189:ARG:HB2	2:E:192:GLU:HG3	2.02	0.42
2:E:441:PHE:O	2:E:445:LEU:HG	2.19	0.42
1:A:96:ASP:HA	1:A:128:ARG:HA	2.01	0.42
1:B:249:SER:O	1:B:250:GLY:C	2.61	0.42
1:C:442:VAL:HG11	1:C:489:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:MET:HE2	2:D:235:THR:CG2	2.49	0.42
2:D:345:TYR:HB3	6:D:600:ADP:C6	2.54	0.42
2:E:166:ILE:O	2:E:170:ILE:HG13	2.18	0.42
2:F:196:LEU:O	2:F:200:MET:HB2	2.19	0.42
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.52	0.42
1:C:169:GLY:O	1:C:175:LYS:HE2	2.18	0.42
2:E:97:VAL:HG13	2:E:232:VAL:HG12	2.02	0.42
2:F:122:GLU:OE1	2:F:122:GLU:HA	2.19	0.42
2:F:400:ASP:O	2:F:404:VAL:HG23	2.20	0.42
3:G:213:ILE:HD13	3:G:213:ILE:HA	1.89	0.42
3:G:254:ARG:O	3:G:258:ILE:HG13	2.20	0.42
1:A:78:ASN:ND2	1:A:80:LYS:HD2	2.34	0.42
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.42
1:C:331:ALA:O	1:C:332:GLY:C	2.63	0.42
2:E:32:ILE:O	2:E:33:LEU:CB	2.68	0.42
2:E:256:ASP:HA	2:E:257:ASN:HA	1.64	0.42
1:A:347:ASP:C	1:A:373:ARG:HH11	2.28	0.42
1:B:218:LYS:HB2	2:E:128:VAL:CG1	2.44	0.42
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.54	0.42
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.50	0.42
2:E:280:GLY:HA2	3:G:262:LEU:HD21	2.01	0.42
2:E:439:LYS:O	2:E:440:GLY:C	2.61	0.42
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.50	0.42
1:B:165:GLU:O	1:B:325:PRO:HD2	2.19	0.42
1:B:175:LYS:NZ	7:B:655:HOH:O	2.21	0.42
1:B:357:PHE:HZ	5:B:600:ANP:O4'	2.02	0.42
1:C:105:GLY:N	1:C:229:THR:O	2.41	0.42
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.50	0.42
2:D:406:ARG:HH11	2:D:406:ARG:HD2	1.60	0.42
2:D:412:ARG:NH1	7:D:696:HOH:O	2.40	0.42
2:E:95:MET:HA	2:E:100:GLU:O	2.20	0.42
2:F:144:ALA:N	2:F:145:PRO:CD	2.82	0.42
2:F:357:ILE:HD13	2:F:357:ILE:HA	1.80	0.42
1:A:32:LEU:HD21	1:A:42:HIS:HB2	2.02	0.42
1:A:338:ILE:N	1:A:339:PRO:CD	2.83	0.42
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.54	0.42
1:B:107:VAL:HG12	1:B:115:ILE:HD11	2.00	0.42
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.42
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.42
1:C:467:ALA:O	1:C:470:SER:HB2	2.20	0.42
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:LEU:HD22	2:E:335:LEU:HD21	2.02	0.42
2:E:182:VAL:HG21	2:E:240:ALA:HB2	2.01	0.42
2:F:251:VAL:HG12	2:F:252:LEU:N	2.35	0.42
1:A:294:TYR:HB2	1:A:337:TYR:CE2	2.54	0.42
1:A:340:THR:O	1:A:344:SER:HB3	2.19	0.42
1:A:390:MET:HE1	1:A:428:LEU:HD21	2.02	0.42
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.35	0.42
2:D:396:LEU:HD22	2:D:400:ASP:HB2	2.00	0.42
2:D:401:LYS:H	2:D:401:LYS:HG2	1.72	0.42
2:E:412:ARG:NH1	2:E:454:GLU:OE1	2.53	0.42
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.42
2:F:438:ILE:H	2:F:438:ILE:HG12	1.73	0.42
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.88	0.42
1:B:94:ILE:O	1:B:95:VAL:C	2.61	0.42
1:B:273:LYS:HB3	7:B:676:HOH:O	2.19	0.42
1:C:345:ILE:HA	2:D:222:MET:HE1	2.02	0.42
1:C:392:LEU:HB3	2:D:458:TYR:OH	2.20	0.42
2:D:94:ILE:HG22	2:D:102:ILE:HD11	2.01	0.42
2:E:185:GLY:HA3	2:E:188:GLU:HG3	2.02	0.42
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.42
2:E:396:LEU:CB	2:E:401:LYS:HG2	2.50	0.42
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.49	0.42
2:F:471:ASP:O	2:F:474:ALA:N	2.53	0.42
1:A:356:LEU:O	1:A:357:PHE:C	2.63	0.41
1:B:99:VAL:HG13	1:B:256:TYR:HB2	2.02	0.41
2:D:95:MET:HE3	2:D:99:GLY:HA2	2.02	0.41
2:D:96:ASN:HB2	2:D:100:GLU:N	2.27	0.41
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.01	0.41
2:D:475:GLU:OE1	2:D:475:GLU:HA	2.20	0.41
2:E:139:VAL:HG21	2:E:348:VAL:HB	2.02	0.41
2:E:231:ARG:O	2:E:234:LEU:N	2.50	0.41
2:E:349:ASP:HA	2:E:350:PRO:HD2	1.86	0.41
3:G:10:LEU:O	3:G:14:LYS:HG3	2.20	0.41
3:G:217:LEU:O	3:G:221:THR:HG23	2.20	0.41
1:A:210:ARG:HG3	2:D:294:GLU:OE2	2.20	0.41
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.41
2:E:425:THR:C	2:E:427:HIS:H	2.28	0.41
3:G:38:LEU:O	3:G:39:LYS:C	2.62	0.41
1:A:238:ASP:HA	7:A:677:HOH:O	2.19	0.41
1:A:267:ILE:HA	1:A:324:LEU:O	2.20	0.41
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.41
2:D:63:MET:CE	2:D:97:VAL:HG11	2.51	0.41
2:D:203:SER:OG	2:D:205:VAL:HG23	2.21	0.41
2:E:360:PRO:HD3	2:E:368:TYR:CG	2.56	0.41
2:E:434:LEU:O	2:E:437:THR:HB	2.21	0.41
3:G:13:ILE:HD13	3:G:242:MET:HG2	2.02	0.41
1:A:383:MET:O	1:A:386:VAL:HG23	2.19	0.41
1:B:36:ASP:OD1	2:E:274:ARG:NE	2.53	0.41
1:B:255:GLU:HG2	1:B:258:ARG:CZ	2.49	0.41
1:B:361:ILE:HD13	1:B:429:LYS:HE2	2.02	0.41
1:C:290:GLY:O	1:C:291:ARG:C	2.61	0.41
1:C:299:PHE:O	1:C:300:TYR:C	2.62	0.41
1:C:423:ARG:HD2	1:C:461:ILE:HD11	2.03	0.41
2:D:139:VAL:O	2:D:140:VAL:C	2.63	0.41
2:D:449:TYR:C	2:D:451:HIS:H	2.28	0.41
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.02	0.41
2:E:388:ILE:HD12	2:E:396:LEU:HD11	2.01	0.41
2:F:47:LEU:HD23	2:F:62:ALA:HA	2.01	0.41
2:F:442:GLN:O	2:F:445:LEU:HB2	2.21	0.41
3:G:209:LEU:HB3	3:G:210:ALA:H	1.60	0.41
1:A:103:LEU:O	1:A:106:ARG:HB2	2.20	0.41
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.41
1:C:224:ASP:OD1	1:C:227:LYS:HE3	2.19	0.41
2:D:38:VAL:HG22	2:D:75:VAL:HG22	2.02	0.41
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.41
2:D:433:PRO:HG2	2:D:436:GLU:CG	2.45	0.41
2:F:423:VAL:O	2:F:423:VAL:HG12	2.20	0.41
1:A:206:ILE:O	1:A:273:LYS:HD2	2.20	0.41
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.35	0.41
1:B:290:GLY:O	1:B:291:ARG:C	2.64	0.41
2:D:281:TYR:CD2	2:D:320:PRO:HG2	2.56	0.41
2:D:360:PRO:HD3	2:D:368:TYR:CD2	2.56	0.41
2:D:449:TYR:C	2:D:451:HIS:N	2.78	0.41
2:E:88:PRO:C	2:E:90:THR:H	2.28	0.41
1:A:407:GLY:CA	1:A:410:LEU:HD21	2.48	0.41
1:B:340:THR:O	1:B:341:ASN:C	2.63	0.41
1:C:142:VAL:C	1:C:143:ARG:HG3	2.46	0.41
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.21	0.41
2:D:112:GLN:NE2	2:D:242:TYR:CE1	2.88	0.41
2:E:35:ALA:C	2:E:36:LEU:HD23	2.46	0.41
2:E:227:GLY:O	2:E:231:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:366:GLU:O	2:E:367:HIS:C	2.63	0.41
2:F:238:THR:O	2:F:239:VAL:C	2.64	0.41
1:A:136:ILE:HD11	2:E:219:TYR:HE2	1.86	0.41
1:A:383:MET:HG3	1:A:387:ALA:HB2	2.02	0.41
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.86	0.41
1:C:362:ARG:HG3	1:C:362:ARG:HH11	1.86	0.41
2:D:35:ALA:HB1	2:D:46:VAL:HG13	2.02	0.41
2:D:112:GLN:NE2	2:D:242:TYR:HE1	2.18	0.41
2:E:359:ASP:O	2:E:362:ILE:N	2.45	0.41
2:E:410:ILE:O	2:E:411:GLN:C	2.63	0.41
1:A:294:TYR:CE2	1:A:338:ILE:HD13	2.56	0.41
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.41
1:B:201:CYS:O	1:B:229:THR:HA	2.21	0.41
1:B:209:LYS:HE3	2:E:151:LYS:HZ3	1.86	0.41
1:B:300:TYR:O	1:B:301:LEU:C	2.64	0.41
1:B:382:ALA:HB1	1:B:442:VAL:HG11	2.02	0.41
1:C:104:LEU:HD21	1:C:257:PHE:CZ	2.56	0.41
1:C:143:ARG:HD2	7:C:641:HOH:O	2.19	0.41
1:C:330:GLN:O	1:C:331:ALA:C	2.64	0.41
1:C:465:GLU:O	1:C:465:GLU:HG2	2.21	0.41
2:D:63:MET:CE	2:D:228:ALA:HA	2.50	0.41
2:D:84:ILE:HB	2:D:95:MET:HE3	2.02	0.41
2:D:86:VAL:HG11	2:D:114:ALA:HB3	2.02	0.41
2:D:402:LEU:O	2:D:406:ARG:HG3	2.21	0.41
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.51	0.41
2:E:397:SER:O	2:E:399:GLU:N	2.54	0.41
2:F:258:ILE:HD11	2:F:292:MET:HE1	2.03	0.41
3:G:42:ARG:HG2	3:G:219:GLU:OE2	2.20	0.41
1:A:422:VAL:O	1:A:426:GLU:HG2	2.21	0.41
1:A:441:GLN:O	1:A:445:ILE:HG12	2.21	0.41
1:B:353:GLU:OE2	1:B:366:ASN:ND2	2.50	0.41
1:C:19:ALA:O	1:C:21:THR:HG23	2.21	0.41
1:C:289:PRO:HB2	7:C:618:HOH:O	2.21	0.41
1:C:485:THR:C	1:C:487:GLY:N	2.76	0.41
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.03	0.41
2:D:64:ASP:CG	2:D:65:GLY:H	2.28	0.41
2:E:105:ARG:NH1	2:E:208:LEU:HD23	2.36	0.41
2:E:387:ILE:HG22	2:E:388:ILE:HD13	2.02	0.41
1:A:74:VAL:CG1	1:A:241:PRO:HG3	2.51	0.40
1:A:147:GLN:OE1	1:A:438:ILE:HD13	2.21	0.40
1:A:268:TYR:HB2	1:A:325:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HA	1:B:234:ALA:O	2.21	0.40
1:B:450:ARG:HA	1:B:450:ARG:HD3	1.87	0.40
2:D:97:VAL:HG11	2:D:231:ARG:HB2	2.03	0.40
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.40
2:E:167:MET:SD	2:E:200:MET:HA	2.61	0.40
2:F:289:MET:HE3	2:F:289:MET:HB2	1.73	0.40
1:A:56:SER:O	1:A:58:GLY:N	2.53	0.40
1:A:105:GLY:HA2	1:A:226:MET:O	2.21	0.40
1:A:398:ARG:HH11	1:A:398:ARG:HD2	1.53	0.40
1:B:336:ALA:HB3	1:B:339:PRO:HD2	2.02	0.40
1:B:344:SER:HA	5:F:600:ANP:O3G	2.21	0.40
1:C:313:ASN:OD1	1:C:313:ASN:C	2.65	0.40
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.56	0.40
2:D:349:ASP:HA	2:D:350:PRO:HD2	1.85	0.40
2:E:167:MET:C	2:E:420:VAL:HG21	2.47	0.40
2:E:282:GLN:H	2:E:282:GLN:NE2	2.19	0.40
2:F:38:VAL:HG11	2:F:69:LEU:CD2	2.50	0.40
3:G:2:THR:HB	3:G:5:ASP:CG	2.46	0.40
1:A:180:ILE:HD11	1:A:216:LEU:CD2	2.52	0.40
1:A:444:VAL:HG12	1:A:469:LEU:HD13	2.03	0.40
1:A:506:ALA:O	1:A:507:GLY:C	2.63	0.40
1:B:221:THR:HG22	1:B:222:ASP:N	2.36	0.40
1:B:239:ALA:HB1	1:B:241:PRO:HD2	2.03	0.40
1:C:384:LYS:HB2	1:C:384:LYS:HE3	1.94	0.40
1:C:390:MET:HE2	1:C:428:LEU:HD11	2.02	0.40
2:D:84:ILE:HB	2:D:85:PRO:HD2	2.04	0.40
2:E:413:PHE:HE2	2:E:440:GLY:HA3	1.87	0.40
2:E:454:GLU:C	2:E:456:ALA:N	2.80	0.40
1:B:363:PRO:C	1:B:365:ILE:H	2.30	0.40
1:B:382:ALA:O	1:B:385:GLN:HB2	2.22	0.40
1:C:43:GLY:O	1:C:44:LEU:C	2.65	0.40
2:D:27:GLU:H	2:D:27:GLU:HG3	1.77	0.40
2:D:256:ASP:HA	2:D:257:ASN:HA	1.87	0.40
2:E:35:ALA:HB1	2:E:46:VAL:CG1	2.52	0.40
2:E:387:ILE:HG22	2:E:388:ILE:N	2.36	0.40
2:E:416:GLN:NE2	2:E:430:LYS:O	2.55	0.40
2:F:228:ALA:O	2:F:232:VAL:HG22	2.21	0.40
1:A:69:ASP:O	1:A:70:ASN:HB3	2.21	0.40
1:A:408:SER:O	1:A:409:ASP:HB2	2.20	0.40
1:C:342:VAL:HA	1:C:345:ILE:HD12	2.03	0.40
2:E:454:GLU:C	2:E:456:ALA:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:357:ILE:O	2:F:359:ASP:N	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	485/510 (95%)	442 (91%)	36 (7%)	7 (1%)	9	19
1	B	485/510 (95%)	435 (90%)	43 (9%)	7 (1%)	9	19
1	C	490/510 (96%)	444 (91%)	38 (8%)	8 (2%)	7	17
2	D	465/482 (96%)	419 (90%)	43 (9%)	3 (1%)	21	38
2	E	464/482 (96%)	408 (88%)	47 (10%)	9 (2%)	6	14
2	F	464/482 (96%)	432 (93%)	30 (6%)	2 (0%)	30	48
3	G	116/272 (43%)	97 (84%)	18 (16%)	1 (1%)	14	28
All	All	2969/3248 (91%)	2677 (90%)	255 (9%)	37 (1%)	10	22

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	393	MET
1	A	57	SER
1	A	405	GLN
1	A	409	ASP
1	B	364	ALA
1	C	332	GLY
1	C	408	SER
1	C	411	ASP
1	C	476	HIS

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Mol	Chain	Res	Type
2	D	28	GLY
2	E	161	GLY
2	E	205	VAL
3	G	81	ILE
1	A	364	ALA
1	A	404	ALA
1	B	236	ALA
1	B	452	TYR
2	E	121	PRO
2	E	455	GLN
1	B	411	ASP
1	C	405	GLN
1	C	475	GLN
2	D	474	ALA
2	E	122	GLU
2	F	327	ALA
1	A	484	ARG
1	B	359	LYS
1	C	409	ASP
2	E	33	LEU
1	B	458	PRO
2	E	28	GLY
2	E	279	VAL
1	B	68	PRO
2	F	279	VAL
2	D	279	VAL
1	A	246	ALA

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	393/412 (95%)	343 (87%)	50 (13%)	4	8
1	B	393/412 (95%)	340 (86%)	53 (14%)	4	7
1	C	397/412 (96%)	359 (90%)	38 (10%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	377/386 (98%)	344 (91%)	33 (9%)	9	20
2	E	376/386 (97%)	335 (89%)	41 (11%)	6	12
2	F	376/386 (97%)	343 (91%)	33 (9%)	9	20
3	G	102/230 (44%)	90 (88%)	12 (12%)	5	10
All	All	2414/2624 (92%)	2154 (89%)	260 (11%)	6	12

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	40	ARG
1	A	45	ARG
1	A	47	VAL
1	A	48	GLN
1	A	50	GLU
1	A	56	SER
1	A	80	LYS
1	A	94	ILE
1	A	99	VAL
1	A	101	GLU
1	A	102	GLU
1	A	121	ILE
1	A	140	ILE
1	A	142	VAL
1	A	143	ARG
1	A	151	LYS
1	A	173	THR
1	A	188	ARG
1	A	193	THR
1	A	195	GLU
1	A	211	SER
1	A	219	ARG
1	A	256	TYR
1	A	270	ASP
1	A	344	SER
1	A	367	VAL
1	A	371	VAL
1	A	380	THR
1	A	386	VAL
1	A	393	GLU
1	A	409	ASP

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Mol	Chain	Res	Type
1	A	410	LEU
1	A	417	LEU
1	A	420	ARG
1	A	430	GLN
1	A	436	MET
1	A	442	VAL
1	A	444	VAL
1	A	449	VAL
1	A	457	GLU
1	A	461	ILE
1	A	472	VAL
1	A	473	ILE
1	A	474	SER
1	A	479	LEU
1	A	485	THR
1	A	489	ILE
1	A	497	LEU
1	A	499	GLU
1	B	38	ILE
1	B	47	VAL
1	B	60	LYS
1	B	79	ASP
1	B	80	LYS
1	B	87	ILE
1	B	99	VAL
1	B	102	GLU
1	B	123	SER
1	B	141	SER
1	B	143	ARG
1	B	173	THR
1	B	186	GLN
1	B	188	ARG
1	B	193	THR
1	B	195	GLU
1	B	211	SER
1	B	216	LEU
1	B	217	VAL
1	B	218	LYS
1	B	221	THR
1	B	227	LYS
1	B	233	SER
1	B	270	ASP

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Mol	Chain	Res	Type
1	B	298	VAL
1	B	327	ILE
1	B	334	VAL
1	B	335	SER
1	B	349	GLN
1	B	351	PHE
1	B	361	ILE
1	B	371	VAL
1	B	374	VAL
1	B	376	SER
1	B	380	THR
1	B	381	ARG
1	B	398	ARG
1	B	399	GLU
1	B	400	VAL
1	B	416	GLN
1	B	423	ARG
1	B	430	GLN
1	B	442	VAL
1	B	444	VAL
1	B	454	ASP
1	B	472	VAL
1	B	474	SER
1	B	479	LEU
1	B	482	LYS
1	B	484	ARG
1	B	485	THR
1	B	490	SER
1	B	505	LEU
1	C	45	ARG
1	C	47	VAL
1	C	56	SER
1	C	63	SER
1	C	64	LEU
1	C	74	VAL
1	C	87	ILE
1	C	91	THR
1	C	99	VAL
1	C	101	GLU
1	C	164	ARG
1	C	184	ILE
1	C	195	GLU

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Mol	Chain	Res	Type
1	C	208	GLN
1	C	216	LEU
1	C	217	VAL
1	C	227	LYS
1	C	267	ILE
1	C	270	ASP
1	C	282	SER
1	C	298	VAL
1	C	334	VAL
1	C	338	ILE
1	C	339	PRO
1	C	349	GLN
1	C	399	GLU
1	C	400	VAL
1	C	406	PHE
1	C	440	GLU
1	C	444	VAL
1	C	469	LEU
1	C	474	SER
1	C	477	GLN
1	C	479	LEU
1	C	485	THR
1	C	501	VAL
1	C	502	THR
1	C	505	LEU
2	D	27	GLU
2	D	37	GLU
2	D	56	SER
2	D	67	GLU
2	D	89	GLU
2	D	95	MET
2	D	97	VAL
2	D	112	GLN
2	D	137	ILE
2	D	139	VAL
2	D	166	ILE
2	D	199	GLU
2	D	205	VAL
2	D	223	ASN
2	D	232	VAL
2	D	249	GLN
2	D	258	ILE

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Mol	Chain	Res	Type
2	D	266	SER
2	D	279	VAL
2	D	282	GLN
2	D	306	SER
2	D	336	SER
2	D	361	ASN
2	D	365	SER
2	D	388	ILE
2	D	397	SER
2	D	401	LYS
2	D	423	VAL
2	D	428	LEU
2	D	431	LEU
2	D	439	LYS
2	D	452	LEU
2	D	475	GLU
2	E	9	THR
2	E	36	LEU
2	E	67	GLU
2	E	89	GLU
2	E	95	MET
2	E	97	VAL
2	E	119	GLU
2	E	127	SER
2	E	128	VAL
2	E	132	ILE
2	E	133	LEU
2	E	139	VAL
2	E	142	LEU
2	E	148	LYS
2	E	164	VAL
2	E	182	VAL
2	E	188	GLU
2	E	194	ASN
2	E	213	SER
2	E	215	VAL
2	E	223	ASN
2	E	257	ASN
2	E	282	GLN
2	E	293	GLN
2	E	297	THR
2	E	333	THR

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Mol	Chain	Res	Type
2	E	358	MET
2	E	365	SER
2	E	385	GLN
2	E	387	ILE
2	E	391	LEU
2	E	393	MET
2	E	394	ASP
2	E	395	GLU
2	E	402	LEU
2	E	412	ARG
2	E	431	LEU
2	E	438	ILE
2	E	452	LEU
2	E	463	ILE
2	E	473	LEU
2	F	10	THR
2	F	27	GLU
2	F	36	LEU
2	F	42	GLU
2	F	67	GLU
2	F	89	GLU
2	F	95	MET
2	F	97	VAL
2	F	112	GLN
2	F	137	ILE
2	F	139	VAL
2	F	166	ILE
2	F	191	ARG
2	F	200	MET
2	F	201	ILE
2	F	210	ASP
2	F	223	ASN
2	F	232	VAL
2	F	279	VAL
2	F	292	MET
2	F	357	ILE
2	F	386	ASP
2	F	387	ILE
2	F	393	MET
2	F	397	SER
2	F	405	SER
2	F	410	ILE

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Mol	Chain	Res	Type
2	F	423	VAL
2	F	428	LEU
2	F	435	LYS
2	F	438	ILE
2	F	455	GLN
2	F	467	VAL
3	G	4	LYS
3	G	11	LYS
3	G	13	ILE
3	G	20	THR
3	G	22	SER
3	G	77	LEU
3	G	82	HIS
3	G	85	VAL
3	G	209	LEU
3	G	214	TYR
3	G	221	THR
3	G	254	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	349	GLN
1	A	396	GLN
1	A	476	HIS
1	B	42	HIS
1	B	65	ASN
1	B	70	ASN
1	B	415	GLN
1	B	466	ASN
1	C	48	GLN
1	C	172	GLN
1	C	208	GLN
1	C	215	GLN
1	C	260	ASN
1	C	416	GLN
2	D	24	GLN
2	D	130	GLN
2	D	198	HIS
2	D	221	GLN
2	D	223	ASN

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Mol	Chain	Res	Type
2	D	282	GLN
2	D	411	GLN
2	D	442	GLN
2	E	39	GLN
2	E	51	GLN
2	E	130	GLN
2	E	223	ASN
2	E	246	GLN
2	E	282	GLN
2	F	51	GLN
2	F	194	ASN
2	F	198	HIS
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	293	GLN
2	F	308	GLN
2	F	361	ASN
2	F	443	GLN
3	G	82	HIS
3	G	211	ASN
3	G	225	GLN

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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
5	ANP	F	600	4	33,33,33	1.14	3 (9%)	45,52,52	1.22	3 (6%)
6	ADP	D	600	4	28,29,29	0.91	1 (3%)	43,45,45	1.20	4 (9%)
5	ANP	A	600	4	33,33,33	1.21	3 (9%)	45,52,52	0.90	3 (6%)
5	ANP	C	600	4	33,33,33	1.58	5 (15%)	45,52,52	1.35	8 (17%)
5	ANP	B	600	4	33,33,33	1.24	4 (12%)	45,52,52	1.35	7 (15%)

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
5	ANP	F	600	4	-	5/18/38/38	0/3/3/3
6	ADP	D	600	4	-	2/16/32/32	0/3/3/3
5	ANP	A	600	4	-	3/18/38/38	0/3/3/3
5	ANP	C	600	4	-	7/18/38/38	0/3/3/3
5	ANP	B	600	4	-	2/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	600	ANP	PG-O3G	-4.54	1.44	1.56
5	B	600	ANP	PG-O2G	-3.66	1.47	1.56
5	C	600	ANP	PB-O3A	3.61	1.63	1.59
5	A	600	ANP	PG-O3G	-3.51	1.47	1.56
5	C	600	ANP	PB-O2B	-3.49	1.47	1.56
5	C	600	ANP	PA-O3A	3.40	1.63	1.59
5	F	600	ANP	PG-O3G	-3.19	1.48	1.56
5	A	600	ANP	PB-O2B	-2.78	1.49	1.56
5	F	600	ANP	PG-O1G	2.46	1.49	1.46
5	A	600	ANP	C2-N1	2.43	1.38	1.33
5	B	600	ANP	PG-O3G	-2.37	1.50	1.56
5	B	600	ANP	PB-O2B	-2.30	1.50	1.56
5	C	600	ANP	C2-N3	-2.29	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	600	ADP	PA-O3A	2.25	1.61	1.59
5	F	600	ANP	PG-O2G	-2.15	1.51	1.56
5	B	600	ANP	C2-N1	2.06	1.37	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	ANP	O4'-C1'-N9	-4.34	99.75	108.09
5	F	600	ANP	O1G-PG-N3B	-3.96	105.94	111.77
5	B	600	ANP	O2A-PA-O3A	3.39	116.44	107.27
5	C	600	ANP	O2G-PG-O1G	-3.37	105.00	113.45
5	C	600	ANP	O3A-PB-N3B	-3.11	97.97	106.59
5	C	600	ANP	O1B-PB-N3B	2.98	116.16	111.77
5	C	600	ANP	O3G-PG-O1G	2.89	120.69	113.45
5	C	600	ANP	O3'-C3'-C2'	-2.80	102.85	111.82
5	F	600	ANP	O1B-PB-N3B	2.79	115.88	111.77
6	D	600	ADP	N6-C6-N1	2.59	124.14	118.38
5	A	600	ANP	O3A-PA-O1A	2.58	118.46	110.70
5	C	600	ANP	O2'-C2'-C3'	-2.52	103.73	111.82
5	A	600	ANP	C2'-C1'-N9	-2.49	107.11	113.30
5	B	600	ANP	C4-N9-C8	2.44	108.30	105.74
5	B	600	ANP	O2G-PG-O3G	2.43	114.11	107.59
5	C	600	ANP	O2B-PB-O3A	2.20	112.00	104.64
5	A	600	ANP	O2'-C2'-C3'	2.17	118.78	111.82
5	F	600	ANP	O5'-C5'-C4'	-2.17	101.60	108.99
5	B	600	ANP	O1G-PG-N3B	-2.16	108.58	111.77
5	B	600	ANP	O2B-PB-O3A	2.16	111.84	104.64
6	D	600	ADP	O3'-C3'-C2'	-2.13	105.00	111.82
6	D	600	ADP	O4'-C1'-N9	-2.12	104.02	108.09
5	C	600	ANP	O1G-PG-N3B	-2.12	108.65	111.77
5	B	600	ANP	O2G-PG-O1G	-2.08	108.25	113.45
6	D	600	ADP	O4'-C4'-C3'	-2.03	101.12	105.15

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	ANP	PB-N3B-PG-O1G
5	A	600	ANP	PG-N3B-PB-O1B
5	B	600	ANP	PB-N3B-PG-O1G
5	B	600	ANP	PG-N3B-PB-O1B
5	C	600	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
5	C	600	ANP	PG-N3B-PB-O1B
5	C	600	ANP	PG-N3B-PB-O3A
5	C	600	ANP	C5'-O5'-PA-O1A
5	C	600	ANP	C5'-O5'-PA-O2A
5	F	600	ANP	PB-N3B-PG-O1G
5	F	600	ANP	PG-N3B-PB-O1B
5	F	600	ANP	PA-O3A-PB-O2B
6	D	600	ADP	PA-O3A-PB-O2B
6	D	600	ADP	PA-O3A-PB-O3B
5	C	600	ANP	C5'-O5'-PA-O3A
5	C	600	ANP	C3'-C4'-C5'-O5'
5	F	600	ANP	PA-O3A-PB-O1B
5	A	600	ANP	PG-N3B-PB-O3A
5	F	600	ANP	PG-N3B-PB-O3A

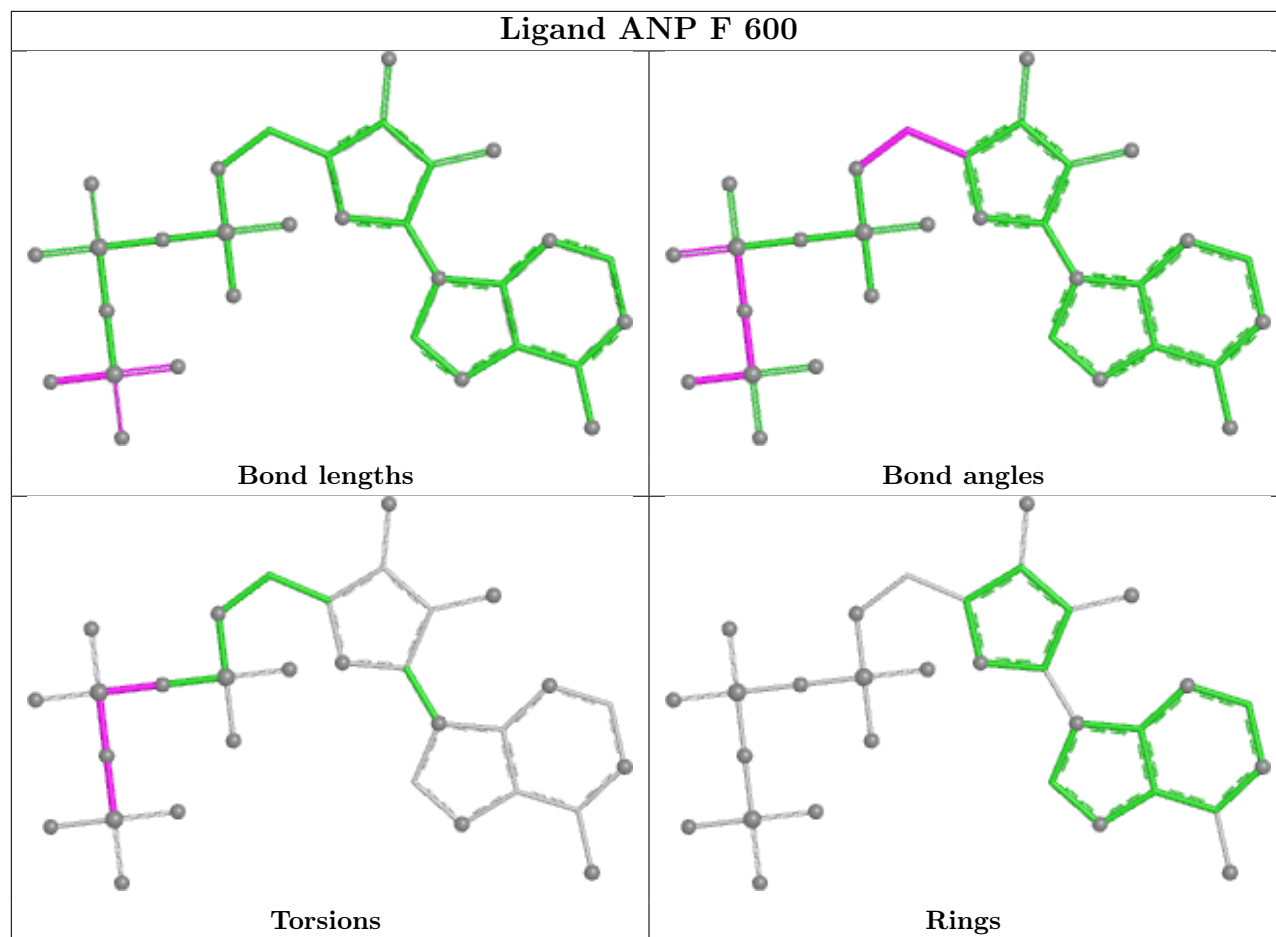
There are no ring outliers.

5 monomers are involved in 17 short contacts:

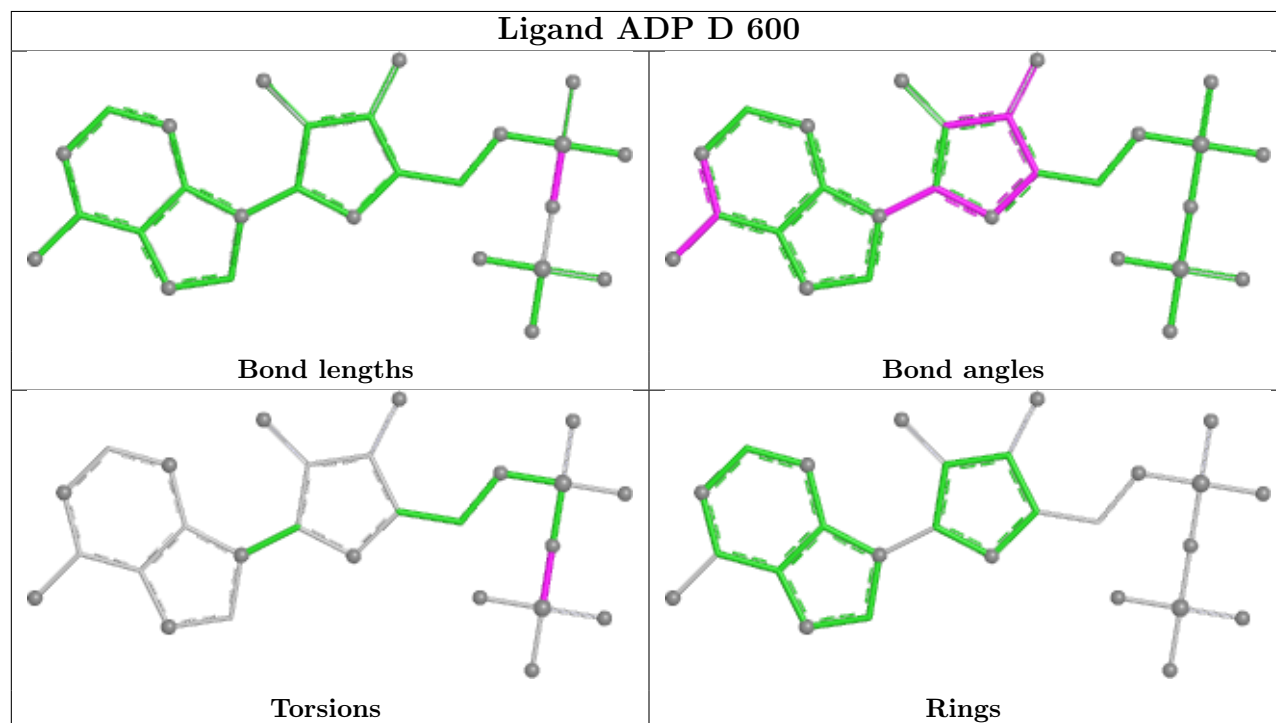
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	600	ANP	4	0
6	D	600	ADP	2	0
5	A	600	ANP	2	0
5	C	600	ANP	4	0
5	B	600	ANP	5	0

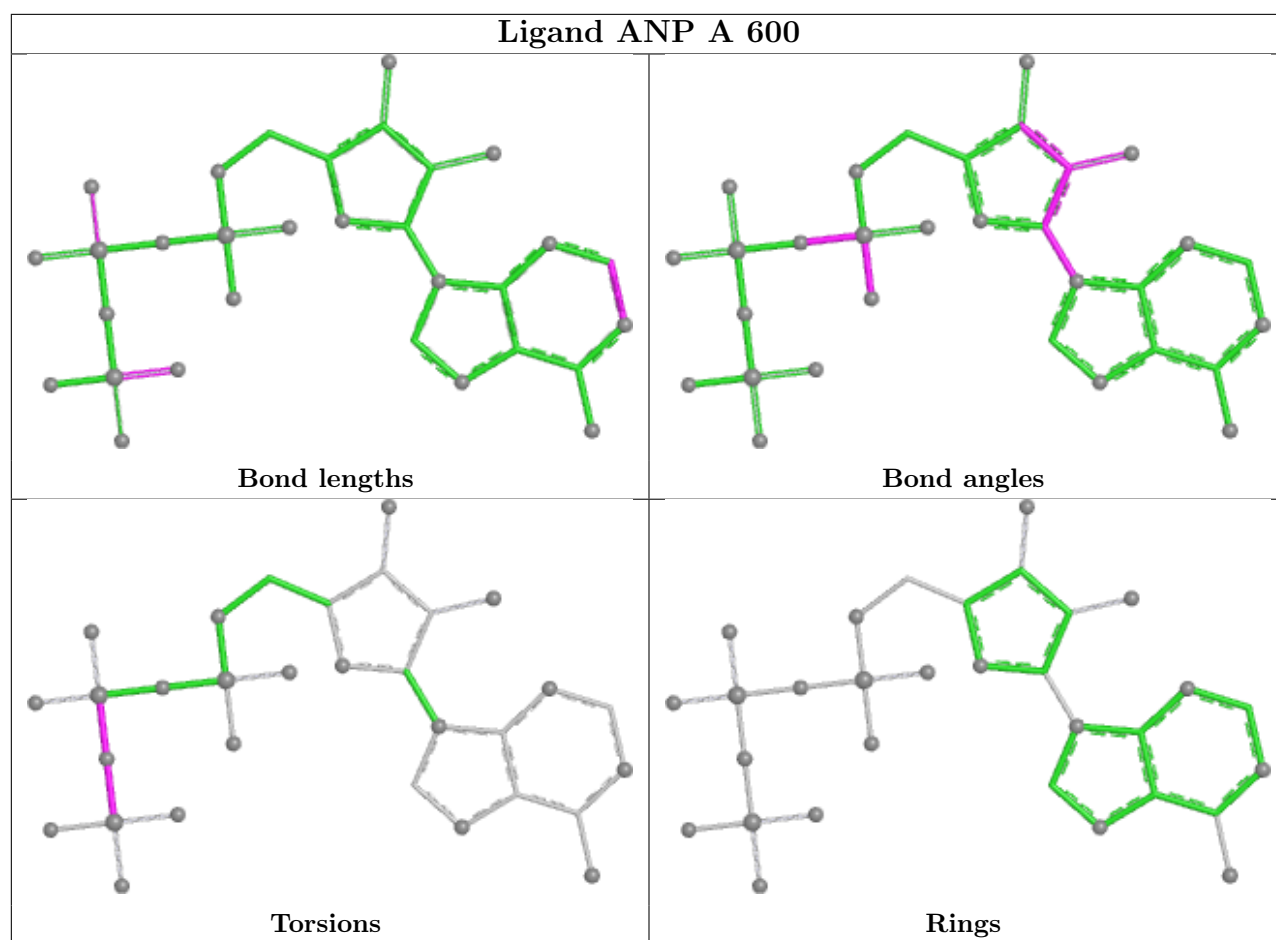
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

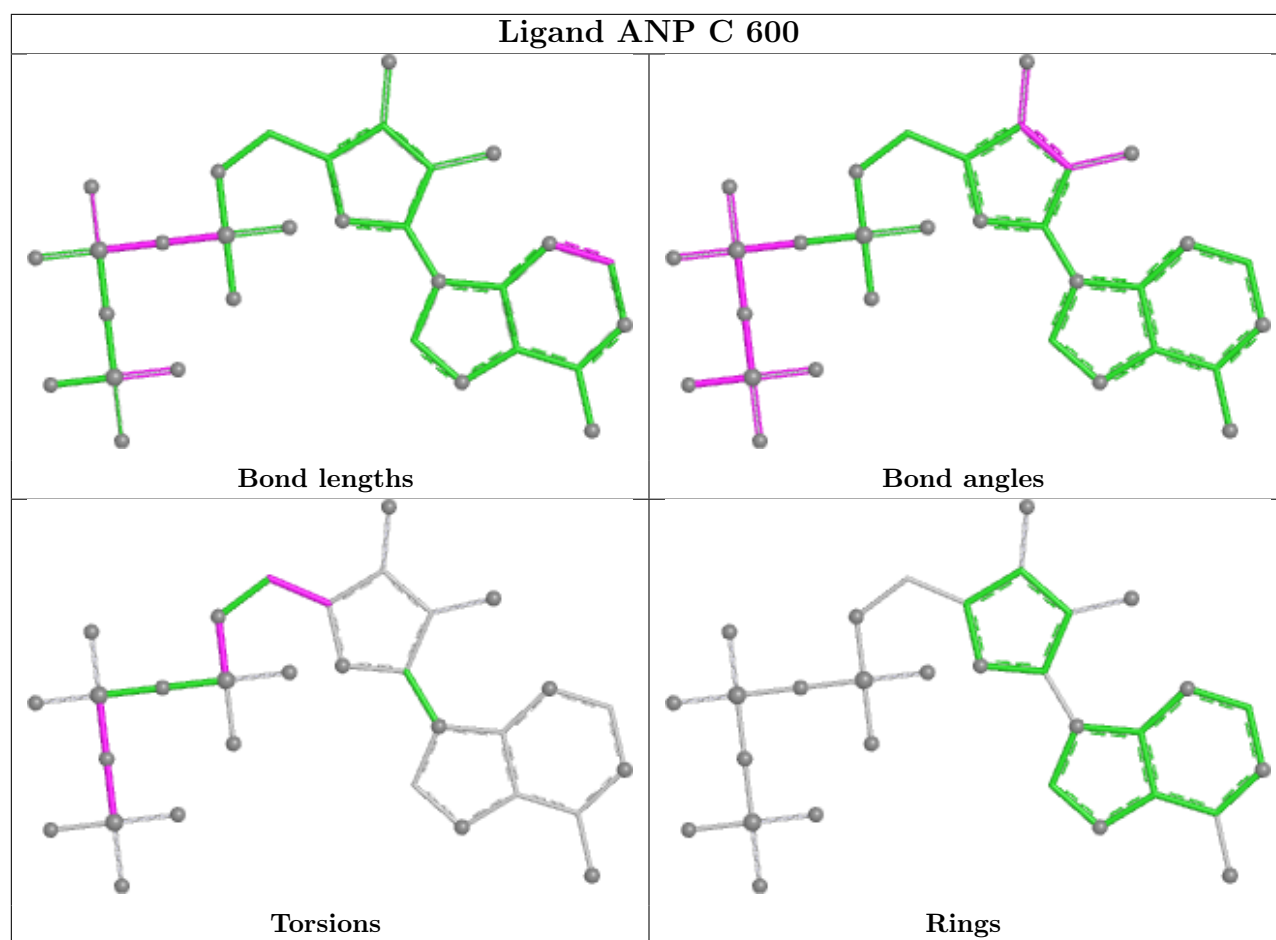
Ligand ANP F 600

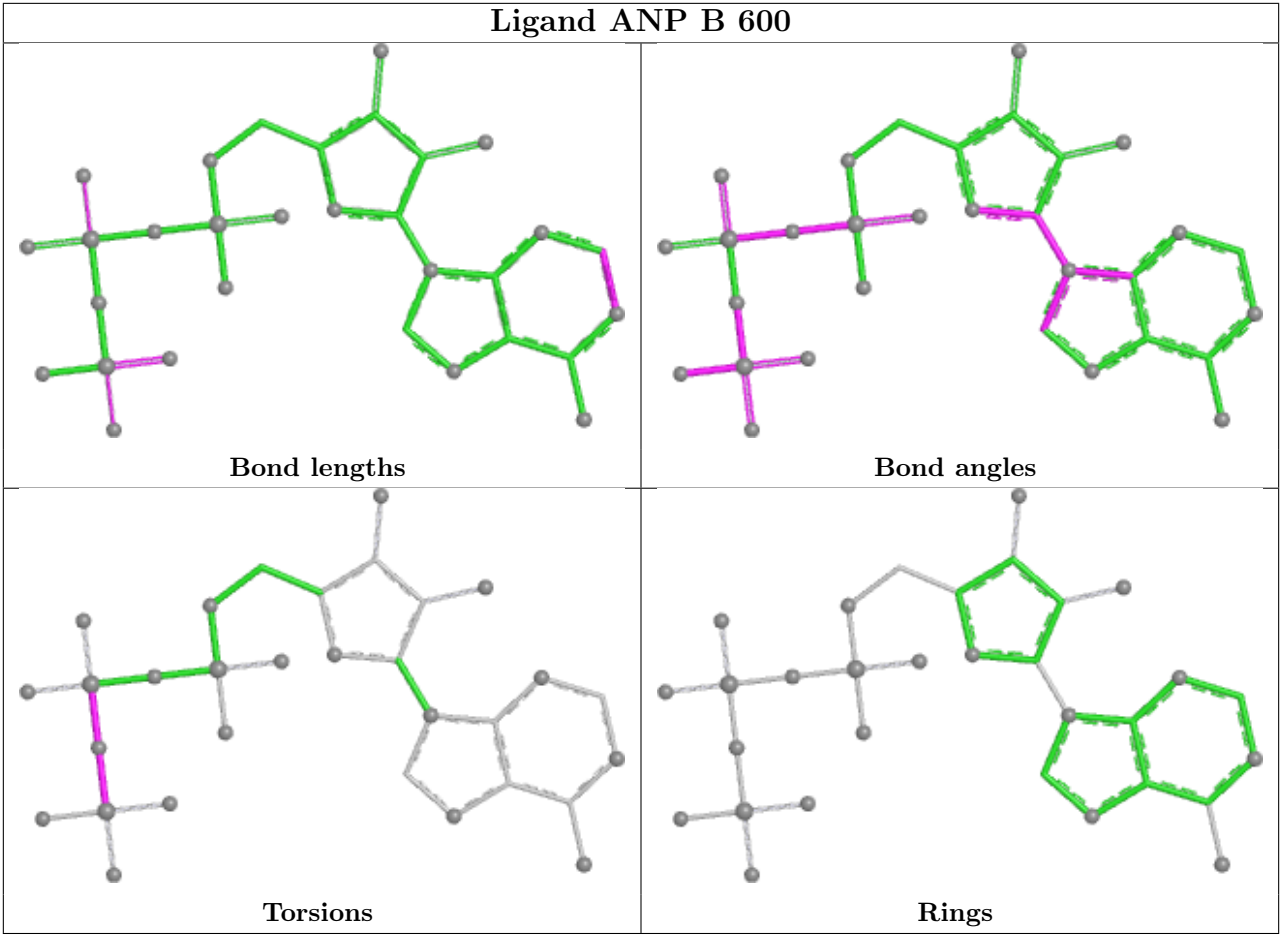


Ligand ADP D 600









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	409:ASP	C	410:LEU	N	1.18
1	B	401:ALA	C	402:ALA	N	1.16

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	487/510 (95%)	-1.06	0 100 100	16, 38, 67, 97	0
1	B	479/510 (93%)	-0.99	0 100 100	15, 37, 75, 98	0
1	C	492/510 (96%)	-1.15	1 (0%) 91 91	13, 33, 63, 95	0
2	D	467/482 (96%)	-1.14	0 100 100	13, 34, 62, 83	0
2	E	466/482 (96%)	-0.86	0 100 100	18, 45, 79, 98	0
2	F	466/482 (96%)	-1.14	1 (0%) 91 91	13, 34, 63, 87	0
3	G	122/272 (44%)	-0.72	0 100 100	12, 60, 100, 100	0
All	All	2979/3248 (91%)	-1.04	2 (0%) 92 92	12, 37, 74, 100	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	407	GLY	2.8
2	F	178	GLY	2.2

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.

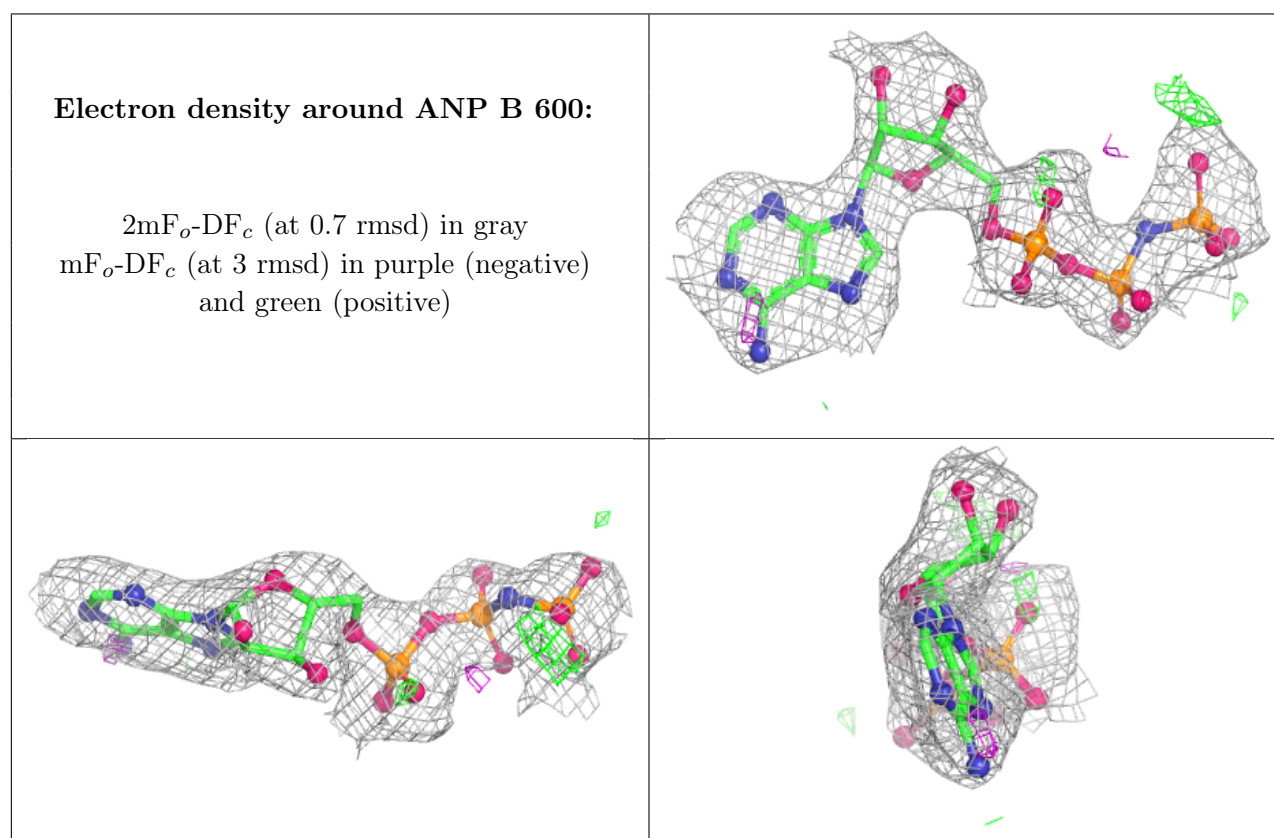
6.4 Ligands [i](#)

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.

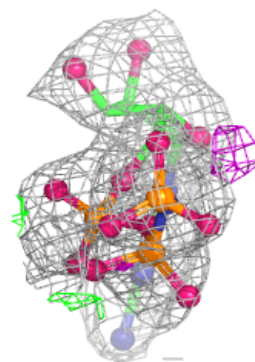
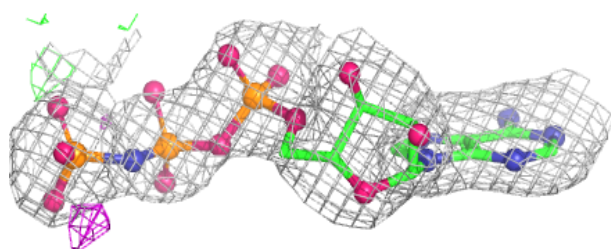
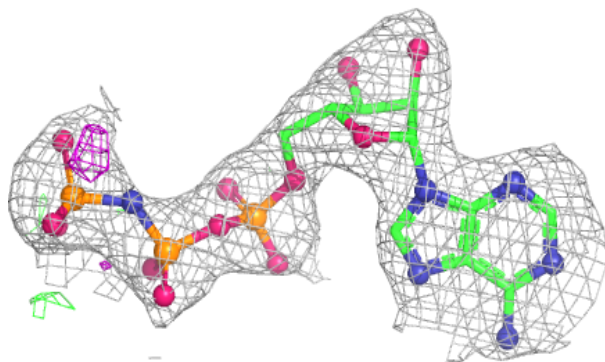
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	C	601	1/1	0.82	0.03	25,25,25,25	0
4	MG	F	601	1/1	0.89	0.03	24,24,24,24	0
4	MG	B	601	1/1	0.92	0.05	36,36,36,36	0
4	MG	A	601	1/1	0.95	0.04	26,26,26,26	0
4	MG	D	601	1/1	0.96	0.03	22,22,22,22	0
5	ANP	B	600	31/31	0.97	0.06	30,34,37,38	0
5	ANP	F	600	31/31	0.98	0.05	26,28,29,31	0
5	ANP	C	600	31/31	0.99	0.03	19,24,26,29	0
5	ANP	A	600	31/31	0.99	0.04	25,27,32,32	0
6	ADP	D	600	27/27	0.99	0.04	20,23,24,25	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.

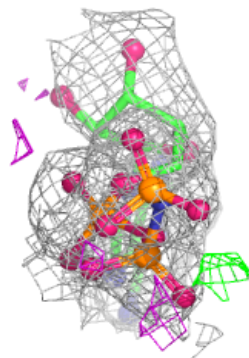
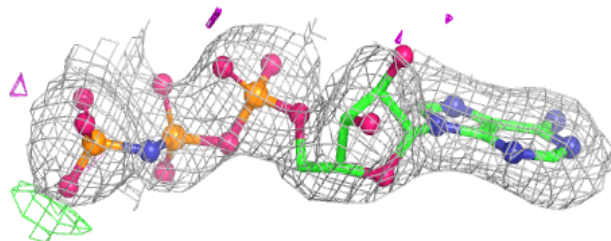
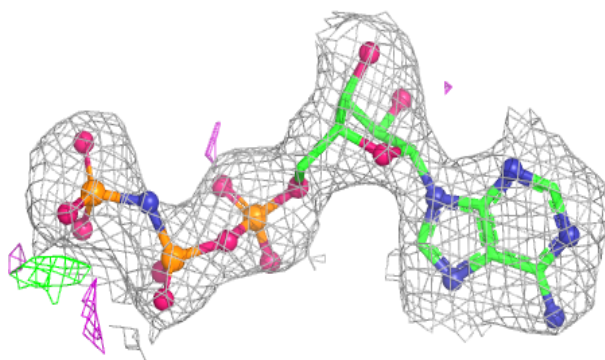


Electron density around ANP F 600:

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

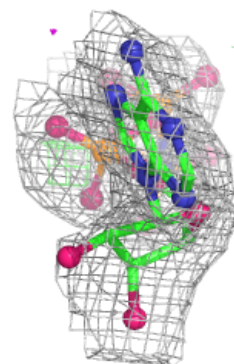
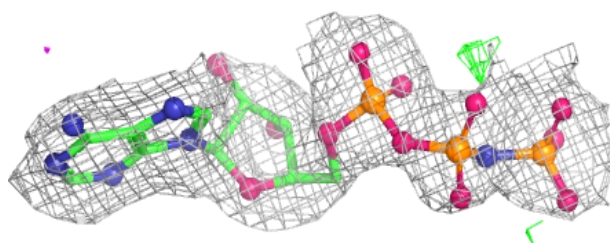
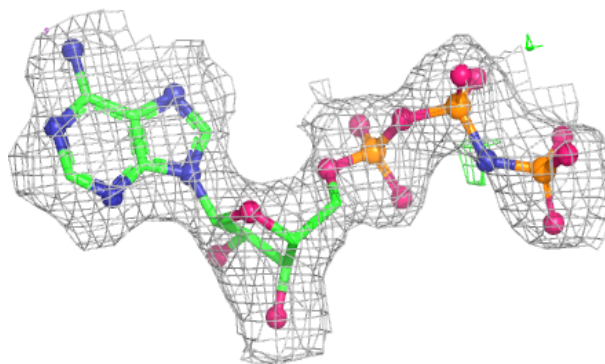
**Electron density around ANP C 600:**

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

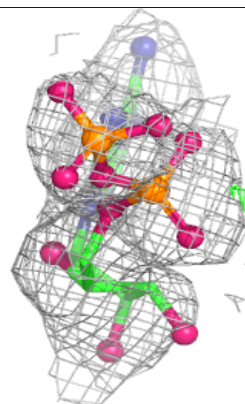
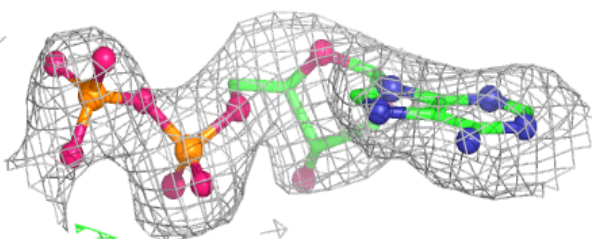
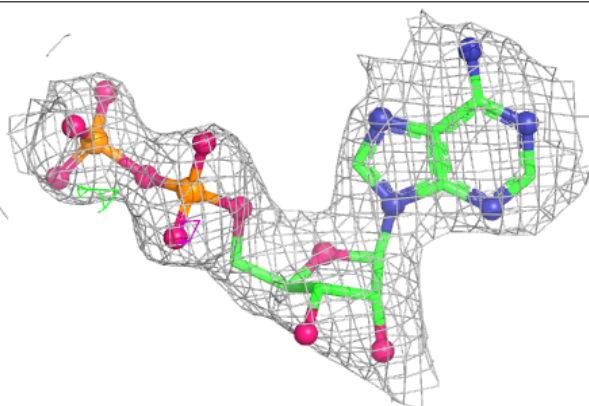


Electron density around ANP A 600:

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

**Electron density around ADP D 600:**

$2mF_o-DF_c$ (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.