



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:23 AM UTC

PDB ID : 2IUU / pdb_00002iuu
Title : P. aeruginosa FtsK motor domain, hexamer
Authors : Massey, T.H.; Mercoglian, C.P.; Yates, J.; Sherratt, D.J.; Lowe, J.
Deposited on : 2006-06-07
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

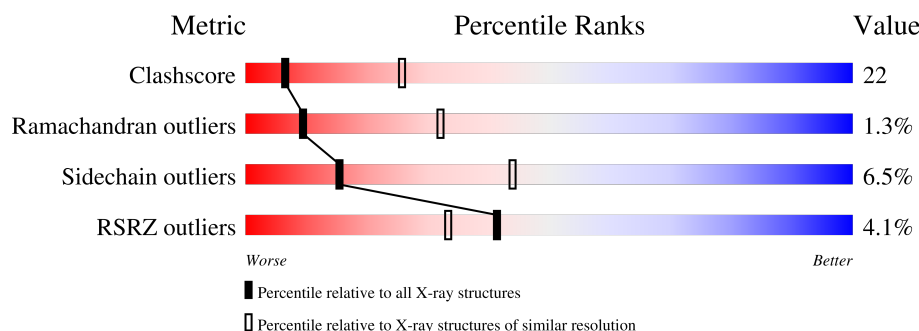
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	491	3% 48% 31% • 17%
1	B	491	3% 48% 31% • 17%
1	C	491	3% 48% 31% • 17%
1	D	491	3% 52% 27% • 17%
1	E	491	4% 46% 33% • 17%
1	F	491	4% 49% 30% • 17%

2 Entry composition [i](#)

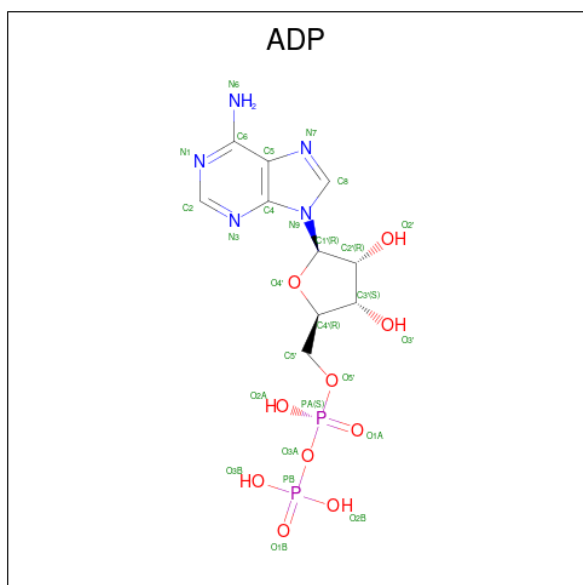
There are 2 unique types of molecules in this entry. The entry contains 18888 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

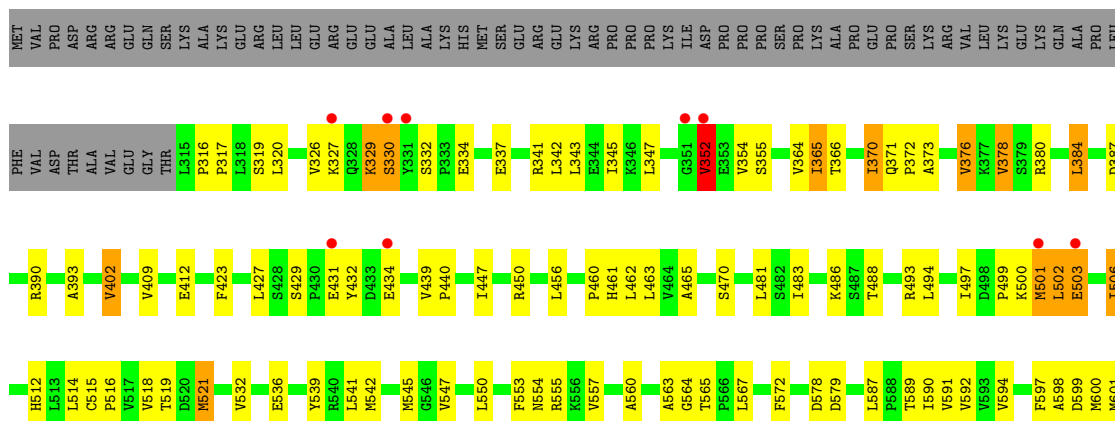
- Molecule 1 is a protein called DNA TRANSLOCASE FTSK.

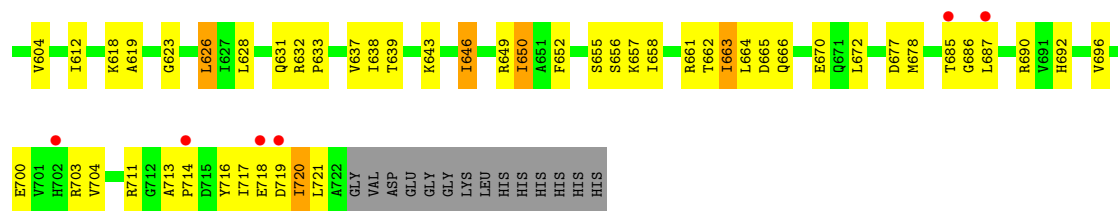
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			
1	B	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			
1	C	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			
1	D	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			
1	E	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			
1	F	408	Total	C	N	O	S	0	0	0
			3121	1983	540	583	15			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

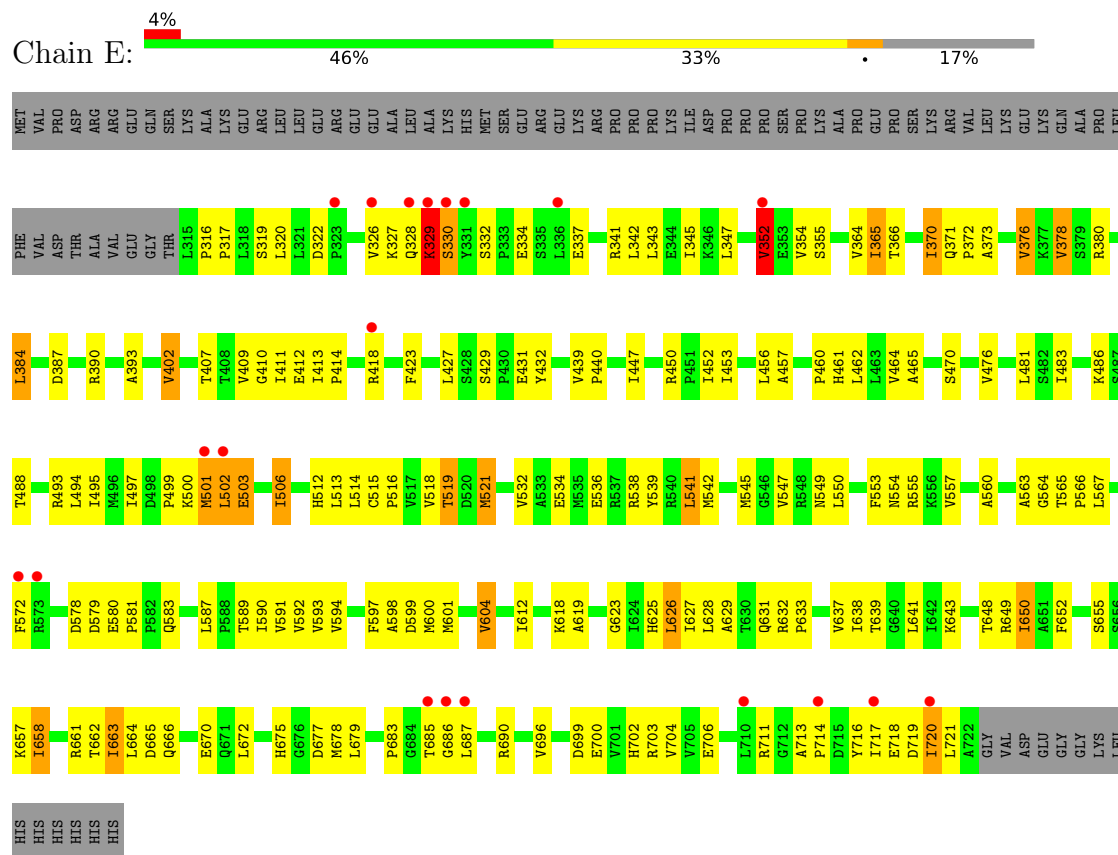


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

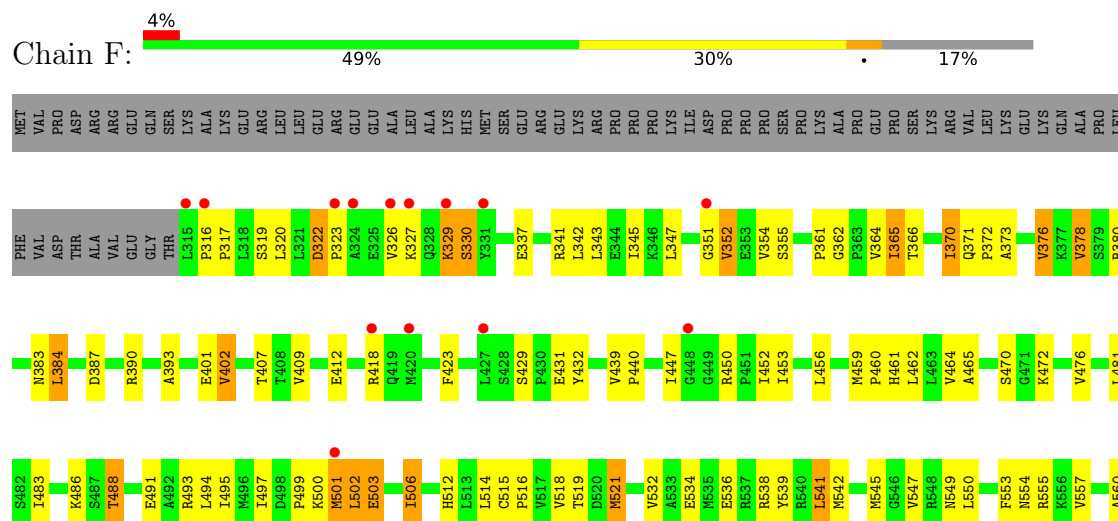


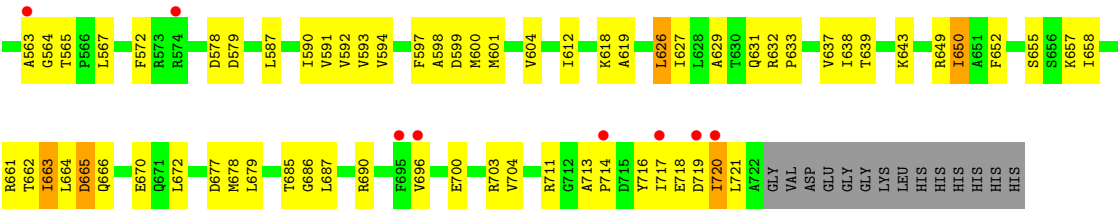


• Molecule 1: DNA TRANSLOCASE FTSK



• Molecule 1: DNA TRANSLOCASE FTSK





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.01Å 221.76Å 134.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.90 100.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (100.00-2.90) 99.6 (100.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.259 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18888	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: ADP

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	0.54	0/3177	1.10	19/4312 (0.4%)
1	B	0.57	0/3177	1.09	15/4312 (0.3%)
1	C	0.59	0/3177	1.10	19/4312 (0.4%)
1	D	0.61	0/3177	1.09	15/4312 (0.3%)
1	E	0.53	0/3177	1.09	16/4312 (0.4%)
1	F	0.54	0/3177	1.09	17/4312 (0.4%)
All	All	0.56	0/19062	1.09	101/25872 (0.4%)

There are no bond length outliers.

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	352	VAL	N-CA-C	12.24	125.37	109.58
1	B	352	VAL	N-CA-C	12.19	125.31	109.58
1	D	352	VAL	N-CA-C	12.04	125.11	109.58
1	C	352	VAL	N-CA-C	11.90	124.93	109.58
1	A	352	VAL	N-CA-C	11.68	124.64	109.58
1	F	352	VAL	N-CA-C	10.64	123.31	109.58
1	C	619	ALA	N-CA-C	8.64	121.65	111.71
1	B	619	ALA	N-CA-C	8.51	121.50	111.71
1	A	720	ILE	N-CA-C	8.45	119.23	110.36
1	A	619	ALA	N-CA-C	8.35	121.31	111.71
1	D	720	ILE	N-CA-C	8.34	119.12	110.36
1	E	720	ILE	N-CA-C	8.29	119.06	110.36
1	B	720	ILE	N-CA-C	8.14	118.92	110.62
1	C	720	ILE	N-CA-C	8.04	118.80	110.36
1	F	351	GLY	N-CA-C	7.92	121.69	112.50
1	D	619	ALA	N-CA-C	7.90	120.80	111.71
1	E	619	ALA	N-CA-C	7.85	120.74	111.71
1	F	720	ILE	N-CA-C	7.68	118.43	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	503	GLU	N-CA-C	7.65	123.92	111.37
1	B	503	GLU	N-CA-C	7.59	123.82	111.37
1	C	503	GLU	N-CA-C	7.59	123.82	111.37
1	E	503	GLU	N-CA-C	7.58	123.81	111.37
1	F	503	GLU	N-CA-C	7.57	123.79	111.37
1	A	503	GLU	N-CA-C	7.56	123.77	111.37
1	A	351	GLY	N-CA-C	7.37	121.05	112.50
1	C	604	VAL	N-CA-C	7.19	118.13	111.45
1	E	316	PRO	CA-C-N	7.07	127.63	119.99
1	E	316	PRO	C-N-CA	7.07	127.63	119.99
1	E	665	ASP	N-CA-C	-7.03	102.25	111.74
1	F	316	PRO	CA-C-N	6.97	127.52	119.99
1	F	316	PRO	C-N-CA	6.97	127.52	119.99
1	C	351	GLY	N-CA-C	6.91	120.51	112.50
1	A	316	PRO	CA-C-N	6.81	127.34	119.99
1	A	316	PRO	C-N-CA	6.81	127.34	119.99
1	C	665	ASP	N-CA-C	-6.71	102.69	111.74
1	D	316	PRO	CA-C-N	6.67	127.20	119.99
1	D	316	PRO	C-N-CA	6.67	127.20	119.99
1	B	655	SER	N-CA-C	6.56	119.25	111.71
1	B	316	PRO	CA-C-N	6.53	127.04	119.99
1	B	316	PRO	C-N-CA	6.53	127.04	119.99
1	F	619	ALA	N-CA-C	6.50	120.31	112.38
1	F	665	ASP	N-CA-C	-6.49	102.98	111.74
1	A	655	SER	N-CA-C	6.45	119.12	111.71
1	C	655	SER	N-CA-C	6.40	119.07	111.71
1	D	655	SER	N-CA-C	6.39	119.06	111.71
1	D	665	ASP	N-CA-C	-6.33	103.19	111.74
1	F	655	SER	N-CA-C	6.24	118.89	111.71
1	F	604	VAL	N-CA-C	6.21	117.23	111.45
1	A	604	VAL	N-CA-C	6.21	117.22	111.45
1	B	604	VAL	N-CA-C	6.17	117.18	111.45
1	C	316	PRO	CA-C-N	5.99	126.46	119.99
1	C	316	PRO	C-N-CA	5.99	126.46	119.99
1	A	646	ILE	CA-C-N	5.98	125.53	119.19
1	A	646	ILE	C-N-CA	5.98	125.53	119.19
1	E	655	SER	N-CA-C	5.96	118.56	111.71
1	D	604	VAL	N-CA-C	5.92	116.96	111.45
1	A	476	VAL	N-CA-C	-5.89	104.77	110.72
1	A	322	ASP	CA-C-N	5.84	126.03	120.31
1	A	322	ASP	C-N-CA	5.84	126.03	120.31
1	C	401	GLU	N-CA-C	5.76	119.41	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	646	ILE	CA-C-N	5.68	125.30	119.56
1	C	646	ILE	C-N-CA	5.68	125.30	119.56
1	A	665	ASP	N-CA-C	-5.68	104.08	111.74
1	B	555	ARG	N-CA-C	-5.61	104.81	111.03
1	D	589	THR	N-CA-C	-5.60	100.85	109.76
1	C	589	THR	N-CA-C	-5.57	100.90	109.76
1	F	322	ASP	CA-C-N	5.50	125.47	120.03
1	F	322	ASP	C-N-CA	5.50	125.47	120.03
1	C	555	ARG	N-CA-C	-5.46	104.97	111.03
1	E	604	VAL	N-CA-C	5.45	117.36	111.58
1	E	589	THR	N-CA-C	-5.39	101.19	109.76
1	E	555	ARG	N-CA-C	-5.38	105.06	111.03
1	F	555	ARG	N-CA-C	-5.37	105.07	111.03
1	B	626	LEU	N-CA-C	5.36	117.97	109.24
1	D	646	ILE	CA-C-N	5.34	124.85	119.19
1	D	646	ILE	C-N-CA	5.34	124.85	119.19
1	E	322	ASP	CA-C-N	5.32	125.30	120.03
1	E	322	ASP	C-N-CA	5.32	125.30	120.03
1	F	401	GLU	N-CA-C	5.32	118.87	112.38
1	A	589	THR	N-CA-C	-5.28	101.36	109.76
1	B	665	ASP	N-CA-C	-5.27	104.63	111.74
1	E	476	VAL	N-CA-C	-5.26	105.41	110.72
1	C	409	VAL	CA-C-N	-5.25	118.56	122.18
1	C	409	VAL	C-N-CA	-5.25	118.56	122.18
1	B	589	THR	N-CA-C	-5.24	101.43	109.76
1	F	612	ILE	CB-CA-C	-5.17	105.26	111.88
1	A	329	LYS	CA-C-O	5.16	120.93	117.94
1	E	316	PRO	N-CA-C	5.16	117.00	110.70
1	C	316	PRO	N-CA-C	5.15	116.98	110.70
1	B	316	PRO	N-CA-C	5.11	116.94	110.70
1	D	656	SER	N-CA-C	5.09	116.54	108.96
1	F	362	GLY	CA-C-N	5.08	124.25	118.97
1	F	362	GLY	C-N-CA	5.08	124.25	118.97
1	D	316	PRO	N-CA-C	5.07	116.89	110.70
1	D	555	ARG	N-CA-C	-5.06	105.41	111.03
1	E	329	LYS	CA-C-O	5.06	120.88	117.94
1	B	401	GLU	N-CA-C	5.04	118.53	112.38
1	B	476	VAL	N-CA-C	-5.04	105.63	110.72
1	A	555	ARG	N-CA-C	-5.02	105.45	111.03
1	A	631	GLN	N-CA-C	-5.02	107.19	113.72
1	C	329	LYS	CA-C-O	5.02	120.85	117.94

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	3121	0	3238	142	0
1	B	3121	0	3238	146	1
1	C	3121	0	3238	144	0
1	D	3121	0	3238	133	1
1	E	3121	0	3238	158	0
1	F	3121	0	3238	144	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
All	All	18888	0	19500	838	1

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 22.

All (838) 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:E:499:PRO:HB3	1:E:521:MET:HE2	1.37	1.02
1:B:497:ILE:HG21	1:B:600:MET:HE2	1.43	1.00
1:E:497:ILE:HG21	1:E:600:MET:HE2	1.45	0.99
1:D:521:MET:HE3	1:D:600:MET:HG3	1.43	0.98
1:D:497:ILE:HG21	1:D:600:MET:HE2	1.47	0.96
1:C:497:ILE:HG21	1:C:600:MET:HE2	1.46	0.95
1:A:497:ILE:HG21	1:A:600:MET:HE2	1.48	0.95
1:F:499:PRO:HB3	1:F:521:MET:HE2	1.47	0.94
1:C:499:PRO:HB3	1:C:521:MET:HE2	1.48	0.94
1:B:521:MET:HE3	1:B:600:MET:HG3	1.48	0.93
1:D:502:LEU:HD13	1:D:503:GLU:HG2	1.53	0.91
1:F:497:ILE:HG21	1:F:600:MET:HE2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:PRO:HB3	1:A:521:MET:HE2	1.52	0.91
1:E:502:LEU:HD13	1:E:503:GLU:HG2	1.49	0.91
1:C:521:MET:HE3	1:C:600:MET:HG3	1.53	0.91
1:B:499:PRO:HB3	1:B:521:MET:HE2	1.52	0.90
1:F:502:LEU:HD13	1:F:503:GLU:HG2	1.51	0.90
1:B:502:LEU:HD13	1:B:503:GLU:HG2	1.54	0.88
1:A:502:LEU:HD13	1:A:503:GLU:HG2	1.55	0.87
1:D:501:MET:HE1	1:E:618:LYS:HE2	1.55	0.87
1:D:506:ILE:HD13	1:D:506:ILE:O	1.75	0.86
1:C:506:ILE:HD13	1:C:506:ILE:O	1.76	0.85
1:C:502:LEU:HD13	1:C:503:GLU:HG2	1.56	0.85
1:F:506:ILE:HD13	1:F:506:ILE:O	1.77	0.85
1:A:521:MET:HE3	1:A:600:MET:HG3	1.58	0.85
1:C:501:MET:HE1	1:D:618:LYS:HE2	1.56	0.84
1:D:499:PRO:HB3	1:D:521:MET:HE2	1.57	0.84
1:E:506:ILE:HD13	1:E:506:ILE:O	1.79	0.83
1:B:506:ILE:O	1:B:506:ILE:HD13	1.78	0.83
1:A:501:MET:HE1	1:B:618:LYS:HE2	1.61	0.83
1:B:501:MET:HE1	1:C:618:LYS:HE2	1.60	0.82
1:F:521:MET:HE3	1:F:600:MET:HG3	1.61	0.82
1:A:618:LYS:HE2	1:F:501:MET:HE1	1.61	0.82
1:E:521:MET:HE3	1:E:600:MET:HG3	1.59	0.82
1:D:329:LYS:HG2	1:D:330:SER:H	1.46	0.81
1:A:329:LYS:HG2	1:A:330:SER:H	1.46	0.81
1:F:597:PHE:CD1	1:F:601:MET:HE2	2.17	0.80
1:D:500:LYS:O	1:D:502:LEU:N	2.12	0.80
1:A:500:LYS:O	1:A:502:LEU:N	2.15	0.80
1:E:329:LYS:HG2	1:E:330:SER:H	1.46	0.80
1:C:500:LYS:O	1:C:502:LEU:N	2.15	0.79
1:B:500:LYS:O	1:B:502:LEU:N	2.15	0.79
1:D:554:ASN:HD21	1:D:587:LEU:H	1.28	0.79
1:C:329:LYS:HG2	1:C:330:SER:H	1.47	0.79
1:E:501:MET:HE1	1:F:618:LYS:HE2	1.63	0.79
1:D:597:PHE:CD1	1:D:601:MET:HE2	2.16	0.79
1:C:554:ASN:HD21	1:C:587:LEU:H	1.30	0.78
1:C:597:PHE:CD1	1:C:601:MET:HE2	2.18	0.78
1:A:663:ILE:HD13	1:A:663:ILE:O	1.84	0.78
1:B:554:ASN:HD21	1:B:587:LEU:H	1.32	0.77
1:E:658:ILE:HD12	1:E:658:ILE:H	1.50	0.77
1:F:601:MET:HE1	1:F:637:VAL:HG13	1.66	0.77
1:D:638:ILE:HD12	1:D:662:THR:HG22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ILE:HD12	1:B:658:ILE:H	1.47	0.77
1:B:329:LYS:HG2	1:B:330:SER:H	1.48	0.76
1:F:329:LYS:HG2	1:F:330:SER:H	1.49	0.76
1:A:547:VAL:HG11	1:A:553:PHE:N	2.01	0.76
1:F:554:ASN:HD21	1:F:587:LEU:H	1.33	0.76
1:A:554:ASN:HD21	1:A:587:LEU:H	1.34	0.76
1:B:500:LYS:C	1:B:502:LEU:H	1.94	0.76
1:F:658:ILE:HD12	1:F:658:ILE:H	1.51	0.76
1:A:597:PHE:CD1	1:A:601:MET:HE2	2.21	0.75
1:E:380:ARG:O	1:E:384:LEU:HD22	1.87	0.75
1:B:601:MET:HE1	1:B:637:VAL:HG13	1.68	0.75
1:A:658:ILE:HD12	1:A:658:ILE:H	1.51	0.75
1:E:554:ASN:HD21	1:E:587:LEU:H	1.34	0.75
1:F:500:LYS:C	1:F:502:LEU:H	1.94	0.75
1:D:500:LYS:C	1:D:502:LEU:H	1.94	0.75
1:C:500:LYS:C	1:C:502:LEU:H	1.94	0.74
1:A:500:LYS:C	1:A:502:LEU:H	1.95	0.74
1:A:506:ILE:HD13	1:A:506:ILE:O	1.86	0.74
1:E:500:LYS:C	1:E:502:LEU:H	1.95	0.74
1:B:547:VAL:HG11	1:B:553:PHE:N	2.01	0.74
1:E:500:LYS:O	1:E:502:LEU:N	2.19	0.74
1:E:601:MET:HE1	1:E:637:VAL:HG13	1.69	0.73
1:F:499:PRO:HB3	1:F:521:MET:CE	2.19	0.73
1:C:658:ILE:HD12	1:C:658:ILE:H	1.53	0.73
1:E:597:PHE:CD1	1:E:601:MET:HE2	2.22	0.73
1:C:440:PRO:HG3	1:C:486:LYS:HD2	1.70	0.73
1:B:597:PHE:CD1	1:B:601:MET:HE2	2.23	0.73
1:D:380:ARG:O	1:D:384:LEU:HD22	1.88	0.73
1:E:440:PRO:HG3	1:E:486:LYS:HD2	1.71	0.73
1:A:685:THR:HG22	1:A:686:GLY:N	2.04	0.73
1:C:365:ILE:HG13	1:C:412:GLU:HB3	1.71	0.73
1:F:500:LYS:O	1:F:502:LEU:N	2.20	0.73
1:E:547:VAL:HG11	1:E:553:PHE:N	2.03	0.72
1:F:365:ILE:HG13	1:F:412:GLU:HB3	1.70	0.72
1:B:685:THR:HG22	1:B:686:GLY:N	2.05	0.72
1:F:638:ILE:HD12	1:F:662:THR:HG22	1.72	0.72
1:A:365:ILE:HG13	1:A:412:GLU:HB3	1.71	0.72
1:B:521:MET:HE3	1:B:600:MET:CG	2.20	0.72
1:E:685:THR:HG22	1:E:686:GLY:N	2.03	0.72
1:D:521:MET:HE3	1:D:600:MET:CG	2.20	0.72
1:B:380:ARG:O	1:B:384:LEU:HD22	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:601:MET:HE1	1:D:637:VAL:HG13	1.70	0.71
1:A:638:ILE:HD12	1:A:662:THR:HG22	1.72	0.71
1:D:658:ILE:H	1:D:658:ILE:HD12	1.56	0.71
1:E:499:PRO:HB3	1:E:521:MET:CE	2.18	0.71
1:B:501:MET:HE1	1:C:618:LYS:CE	2.21	0.70
1:B:545:MET:HE2	1:B:553:PHE:CE1	2.26	0.70
1:F:547:VAL:HG11	1:F:553:PHE:N	2.07	0.70
1:C:717:ILE:O	1:C:720:ILE:HG22	1.91	0.70
1:E:545:MET:HE2	1:E:553:PHE:CE1	2.27	0.70
1:A:380:ARG:O	1:A:384:LEU:HD22	1.90	0.70
1:B:663:ILE:HD13	1:B:663:ILE:O	1.91	0.70
1:F:717:ILE:HG22	1:F:719:ASP:HB3	1.74	0.70
1:C:501:MET:HE1	1:D:618:LYS:CE	2.21	0.69
1:C:601:MET:HE1	1:C:637:VAL:HG13	1.74	0.69
1:F:711:ARG:HG3	1:F:711:ARG:HH21	1.55	0.69
1:F:685:THR:HG22	1:F:686:GLY:N	2.06	0.69
1:A:440:PRO:HG3	1:A:486:LYS:HD2	1.73	0.69
1:B:500:LYS:HE3	1:B:599:ASP:OD2	1.93	0.69
1:D:663:ILE:O	1:D:663:ILE:HD13	1.93	0.69
1:E:493:ARG:HD2	1:E:512:HIS:O	1.93	0.69
1:F:717:ILE:O	1:F:720:ILE:HG22	1.92	0.69
1:B:717:ILE:HG22	1:B:719:ASP:HB3	1.75	0.69
1:D:685:THR:HG22	1:D:686:GLY:N	2.07	0.69
1:C:685:THR:HG22	1:C:686:GLY:N	2.06	0.68
1:D:547:VAL:HG11	1:D:553:PHE:N	2.08	0.68
1:F:380:ARG:O	1:F:384:LEU:HD22	1.93	0.68
1:B:711:ARG:HH21	1:B:711:ARG:HG3	1.59	0.68
1:F:601:MET:CE	1:F:637:VAL:HG13	2.23	0.68
1:A:717:ILE:HG22	1:A:719:ASP:HB3	1.73	0.68
1:D:717:ILE:HG22	1:D:719:ASP:HB3	1.74	0.68
1:F:500:LYS:HE3	1:F:599:ASP:OD2	1.94	0.68
1:C:387:ASP:OD2	1:D:378:VAL:HG23	1.93	0.68
1:C:380:ARG:O	1:C:384:LEU:HD22	1.92	0.68
1:C:711:ARG:HH21	1:C:711:ARG:HG3	1.58	0.68
1:C:717:ILE:HG22	1:C:719:ASP:HB3	1.75	0.67
1:C:663:ILE:HD13	1:C:663:ILE:O	1.95	0.67
1:E:365:ILE:HG13	1:E:412:GLU:HB3	1.75	0.67
1:E:717:ILE:O	1:E:720:ILE:HG22	1.94	0.67
1:A:545:MET:HE2	1:A:553:PHE:CE1	2.30	0.67
1:D:501:MET:HE1	1:E:618:LYS:CE	2.25	0.67
1:F:554:ASN:HA	1:F:557:VAL:HG12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:VAL:HG11	1:C:553:PHE:N	2.11	0.66
1:E:429:SER:HB2	1:E:431:GLU:OE2	1.94	0.66
1:A:499:PRO:HB3	1:A:521:MET:CE	2.24	0.66
1:B:601:MET:CE	1:B:637:VAL:HG13	2.24	0.66
1:C:545:MET:HE2	1:C:553:PHE:CE1	2.30	0.66
1:D:601:MET:CE	1:D:637:VAL:HG13	2.26	0.66
1:E:601:MET:CE	1:E:637:VAL:HG13	2.25	0.66
1:F:545:MET:HE2	1:F:553:PHE:CE1	2.31	0.66
1:E:717:ILE:HG22	1:E:719:ASP:HB3	1.77	0.66
1:F:440:PRO:HG3	1:F:486:LYS:HD2	1.78	0.66
1:C:521:MET:HE3	1:C:600:MET:CG	2.26	0.66
1:E:341:ARG:O	1:E:345:ILE:HG12	1.96	0.65
1:B:572:PHE:HZ	1:B:579:ASP:HB3	1.61	0.65
1:A:717:ILE:O	1:A:720:ILE:HG22	1.95	0.65
1:A:700:GLU:O	1:A:704:VAL:HG23	1.95	0.65
1:B:440:PRO:HG3	1:B:486:LYS:HD2	1.78	0.65
1:D:462:LEU:HD11	1:D:650:ILE:HD13	1.79	0.65
1:F:423:PHE:HE1	1:F:481:LEU:HB3	1.62	0.65
1:A:402:VAL:HG13	1:A:687:LEU:HD11	1.78	0.65
1:E:501:MET:HE1	1:F:618:LYS:CE	2.27	0.65
1:E:663:ILE:HD13	1:E:663:ILE:O	1.97	0.65
1:B:497:ILE:HG21	1:B:600:MET:CE	2.24	0.65
1:E:439:VAL:HG12	1:E:483:ILE:HD12	1.78	0.65
1:A:618:LYS:CE	1:F:501:MET:HE1	2.27	0.65
1:D:365:ILE:HG13	1:D:412:GLU:HB3	1.78	0.65
1:D:493:ARG:HD2	1:D:512:HIS:O	1.97	0.65
1:D:554:ASN:HA	1:D:557:VAL:HG12	1.79	0.65
1:D:545:MET:HE2	1:D:553:PHE:CE1	2.32	0.65
1:A:601:MET:HE1	1:A:637:VAL:HG13	1.79	0.64
1:D:717:ILE:O	1:D:720:ILE:HG22	1.97	0.64
1:E:554:ASN:HA	1:E:557:VAL:HG12	1.80	0.64
1:A:497:ILE:HG21	1:A:600:MET:CE	2.25	0.64
1:C:638:ILE:HD12	1:C:662:THR:HG22	1.79	0.64
1:F:663:ILE:HD13	1:F:663:ILE:O	1.98	0.64
1:B:717:ILE:O	1:B:720:ILE:HG22	1.97	0.64
1:E:462:LEU:HD11	1:E:650:ILE:CD1	2.27	0.64
1:B:439:VAL:HG12	1:B:483:ILE:HD12	1.79	0.64
1:E:327:LYS:HG3	1:E:327:LYS:O	1.98	0.64
1:B:499:PRO:HB3	1:B:521:MET:CE	2.28	0.64
1:E:572:PHE:HZ	1:E:579:ASP:HB3	1.62	0.64
1:E:638:ILE:HD12	1:E:662:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:402:VAL:HG13	1:F:687:LEU:HD11	1.79	0.64
1:A:387:ASP:OD2	1:B:378:VAL:HG23	1.98	0.64
1:B:365:ILE:HG13	1:B:412:GLU:HB3	1.78	0.64
1:D:329:LYS:HG2	1:D:330:SER:N	2.13	0.64
1:D:700:GLU:O	1:D:704:VAL:HG23	1.98	0.64
1:A:493:ARG:HD2	1:A:512:HIS:O	1.97	0.63
1:D:327:LYS:O	1:D:327:LYS:HG3	1.98	0.63
1:A:501:MET:HE1	1:B:618:LYS:CE	2.27	0.63
1:B:327:LYS:HG3	1:B:327:LYS:O	1.99	0.63
1:C:329:LYS:HG2	1:C:330:SER:N	2.13	0.63
1:C:497:ILE:HD13	1:C:600:MET:HE1	1.79	0.63
1:E:329:LYS:CG	1:E:330:SER:H	2.11	0.63
1:A:572:PHE:HZ	1:A:579:ASP:HB3	1.63	0.63
1:E:500:LYS:HE3	1:E:599:ASP:OD2	1.98	0.63
1:F:327:LYS:O	1:F:327:LYS:HG3	1.98	0.63
1:F:493:ARG:HD2	1:F:512:HIS:O	1.99	0.63
1:A:711:ARG:HG3	1:A:711:ARG:HH21	1.63	0.63
1:C:327:LYS:O	1:C:327:LYS:HG3	1.97	0.63
1:D:440:PRO:HG3	1:D:486:LYS:HD2	1.80	0.63
1:A:329:LYS:HG2	1:A:330:SER:N	2.13	0.63
1:B:638:ILE:HD12	1:B:662:THR:HG22	1.80	0.63
1:F:462:LEU:HD11	1:F:650:ILE:HD13	1.80	0.63
1:B:514:LEU:HD11	1:B:590:ILE:HD12	1.80	0.63
1:F:572:PHE:HZ	1:F:579:ASP:HB3	1.64	0.63
1:A:354:VAL:HG23	1:A:372:PRO:HA	1.81	0.62
1:E:711:ARG:HH21	1:E:711:ARG:HG3	1.64	0.62
1:B:329:LYS:HG2	1:B:330:SER:N	2.14	0.62
1:C:370:ILE:HD13	1:C:409:VAL:O	1.99	0.62
1:E:387:ASP:OD2	1:F:378:VAL:HG23	2.00	0.62
1:C:601:MET:CE	1:C:637:VAL:HG13	2.30	0.62
1:D:370:ILE:HD13	1:D:409:VAL:O	1.99	0.62
1:F:370:ILE:HD13	1:F:409:VAL:O	1.99	0.62
1:A:429:SER:HB2	1:A:431:GLU:OE2	1.99	0.62
1:B:658:ILE:HD12	1:B:658:ILE:N	2.14	0.62
1:B:685:THR:HG22	1:B:686:GLY:H	1.65	0.62
1:C:514:LEU:HD11	1:C:590:ILE:HD12	1.80	0.62
1:A:494:LEU:HD23	1:A:591:VAL:HB	1.81	0.62
1:D:572:PHE:HZ	1:D:579:ASP:HB3	1.65	0.62
1:C:554:ASN:HA	1:C:557:VAL:HG12	1.82	0.62
1:F:370:ILE:HD13	1:F:370:ILE:H	1.65	0.62
1:E:354:VAL:HG23	1:E:372:PRO:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:VAL:HG12	1:D:483:ILE:HD12	1.82	0.61
1:D:711:ARG:HH21	1:D:711:ARG:HG3	1.65	0.61
1:B:341:ARG:O	1:B:345:ILE:HG12	2.01	0.61
1:B:497:ILE:HD12	1:B:594:VAL:HG22	1.82	0.61
1:C:370:ILE:HD13	1:C:370:ILE:H	1.66	0.61
1:C:541:LEU:O	1:C:545:MET:HG2	2.01	0.61
1:F:329:LYS:HG2	1:F:330:SER:N	2.15	0.61
1:F:462:LEU:HD11	1:F:650:ILE:CD1	2.30	0.61
1:A:423:PHE:HE1	1:A:481:LEU:HB3	1.63	0.61
1:B:497:ILE:HD13	1:B:600:MET:HE1	1.81	0.61
1:A:631:GLN:O	1:A:633:PRO:HD3	2.01	0.61
1:B:429:SER:HB2	1:B:431:GLU:OE2	2.00	0.61
1:C:439:VAL:HG12	1:C:483:ILE:HD12	1.82	0.61
1:C:497:ILE:HG21	1:C:600:MET:CE	2.28	0.61
1:E:497:ILE:HD12	1:E:594:VAL:HG22	1.83	0.61
1:F:429:SER:HB2	1:F:431:GLU:OE2	2.00	0.61
1:A:327:LYS:O	1:A:327:LYS:HG3	2.01	0.60
1:D:500:LYS:HE3	1:D:599:ASP:OD2	2.01	0.60
1:A:341:ARG:O	1:A:345:ILE:HG12	2.01	0.60
1:A:370:ILE:HD13	1:A:409:VAL:O	2.02	0.60
1:C:465:ALA:HB3	1:C:663:ILE:HG13	1.83	0.60
1:F:341:ARG:O	1:F:345:ILE:HG12	2.00	0.60
1:A:554:ASN:HA	1:A:557:VAL:HG12	1.82	0.60
1:D:354:VAL:HG23	1:D:372:PRO:HA	1.83	0.60
1:D:497:ILE:HD12	1:D:594:VAL:HG22	1.83	0.60
1:F:598:ALA:HA	1:F:601:MET:HE3	1.83	0.60
1:C:429:SER:HB2	1:C:431:GLU:OE2	2.01	0.60
1:C:700:GLU:O	1:C:704:VAL:HG23	2.01	0.60
1:E:521:MET:HE3	1:E:600:MET:CG	2.29	0.60
1:A:658:ILE:HD12	1:A:658:ILE:N	2.17	0.60
1:E:329:LYS:HG2	1:E:330:SER:N	2.14	0.60
1:D:429:SER:HB2	1:D:431:GLU:OE2	2.02	0.60
1:E:423:PHE:HE1	1:E:481:LEU:HB3	1.65	0.60
1:C:497:ILE:HD12	1:C:594:VAL:HG22	1.84	0.59
1:E:465:ALA:HB3	1:E:663:ILE:HG13	1.84	0.59
1:C:713:ALA:HB1	1:C:714:PRO:HD2	1.84	0.59
1:F:532:VAL:O	1:F:536:GLU:HG2	2.02	0.59
1:A:378:VAL:HG23	1:F:387:ASP:OD2	2.03	0.59
1:E:658:ILE:HD12	1:E:658:ILE:N	2.15	0.59
1:A:685:THR:HG22	1:A:686:GLY:H	1.65	0.59
1:B:423:PHE:HE1	1:B:481:LEU:HB3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:ASN:HA	1:B:557:VAL:HG12	1.83	0.59
1:D:341:ARG:O	1:D:345:ILE:HG12	2.02	0.59
1:E:370:ILE:HD13	1:E:370:ILE:H	1.66	0.59
1:E:370:ILE:HD13	1:E:409:VAL:O	2.03	0.59
1:E:462:LEU:HD11	1:E:650:ILE:HD13	1.83	0.59
1:E:598:ALA:HA	1:E:601:MET:HE3	1.85	0.59
1:A:497:ILE:HD13	1:A:600:MET:HE1	1.84	0.59
1:A:601:MET:CE	1:A:637:VAL:HG13	2.33	0.59
1:C:572:PHE:HZ	1:C:579:ASP:HB3	1.66	0.59
1:B:465:ALA:HB1	1:B:633:PRO:HG3	1.83	0.59
1:C:500:LYS:HE3	1:C:599:ASP:OD2	2.02	0.59
1:A:497:ILE:HD12	1:A:594:VAL:HG22	1.85	0.58
1:D:465:ALA:HB3	1:D:663:ILE:HG13	1.84	0.58
1:F:700:GLU:O	1:F:704:VAL:HG23	2.03	0.58
1:B:402:VAL:HG13	1:B:687:LEU:HD11	1.85	0.58
1:F:658:ILE:HD12	1:F:658:ILE:N	2.15	0.58
1:D:329:LYS:H	1:D:329:LYS:HD3	1.69	0.58
1:C:341:ARG:O	1:C:345:ILE:HG12	2.04	0.58
1:F:354:VAL:HG23	1:F:372:PRO:HA	1.85	0.58
1:F:439:VAL:HG12	1:F:483:ILE:HD12	1.85	0.58
1:C:465:ALA:HB1	1:C:633:PRO:HG3	1.86	0.58
1:A:500:LYS:HE3	1:A:599:ASP:OD2	2.03	0.58
1:C:499:PRO:HB3	1:C:521:MET:CE	2.27	0.58
1:D:599:ASP:OD1	1:D:632:ARG:NH1	2.37	0.58
1:D:462:LEU:HD11	1:D:650:ILE:CD1	2.32	0.57
1:B:663:ILE:HD13	1:B:663:ILE:C	2.29	0.57
1:F:514:LEU:HD11	1:F:590:ILE:HD12	1.84	0.57
1:A:663:ILE:HD13	1:A:663:ILE:C	2.29	0.57
1:C:402:VAL:HG13	1:C:687:LEU:HD11	1.86	0.57
1:C:550:LEU:HD11	1:C:587:LEU:HB2	1.86	0.57
1:C:685:THR:HG22	1:C:686:GLY:H	1.67	0.57
1:E:497:ILE:HD13	1:E:600:MET:HE1	1.86	0.57
1:F:494:LEU:HD23	1:F:591:VAL:HB	1.86	0.57
1:A:661:ARG:HA	1:A:666:GLN:H	1.68	0.57
1:E:329:LYS:CG	1:E:330:SER:N	2.67	0.57
1:B:521:MET:HE3	1:B:600:MET:CB	2.33	0.57
1:D:329:LYS:CG	1:D:330:SER:N	2.66	0.57
1:E:685:THR:CG2	1:E:686:GLY:N	2.67	0.57
1:B:370:ILE:HD13	1:B:370:ILE:H	1.70	0.57
1:B:550:LEU:HD11	1:B:587:LEU:HB2	1.85	0.57
1:B:493:ARG:HD2	1:B:512:HIS:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:ALA:HA	1:B:601:MET:HE3	1.87	0.57
1:A:329:LYS:CG	1:A:330:SER:N	2.67	0.57
1:D:423:PHE:HE1	1:D:481:LEU:HB3	1.68	0.57
1:A:462:LEU:HD11	1:A:650:ILE:HD13	1.87	0.57
1:D:514:LEU:HD11	1:D:590:ILE:HD12	1.87	0.57
1:F:365:ILE:HG12	1:F:366:THR:N	2.19	0.57
1:A:465:ALA:HB3	1:A:663:ILE:HG13	1.87	0.57
1:A:685:THR:CG2	1:A:686:GLY:N	2.68	0.57
1:B:365:ILE:HD11	1:B:447:ILE:HB	1.86	0.57
1:C:354:VAL:HG23	1:C:372:PRO:HA	1.87	0.56
1:C:658:ILE:HD12	1:C:658:ILE:N	2.18	0.56
1:A:439:VAL:HG12	1:A:483:ILE:HD12	1.87	0.56
1:A:521:MET:HE3	1:A:600:MET:CG	2.34	0.56
1:B:329:LYS:CG	1:B:330:SER:N	2.68	0.56
1:B:465:ALA:HB3	1:B:663:ILE:HG13	1.87	0.56
1:B:685:THR:CG2	1:B:686:GLY:N	2.69	0.56
1:B:700:GLU:O	1:B:704:VAL:HG23	2.04	0.56
1:E:365:ILE:HD11	1:E:447:ILE:HB	1.86	0.56
1:E:470:SER:HB2	1:E:652:PHE:HB3	1.87	0.56
1:A:560:ALA:CB	1:A:567:LEU:HG	2.34	0.56
1:D:658:ILE:HD12	1:D:658:ILE:N	2.20	0.56
1:E:685:THR:HG22	1:E:686:GLY:H	1.69	0.56
1:C:329:LYS:CG	1:C:330:SER:N	2.66	0.56
1:D:370:ILE:HD13	1:D:370:ILE:H	1.71	0.56
1:E:550:LEU:HD11	1:E:587:LEU:HB2	1.86	0.56
1:E:658:ILE:H	1:E:658:ILE:CD1	2.18	0.56
1:F:329:LYS:H	1:F:329:LYS:HD3	1.70	0.56
1:F:560:ALA:CB	1:F:567:LEU:HG	2.35	0.56
1:D:365:ILE:HD11	1:D:447:ILE:HB	1.87	0.56
1:D:387:ASP:OD2	1:E:378:VAL:HG23	2.05	0.56
1:E:329:LYS:HD3	1:E:329:LYS:H	1.71	0.56
1:E:532:VAL:O	1:E:536:GLU:HG2	2.05	0.56
1:A:514:LEU:HD11	1:A:590:ILE:HD12	1.87	0.56
1:C:599:ASP:OD1	1:C:632:ARG:NH1	2.39	0.56
1:F:470:SER:HB2	1:F:652:PHE:HB3	1.88	0.56
1:E:402:VAL:HG13	1:E:687:LEU:HD11	1.88	0.56
1:F:550:LEU:HD11	1:F:587:LEU:HB2	1.87	0.56
1:B:462:LEU:HD11	1:B:650:ILE:CD1	2.36	0.56
1:A:470:SER:HB2	1:A:652:PHE:HB3	1.88	0.56
1:D:499:PRO:HB3	1:D:521:MET:CE	2.32	0.56
1:F:685:THR:CG2	1:F:686:GLY:N	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:ARG:HD2	1:C:512:HIS:O	2.06	0.55
1:C:423:PHE:HE1	1:C:481:LEU:HB3	1.69	0.55
1:E:521:MET:HE3	1:E:600:MET:CB	2.35	0.55
1:A:370:ILE:HD13	1:A:370:ILE:H	1.71	0.55
1:C:685:THR:CG2	1:C:686:GLY:N	2.69	0.55
1:B:354:VAL:HG23	1:B:372:PRO:HA	1.88	0.55
1:B:488:THR:HG23	1:B:491:GLU:OE2	2.06	0.55
1:C:560:ALA:CB	1:C:567:LEU:HG	2.35	0.55
1:E:465:ALA:HB1	1:E:633:PRO:HG3	1.88	0.55
1:F:500:LYS:C	1:F:502:LEU:N	2.63	0.55
1:A:347:LEU:HB3	1:A:352:VAL:HG23	1.89	0.55
1:A:462:LEU:HD11	1:A:650:ILE:CD1	2.35	0.55
1:D:532:VAL:O	1:D:536:GLU:HG2	2.06	0.55
1:E:494:LEU:HD23	1:E:591:VAL:HB	1.87	0.55
1:E:560:ALA:CB	1:E:567:LEU:HG	2.36	0.55
1:F:658:ILE:H	1:F:658:ILE:CD1	2.19	0.55
1:F:661:ARG:HA	1:F:666:GLN:H	1.71	0.55
1:C:494:LEU:HD23	1:C:591:VAL:HB	1.89	0.55
1:F:713:ALA:HB1	1:F:714:PRO:HD2	1.89	0.55
1:A:713:ALA:HB1	1:A:714:PRO:HD2	1.89	0.55
1:E:661:ARG:HA	1:E:666:GLN:H	1.71	0.54
1:E:700:GLU:O	1:E:704:VAL:HG23	2.07	0.54
1:A:677:ASP:OD1	1:A:690:ARG:NH1	2.36	0.54
1:A:658:ILE:H	1:A:658:ILE:CD1	2.19	0.54
1:D:465:ALA:HB1	1:D:633:PRO:HG3	1.89	0.54
1:F:347:LEU:HB3	1:F:352:VAL:HG23	1.89	0.54
1:D:550:LEU:HD11	1:D:587:LEU:HB2	1.90	0.54
1:C:329:LYS:H	1:C:329:LYS:HD3	1.71	0.54
1:D:685:THR:CG2	1:D:686:GLY:N	2.70	0.54
1:F:329:LYS:CG	1:F:330:SER:N	2.68	0.54
1:A:329:LYS:H	1:A:329:LYS:HD3	1.72	0.54
1:F:649:ARG:HB3	1:F:663:ILE:CD1	2.37	0.54
1:A:365:ILE:HD11	1:A:447:ILE:HB	1.88	0.54
1:C:462:LEU:HD11	1:C:650:ILE:CD1	2.38	0.54
1:D:554:ASN:HA	1:D:557:VAL:CG1	2.37	0.54
1:B:592:VAL:HB	1:B:626:LEU:HD12	1.89	0.54
1:E:599:ASP:OD1	1:E:632:ARG:NH1	2.40	0.54
1:A:550:LEU:HD11	1:A:587:LEU:HB2	1.89	0.54
1:F:521:MET:HE3	1:F:600:MET:CG	2.34	0.54
1:B:370:ILE:HD13	1:B:409:VAL:O	2.08	0.53
1:E:713:ALA:HB1	1:E:714:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ALA:HB1	1:A:633:PRO:HG3	1.88	0.53
1:B:452:ILE:C	1:B:453:ILE:HD12	2.33	0.53
1:B:685:THR:CG2	1:B:686:GLY:H	2.21	0.53
1:C:717:ILE:N	1:C:717:ILE:HD12	2.23	0.53
1:D:560:ALA:CB	1:D:567:LEU:HG	2.38	0.53
1:D:598:ALA:HA	1:D:601:MET:HE3	1.91	0.53
1:E:516:PRO:HG3	1:E:716:TYR:CE1	2.44	0.53
1:D:597:PHE:HD1	1:D:601:MET:HE2	1.69	0.53
1:D:677:ASP:OD1	1:D:690:ARG:NH1	2.39	0.53
1:F:663:ILE:HD13	1:F:663:ILE:C	2.33	0.53
1:F:717:ILE:N	1:F:717:ILE:HD12	2.23	0.53
1:D:663:ILE:HD13	1:D:663:ILE:C	2.32	0.53
1:F:554:ASN:HA	1:F:557:VAL:CG1	2.39	0.53
1:A:500:LYS:C	1:A:502:LEU:N	2.63	0.53
1:C:661:ARG:HA	1:C:666:GLN:H	1.73	0.53
1:A:365:ILE:HG12	1:A:366:THR:N	2.24	0.53
1:D:494:LEU:HD23	1:D:591:VAL:HB	1.90	0.53
1:A:631:GLN:C	1:A:633:PRO:HD3	2.33	0.53
1:B:329:LYS:H	1:B:329:LYS:HD3	1.74	0.53
1:B:717:ILE:HD12	1:B:717:ILE:N	2.24	0.53
1:E:514:LEU:HD11	1:E:590:ILE:HD12	1.90	0.53
1:F:685:THR:HG22	1:F:686:GLY:H	1.73	0.53
1:B:534:GLU:O	1:B:538:ARG:HG3	2.09	0.53
1:B:658:ILE:H	1:B:658:ILE:CD1	2.17	0.53
1:C:532:VAL:O	1:C:536:GLU:HG2	2.09	0.53
1:A:717:ILE:N	1:A:717:ILE:HD12	2.24	0.53
1:B:631:GLN:C	1:B:633:PRO:HD3	2.33	0.53
1:C:521:MET:HE3	1:C:600:MET:CB	2.39	0.53
1:C:534:GLU:O	1:C:538:ARG:HG3	2.09	0.53
1:D:497:ILE:HG21	1:D:600:MET:CE	2.32	0.53
1:F:497:ILE:HD12	1:F:594:VAL:HG22	1.91	0.53
1:F:541:LEU:O	1:F:545:MET:HG2	2.08	0.52
1:D:657:LYS:HG2	1:D:670:GLU:OE1	2.09	0.52
1:B:560:ALA:CB	1:B:567:LEU:HG	2.38	0.52
1:E:663:ILE:HD13	1:E:663:ILE:C	2.34	0.52
1:A:317:PRO:C	1:A:319:SER:H	2.18	0.52
1:A:685:THR:CG2	1:A:686:GLY:H	2.21	0.52
1:D:470:SER:HB2	1:D:652:PHE:HB3	1.92	0.52
1:D:661:ARG:HA	1:D:666:GLN:H	1.74	0.52
1:D:672:LEU:HD13	1:D:678:MET:HA	1.91	0.52
1:F:465:ALA:HB1	1:F:633:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:LYS:C	1:D:502:LEU:N	2.62	0.52
1:D:685:THR:HG22	1:D:686:GLY:H	1.74	0.52
1:F:464:VAL:O	1:F:629:ALA:HA	2.10	0.52
1:C:329:LYS:CG	1:C:330:SER:H	2.12	0.52
1:D:402:VAL:HG13	1:D:687:LEU:HD11	1.92	0.52
1:B:657:LYS:HG2	1:B:670:GLU:OE1	2.10	0.52
1:F:545:MET:HE2	1:F:553:PHE:CD1	2.45	0.52
1:C:354:VAL:HG22	1:C:355:SER:N	2.25	0.51
1:C:462:LEU:HD11	1:C:650:ILE:HD13	1.92	0.51
1:C:663:ILE:HD13	1:C:663:ILE:C	2.35	0.51
1:D:460:PRO:HG2	1:D:461:HIS:CD2	2.45	0.51
1:E:685:THR:CG2	1:E:686:GLY:H	2.24	0.51
1:A:329:LYS:CG	1:A:330:SER:H	2.11	0.51
1:A:699:ASP:HB3	1:A:703:ARG:HH11	1.75	0.51
1:C:631:GLN:C	1:C:633:PRO:HD3	2.35	0.51
1:F:465:ALA:HB3	1:F:663:ILE:HG13	1.92	0.51
1:B:387:ASP:OD2	1:C:378:VAL:HG23	2.10	0.51
1:C:598:ALA:HA	1:C:601:MET:HE3	1.92	0.51
1:E:677:ASP:OD1	1:E:690:ARG:NH1	2.36	0.51
1:D:347:LEU:HB3	1:D:352:VAL:HG23	1.92	0.51
1:D:390:ARG:HE	1:E:378:VAL:CG2	2.22	0.51
1:B:354:VAL:HG23	1:B:371:GLN:C	2.36	0.51
1:C:516:PRO:HG3	1:C:716:TYR:CE1	2.44	0.51
1:C:354:VAL:HG22	1:C:355:SER:H	1.76	0.51
1:F:677:ASP:OD1	1:F:690:ARG:NH1	2.39	0.51
1:C:685:THR:CG2	1:C:686:GLY:H	2.23	0.51
1:A:547:VAL:HG12	1:A:549:ASN:H	1.76	0.51
1:F:488:THR:HG23	1:F:491:GLU:OE2	2.12	0.51
1:A:354:VAL:HG21	1:A:370:ILE:CG1	2.41	0.50
1:C:317:PRO:C	1:C:319:SER:H	2.17	0.50
1:C:495:ILE:HG13	1:C:514:LEU:HD12	1.93	0.50
1:B:462:LEU:HD11	1:B:650:ILE:HD13	1.92	0.50
1:B:470:SER:HB2	1:B:652:PHE:HB3	1.93	0.50
1:B:494:LEU:HD23	1:B:591:VAL:HB	1.93	0.50
1:F:539:TYR:HA	1:F:542:MET:HE3	1.94	0.50
1:B:713:ALA:HB1	1:B:714:PRO:HD2	1.92	0.50
1:A:554:ASN:HA	1:A:557:VAL:CG1	2.41	0.50
1:B:599:ASP:OD1	1:B:632:ARG:NH1	2.44	0.50
1:D:354:VAL:HG21	1:D:370:ILE:CG1	2.41	0.50
1:E:592:VAL:HB	1:E:626:LEU:HD12	1.94	0.50
1:E:717:ILE:O	1:E:719:ASP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:ALA:O	1:E:376:VAL:HG13	2.11	0.50
1:B:545:MET:HE2	1:B:553:PHE:CD1	2.46	0.50
1:F:592:VAL:HB	1:F:626:LEU:HD12	1.94	0.50
1:B:672:LEU:HD13	1:B:678:MET:HA	1.94	0.50
1:E:663:ILE:HG23	1:E:664:LEU:HG	1.93	0.50
1:C:500:LYS:C	1:C:502:LEU:N	2.62	0.50
1:D:717:ILE:HD12	1:D:717:ILE:N	2.26	0.50
1:F:497:ILE:HD13	1:F:600:MET:HE1	1.94	0.50
1:B:317:PRO:C	1:B:319:SER:H	2.19	0.50
1:B:500:LYS:C	1:B:502:LEU:N	2.62	0.50
1:F:599:ASP:OD1	1:F:632:ARG:NH1	2.45	0.49
1:C:592:VAL:HB	1:C:626:LEU:HD12	1.94	0.49
1:C:597:PHE:HD1	1:C:601:MET:HE2	1.72	0.49
1:E:317:PRO:C	1:E:319:SER:H	2.20	0.49
1:E:380:ARG:O	1:E:384:LEU:CD2	2.59	0.49
1:E:699:ASP:HB3	1:E:703:ARG:HH11	1.76	0.49
1:A:717:ILE:O	1:A:719:ASP:N	2.46	0.49
1:B:563:ALA:C	1:B:565:THR:H	2.19	0.49
1:D:373:ALA:O	1:D:376:VAL:HG13	2.12	0.49
1:E:462:LEU:HD11	1:E:650:ILE:HD12	1.94	0.49
1:E:717:ILE:N	1:E:717:ILE:HD12	2.27	0.49
1:A:592:VAL:HB	1:A:626:LEU:HD12	1.94	0.49
1:B:563:ALA:O	1:B:565:THR:N	2.46	0.49
1:B:717:ILE:O	1:B:719:ASP:N	2.46	0.49
1:C:365:ILE:HG12	1:C:366:THR:N	2.28	0.49
1:E:460:PRO:HG2	1:E:461:HIS:CD2	2.48	0.49
1:E:500:LYS:C	1:E:502:LEU:N	2.63	0.49
1:B:373:ALA:O	1:B:376:VAL:HG13	2.12	0.49
1:D:717:ILE:O	1:D:719:ASP:N	2.46	0.49
1:F:364:VAL:HG22	1:F:418:ARG:HG3	1.95	0.49
1:E:390:ARG:HE	1:F:378:VAL:CG2	2.26	0.49
1:F:317:PRO:C	1:F:319:SER:H	2.21	0.49
1:A:549:ASN:OD1	1:A:551:ALA:HB3	2.13	0.49
1:B:393:ALA:HB2	1:C:407:THR:CG2	2.43	0.49
1:C:672:LEU:HD13	1:C:678:MET:HA	1.93	0.49
1:D:497:ILE:HD13	1:D:600:MET:HE1	1.95	0.49
1:D:713:ALA:HB1	1:D:714:PRO:HD2	1.94	0.49
1:A:598:ALA:HA	1:A:601:MET:HE3	1.95	0.49
1:C:364:VAL:HG22	1:C:418:ARG:HG3	1.95	0.49
1:E:545:MET:HE2	1:E:553:PHE:CD1	2.48	0.49
1:A:545:MET:HE2	1:A:553:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:THR:O	1:B:643:LYS:HG3	2.13	0.48
1:D:521:MET:HE3	1:D:600:MET:CB	2.42	0.48
1:F:672:LEU:HD13	1:F:678:MET:HA	1.95	0.48
1:F:711:ARG:HG3	1:F:711:ARG:NH2	2.24	0.48
1:B:332:SER:OG	1:B:334:GLU:HG3	2.13	0.48
1:C:563:ALA:C	1:C:565:THR:H	2.21	0.48
1:B:516:PRO:HG3	1:B:716:TYR:CE1	2.49	0.48
1:E:493:ARG:NH2	1:E:513:LEU:O	2.46	0.48
1:E:534:GLU:O	1:E:538:ARG:HG3	2.13	0.48
1:C:493:ARG:NH2	1:C:513:LEU:O	2.46	0.48
1:C:716:TYR:C	1:C:717:ILE:HD12	2.39	0.48
1:B:549:ASN:OD1	1:B:551:ALA:HB3	2.14	0.48
1:D:631:GLN:O	1:D:633:PRO:HD3	2.13	0.48
1:E:578:ASP:O	1:E:579:ASP:C	2.56	0.48
1:F:515:CYS:HB3	1:F:720:ILE:HG21	1.95	0.48
1:B:365:ILE:HG12	1:B:366:THR:N	2.28	0.48
1:B:380:ARG:O	1:B:384:LEU:CD2	2.61	0.48
1:B:554:ASN:HA	1:B:557:VAL:CG1	2.43	0.48
1:F:380:ARG:O	1:F:384:LEU:CD2	2.61	0.48
1:C:677:ASP:OD1	1:C:690:ARG:NH1	2.40	0.48
1:F:717:ILE:O	1:F:719:ASP:N	2.47	0.48
1:C:470:SER:HB2	1:C:652:PHE:HB3	1.95	0.48
1:D:463:LEU:HG	1:D:646:ILE:HG21	1.96	0.48
1:E:457:ALA:HA	1:E:625:HIS:CD2	2.48	0.48
1:A:532:VAL:O	1:A:536:GLU:HG2	2.14	0.48
1:C:717:ILE:O	1:C:719:ASP:N	2.46	0.48
1:E:347:LEU:HB3	1:E:352:VAL:HG23	1.96	0.48
1:B:354:VAL:HG21	1:B:370:ILE:CG1	2.44	0.48
1:B:532:VAL:O	1:B:536:GLU:HG2	2.13	0.48
1:B:661:ARG:HA	1:B:666:GLN:H	1.79	0.48
1:E:554:ASN:HA	1:E:557:VAL:CG1	2.43	0.48
1:A:452:ILE:C	1:A:453:ILE:HD12	2.38	0.47
1:A:648:THR:OG1	1:A:683:PRO:HD3	2.13	0.47
1:B:711:ARG:HG3	1:B:711:ARG:NH2	2.27	0.47
1:C:354:VAL:HG21	1:C:370:ILE:CG1	2.43	0.47
1:C:649:ARG:HB3	1:C:663:ILE:CD1	2.44	0.47
1:A:563:ALA:C	1:A:565:THR:H	2.22	0.47
1:C:649:ARG:HB3	1:C:663:ILE:HD13	1.96	0.47
1:D:578:ASP:O	1:D:579:ASP:C	2.57	0.47
1:E:639:THR:O	1:E:643:LYS:HG3	2.14	0.47
1:F:354:VAL:HG21	1:F:370:ILE:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:ILE:HD11	1:C:447:ILE:HB	1.96	0.47
1:D:658:ILE:H	1:D:658:ILE:CD1	2.23	0.47
1:E:354:VAL:HG23	1:E:372:PRO:CA	2.45	0.47
1:F:460:PRO:HG2	1:F:461:HIS:CD2	2.49	0.47
1:F:631:GLN:O	1:F:633:PRO:HD3	2.13	0.47
1:B:460:PRO:HG2	1:B:461:HIS:CD2	2.49	0.47
1:C:658:ILE:H	1:C:658:ILE:CD1	2.23	0.47
1:B:354:VAL:HG22	1:B:355:SER:N	2.30	0.47
1:D:354:VAL:HG22	1:D:355:SER:N	2.30	0.47
1:A:515:CYS:HB3	1:A:720:ILE:HG21	1.96	0.47
1:D:516:PRO:HG3	1:D:716:TYR:CE1	2.50	0.47
1:F:365:ILE:HD11	1:F:447:ILE:HB	1.96	0.47
1:A:663:ILE:HG23	1:A:664:LEU:HG	1.97	0.47
1:C:317:PRO:C	1:C:319:SER:N	2.73	0.47
1:D:354:VAL:HG22	1:D:355:SER:H	1.80	0.47
1:F:563:ALA:C	1:F:565:THR:H	2.23	0.47
1:F:685:THR:CG2	1:F:686:GLY:H	2.26	0.47
1:F:373:ALA:O	1:F:376:VAL:HG13	2.14	0.47
1:F:578:ASP:O	1:F:579:ASP:C	2.58	0.47
1:A:460:PRO:HG2	1:A:461:HIS:CD2	2.50	0.46
1:A:534:GLU:O	1:A:538:ARG:HG3	2.14	0.46
1:E:563:ALA:C	1:E:565:THR:H	2.23	0.46
1:B:699:ASP:HB3	1:B:703:ARG:HH11	1.80	0.46
1:D:354:VAL:HG23	1:D:371:GLN:C	2.40	0.46
1:D:550:LEU:HD22	1:D:623:GLY:HA3	1.96	0.46
1:C:320:LEU:O	1:C:703:ARG:NH2	2.45	0.46
1:C:545:MET:HE2	1:C:553:PHE:CD1	2.49	0.46
1:C:578:ASP:O	1:C:579:ASP:C	2.57	0.46
1:F:354:VAL:HG22	1:F:355:SER:H	1.80	0.46
1:A:516:PRO:HG3	1:A:716:TYR:CE1	2.51	0.46
1:A:539:TYR:HA	1:A:542:MET:HE3	1.97	0.46
1:B:663:ILE:HG23	1:B:664:LEU:HG	1.97	0.46
1:D:663:ILE:HG23	1:D:664:LEU:HG	1.96	0.46
1:E:464:VAL:O	1:E:629:ALA:HA	2.15	0.46
1:F:495:ILE:HG13	1:F:514:LEU:HD12	1.97	0.46
1:F:516:PRO:HG3	1:F:716:TYR:CE1	2.51	0.46
1:C:465:ALA:CB	1:C:663:ILE:HG13	2.45	0.46
1:D:685:THR:CG2	1:D:686:GLY:H	2.27	0.46
1:A:317:PRO:C	1:A:319:SER:N	2.74	0.46
1:A:716:TYR:C	1:A:717:ILE:HD12	2.41	0.46
1:C:554:ASN:HA	1:C:557:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:541:LEU:O	1:E:545:MET:HG2	2.15	0.46
1:E:631:GLN:C	1:E:633:PRO:HD3	2.40	0.46
1:F:521:MET:HE3	1:F:600:MET:CB	2.46	0.46
1:A:578:ASP:O	1:A:579:ASP:C	2.58	0.46
1:B:648:THR:OG1	1:B:683:PRO:HD3	2.16	0.46
1:B:716:TYR:C	1:B:717:ILE:HD12	2.41	0.46
1:D:329:LYS:H	1:D:329:LYS:CD	2.28	0.46
1:D:592:VAL:HB	1:D:626:LEU:HD12	1.98	0.46
1:F:547:VAL:HG12	1:F:549:ASN:H	1.79	0.46
1:B:329:LYS:CG	1:B:330:SER:H	2.13	0.46
1:B:317:PRO:C	1:B:319:SER:N	2.74	0.45
1:F:657:LYS:HG2	1:F:670:GLU:OE1	2.15	0.45
1:F:663:ILE:HG23	1:F:664:LEU:HG	1.97	0.45
1:B:390:ARG:HE	1:C:378:VAL:CG2	2.29	0.45
1:B:578:ASP:O	1:B:579:ASP:C	2.58	0.45
1:B:631:GLN:O	1:B:633:PRO:HD3	2.16	0.45
1:A:494:LEU:CD2	1:A:591:VAL:HB	2.44	0.45
1:A:672:LEU:HD13	1:A:678:MET:HA	1.98	0.45
1:C:699:ASP:HB3	1:C:703:ARG:HH11	1.81	0.45
1:D:563:ALA:C	1:D:565:THR:H	2.25	0.45
1:F:329:LYS:HD3	1:F:329:LYS:N	2.31	0.45
1:B:541:LEU:O	1:B:545:MET:HG2	2.16	0.45
1:C:560:ALA:HB2	1:C:567:LEU:HG	1.98	0.45
1:F:649:ARG:HB3	1:F:663:ILE:HD13	1.98	0.45
1:A:364:VAL:HG22	1:A:418:ARG:HG3	1.98	0.45
1:C:711:ARG:HG3	1:C:711:ARG:NH2	2.28	0.45
1:F:560:ALA:HB2	1:F:567:LEU:HG	1.98	0.45
1:B:320:LEU:O	1:B:703:ARG:NH2	2.42	0.45
1:C:515:CYS:SG	1:C:720:ILE:HD13	2.57	0.45
1:E:329:LYS:H	1:E:329:LYS:CD	2.30	0.45
1:E:452:ILE:C	1:E:453:ILE:HD12	2.41	0.45
1:F:354:VAL:HG22	1:F:355:SER:N	2.32	0.45
1:C:329:LYS:H	1:C:329:LYS:CD	2.30	0.45
1:C:432:TYR:HB2	1:C:453:ILE:HG12	1.99	0.45
1:D:649:ARG:HB3	1:D:663:ILE:CD1	2.46	0.45
1:E:332:SER:OG	1:E:334:GLU:HG3	2.16	0.45
1:F:354:VAL:HG23	1:F:372:PRO:CA	2.46	0.45
1:F:597:PHE:HD1	1:F:601:MET:HE2	1.77	0.45
1:F:672:LEU:HD21	1:F:679:LEU:HG	1.98	0.45
1:B:347:LEU:HB3	1:B:352:VAL:HG23	1.98	0.45
1:C:354:VAL:HG23	1:C:371:GLN:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:ILE:HG23	1:C:664:LEU:HG	1.98	0.45
1:D:639:THR:O	1:D:643:LYS:HG3	2.17	0.45
1:A:378:VAL:CG1	1:A:401:GLU:HG2	2.46	0.45
1:A:657:LYS:HG2	1:A:670:GLU:OE1	2.17	0.45
1:B:409:VAL:HG12	1:B:410:GLY:N	2.32	0.45
1:C:332:SER:OG	1:C:334:GLU:HG3	2.16	0.45
1:D:465:ALA:CB	1:D:663:ILE:HG13	2.47	0.45
1:E:354:VAL:HG21	1:E:370:ILE:CG1	2.46	0.45
1:E:450:ARG:HG2	1:E:450:ARG:HH21	1.82	0.45
1:E:672:LEU:HD21	1:E:679:LEU:HG	1.99	0.45
1:F:354:VAL:HG23	1:F:371:GLN:C	2.41	0.45
1:F:459:MET:N	1:F:460:PRO:HA	2.32	0.45
1:F:472:LYS:O	1:F:476:VAL:HG23	2.17	0.45
1:A:464:VAL:O	1:A:629:ALA:HA	2.16	0.45
1:E:672:LEU:HD13	1:E:678:MET:HA	1.99	0.45
1:A:354:VAL:HG23	1:A:372:PRO:CA	2.46	0.44
1:B:465:ALA:CB	1:B:663:ILE:HG13	2.47	0.44
1:D:329:LYS:HD3	1:D:329:LYS:N	2.29	0.44
1:E:649:ARG:HB3	1:E:663:ILE:CD1	2.47	0.44
1:F:497:ILE:HG21	1:F:600:MET:CE	2.35	0.44
1:B:495:ILE:HG13	1:B:514:LEU:HD12	1.98	0.44
1:B:649:ARG:HB3	1:B:663:ILE:CD1	2.48	0.44
1:C:452:ILE:C	1:C:453:ILE:HD12	2.42	0.44
1:E:393:ALA:HB2	1:F:407:THR:CG2	2.48	0.44
1:F:329:LYS:H	1:F:329:LYS:CD	2.29	0.44
1:A:599:ASP:OD1	1:A:632:ARG:NH1	2.51	0.44
1:C:373:ALA:O	1:C:376:VAL:HG13	2.17	0.44
1:C:459:MET:N	1:C:460:PRO:HA	2.33	0.44
1:E:365:ILE:HG12	1:E:366:THR:N	2.32	0.44
1:A:329:LYS:H	1:A:329:LYS:CD	2.31	0.44
1:A:378:VAL:CG2	1:F:390:ARG:HE	2.31	0.44
1:D:354:VAL:HG23	1:D:372:PRO:CA	2.46	0.44
1:D:393:ALA:HB2	1:E:407:THR:CG2	2.48	0.44
1:B:450:ARG:HG2	1:B:450:ARG:HH21	1.82	0.44
1:C:427:LEU:HD22	1:C:432:TYR:CZ	2.52	0.44
1:D:332:SER:OG	1:D:334:GLU:HG3	2.18	0.44
1:E:593:VAL:HG12	1:E:627:ILE:HB	1.99	0.44
1:F:450:ARG:HG2	1:F:450:ARG:HH21	1.83	0.44
1:C:380:ARG:O	1:C:384:LEU:CD2	2.62	0.44
1:C:550:LEU:HD22	1:C:623:GLY:HA3	1.99	0.44
1:C:631:GLN:O	1:C:633:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:LEU:O	1:D:703:ARG:NH2	2.43	0.44
1:F:534:GLU:O	1:F:538:ARG:HG3	2.18	0.44
1:A:322:ASP:HA	1:A:323:PRO:HD3	1.83	0.44
1:A:612:ILE:HD12	1:A:628:LEU:HD11	1.99	0.44
1:C:497:ILE:HD13	1:C:600:MET:CE	2.47	0.44
1:C:612:ILE:HD12	1:C:628:LEU:HD11	1.99	0.44
1:D:545:MET:HE2	1:D:553:PHE:CD1	2.52	0.44
1:E:497:ILE:HG21	1:E:600:MET:CE	2.31	0.44
1:F:432:TYR:HB2	1:F:453:ILE:HG12	1.99	0.44
1:A:563:ALA:O	1:A:565:THR:N	2.51	0.44
1:B:354:VAL:HG23	1:B:372:PRO:CA	2.48	0.44
1:B:717:ILE:C	1:B:719:ASP:N	2.76	0.44
1:C:518:VAL:HG22	1:C:721:LEU:HD21	2.00	0.44
1:A:329:LYS:HD3	1:A:329:LYS:N	2.32	0.43
1:D:633:PRO:C	1:D:662:THR:HG21	2.43	0.43
1:F:494:LEU:CD2	1:F:591:VAL:HB	2.48	0.43
1:A:717:ILE:C	1:A:719:ASP:N	2.75	0.43
1:C:717:ILE:C	1:C:719:ASP:N	2.76	0.43
1:D:717:ILE:C	1:D:719:ASP:N	2.76	0.43
1:E:521:MET:HB3	1:E:604:VAL:HG23	2.00	0.43
1:E:631:GLN:O	1:E:633:PRO:HD3	2.18	0.43
1:A:332:SER:OG	1:A:334:GLU:HG3	2.18	0.43
1:C:563:ALA:O	1:C:565:THR:N	2.51	0.43
1:D:317:PRO:C	1:D:319:SER:H	2.25	0.43
1:E:329:LYS:HD3	1:E:329:LYS:N	2.32	0.43
1:E:409:VAL:HG12	1:E:410:GLY:N	2.33	0.43
1:C:547:VAL:HG12	1:C:549:ASN:H	1.82	0.43
1:E:539:TYR:HA	1:E:542:MET:HE3	2.00	0.43
1:A:354:VAL:HG23	1:A:371:GLN:C	2.44	0.43
1:B:446:ASP:OD2	1:B:450:ARG:HB2	2.19	0.43
1:D:364:VAL:HB	1:D:692:HIS:CE1	2.54	0.43
1:E:432:TYR:HB2	1:E:453:ILE:HG12	2.01	0.43
1:F:631:GLN:C	1:F:633:PRO:HD3	2.43	0.43
1:C:450:ARG:HG2	1:C:450:ARG:HH21	1.82	0.43
1:E:494:LEU:CD2	1:E:591:VAL:HB	2.49	0.43
1:E:547:VAL:HG12	1:E:549:ASN:H	1.81	0.43
1:F:717:ILE:C	1:F:719:ASP:N	2.76	0.43
1:A:427:LEU:HD22	1:A:432:TYR:CE2	2.54	0.43
1:B:678:MET:HG2	1:B:691:VAL:O	2.19	0.43
1:C:347:LEU:HB3	1:C:352:VAL:HG23	2.01	0.43
1:D:341:ARG:N	1:D:341:ARG:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:CYS:HB3	1:D:720:ILE:HG21	2.01	0.43
1:E:716:TYR:C	1:E:717:ILE:HD12	2.44	0.43
1:F:320:LEU:O	1:F:703:ARG:NH2	2.44	0.43
1:E:515:CYS:HB3	1:E:720:ILE:HG21	2.00	0.43
1:B:515:CYS:HB3	1:B:720:ILE:HG21	2.00	0.43
1:E:560:ALA:HB2	1:E:567:LEU:HG	2.00	0.43
1:E:648:THR:OG1	1:E:683:PRO:HD3	2.19	0.43
1:F:716:TYR:C	1:F:717:ILE:HD12	2.43	0.43
1:A:566:PRO:HB2	1:A:583:GLN:OE1	2.19	0.43
1:A:678:MET:HG2	1:A:691:VAL:O	2.19	0.43
1:B:541:LEU:HD22	1:B:553:PHE:CE1	2.54	0.43
1:C:322:ASP:HA	1:C:323:PRO:HD3	1.84	0.43
1:D:563:ALA:O	1:D:565:THR:N	2.52	0.43
1:D:711:ARG:HG3	1:D:711:ARG:NH2	2.31	0.43
1:E:317:PRO:C	1:E:319:SER:N	2.75	0.43
1:F:518:VAL:HG22	1:F:721:LEU:HD21	2.01	0.43
1:B:329:LYS:H	1:B:329:LYS:CD	2.32	0.42
1:F:373:ALA:O	1:F:376:VAL:CG1	2.66	0.42
1:F:563:ALA:O	1:F:565:THR:N	2.52	0.42
1:A:446:ASP:OD2	1:A:450:ARG:HB2	2.20	0.42
1:A:711:ARG:HG3	1:A:711:ARG:NH2	2.31	0.42
1:B:547:VAL:HG12	1:B:549:ASN:H	1.84	0.42
1:C:329:LYS:HD3	1:C:329:LYS:N	2.32	0.42
1:F:361:PRO:HA	1:F:366:THR:HG23	2.00	0.42
1:A:643:LYS:O	1:A:644:ALA:C	2.62	0.42
1:B:566:PRO:CB	1:B:583:GLN:OE1	2.67	0.42
1:B:493:ARG:NH2	1:B:513:LEU:O	2.53	0.42
1:C:539:TYR:OH	1:C:621:ALA:HB3	2.19	0.42
1:C:657:LYS:HG2	1:C:670:GLU:OE1	2.20	0.42
1:D:380:ARG:O	1:D:384:LEU:CD2	2.61	0.42
1:D:518:VAL:HG22	1:D:721:LEU:HD21	2.01	0.42
1:E:364:VAL:HG22	1:E:418:ARG:HG3	2.00	0.42
1:E:465:ALA:CB	1:E:663:ILE:HG13	2.49	0.42
1:A:450:ARG:HG2	1:A:450:ARG:HH21	1.84	0.42
1:A:465:ALA:CB	1:A:663:ILE:HG13	2.49	0.42
1:D:631:GLN:C	1:D:633:PRO:HD3	2.44	0.42
1:E:702:HIS:O	1:E:706:GLU:HG2	2.20	0.42
1:A:495:ILE:HG13	1:A:514:LEU:HD12	2.02	0.42
1:E:354:VAL:HG23	1:E:371:GLN:C	2.44	0.42
1:A:649:ARG:HB3	1:A:663:ILE:CD1	2.49	0.42
1:B:464:VAL:O	1:B:629:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:PRO:HB2	1:B:583:GLN:OE1	2.18	0.42
1:D:720:ILE:HG23	1:D:721:LEU:N	2.35	0.42
1:E:495:ILE:HG13	1:E:514:LEU:HD12	2.02	0.42
1:E:711:ARG:HG3	1:E:711:ARG:NH2	2.30	0.42
1:F:317:PRO:C	1:F:319:SER:N	2.76	0.42
1:A:427:LEU:HD22	1:A:432:TYR:CZ	2.54	0.42
1:D:365:ILE:HG12	1:D:366:THR:N	2.34	0.42
1:D:427:LEU:HD22	1:D:432:TYR:CE2	2.55	0.42
1:E:390:ARG:HH11	1:F:378:VAL:CG2	2.33	0.42
1:B:601:MET:HE1	1:B:637:VAL:CG1	2.46	0.42
1:E:550:LEU:HD22	1:E:623:GLY:HA3	2.02	0.42
1:D:716:TYR:C	1:D:717:ILE:HD12	2.45	0.42
1:E:370:ILE:HD12	1:E:411:ILE:HG13	2.01	0.42
1:E:413:ILE:HA	1:E:414:PRO:HD3	1.94	0.42
1:B:329:LYS:HD3	1:B:329:LYS:N	2.34	0.41
1:B:370:ILE:HD12	1:B:411:ILE:HG13	2.02	0.41
1:C:420:MET:HE2	2:C:1723:ADP:C2	2.55	0.41
1:E:328:GLN:HE21	1:E:328:GLN:HB2	1.66	0.41
1:E:612:ILE:HD12	1:E:628:LEU:HD11	2.01	0.41
1:E:638:ILE:HG22	1:E:643:LYS:CG	2.50	0.41
1:A:560:ALA:HB2	1:A:567:LEU:HG	2.00	0.41
1:B:638:ILE:HG22	1:B:643:LYS:CG	2.51	0.41
1:C:390:ARG:HH11	1:D:378:VAL:CG2	2.33	0.41
1:A:459:MET:N	1:A:460:PRO:HA	2.36	0.41
1:B:462:LEU:HD11	1:B:650:ILE:HD12	2.02	0.41
1:A:515:CYS:SG	1:A:720:ILE:HD13	2.60	0.41
1:A:566:PRO:CB	1:A:583:GLN:OE1	2.69	0.41
1:B:672:LEU:HD21	1:B:679:LEU:HG	2.02	0.41
1:D:390:ARG:NE	1:E:378:VAL:HG22	2.36	0.41
1:D:560:ALA:HB2	1:D:567:LEU:HG	2.01	0.41
1:F:452:ILE:C	1:F:453:ILE:HD12	2.45	0.41
1:A:407:THR:CG2	1:F:393:ALA:HB2	2.51	0.41
1:C:373:ALA:O	1:C:376:VAL:CG1	2.68	0.41
1:E:580:GLU:HA	1:E:581:PRO:HD3	1.93	0.41
1:E:354:VAL:HG22	1:E:355:SER:N	2.35	0.41
1:A:315:LEU:N	1:A:711:ARG:HE	2.19	0.41
1:B:354:VAL:HG21	1:B:370:ILE:HG13	2.03	0.41
1:B:420:MET:HE2	2:B:1723:ADP:C2	2.56	0.41
1:B:459:MET:N	1:B:460:PRO:HA	2.35	0.41
1:E:563:ALA:O	1:E:565:THR:N	2.53	0.41
1:E:717:ILE:C	1:E:719:ASP:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:HG21	1:A:370:ILE:HG13	2.03	0.41
1:B:463:LEU:HG	1:B:646:ILE:HG21	2.02	0.41
1:C:580:GLU:HA	1:C:581:PRO:HD3	1.95	0.41
1:E:320:LEU:O	1:E:703:ARG:NH2	2.47	0.41
1:F:341:ARG:N	1:F:341:ARG:HD2	2.35	0.41
1:B:373:ALA:O	1:B:376:VAL:CG1	2.68	0.41
1:C:512:HIS:HE1	1:C:708:TRP:CD2	2.39	0.41
1:C:549:ASN:OD1	1:C:551:ALA:HB3	2.21	0.41
1:E:341:ARG:N	1:E:341:ARG:HD2	2.35	0.41
1:E:347:LEU:HD23	1:E:347:LEU:HA	1.92	0.41
1:F:665:ASP:O	1:F:666:GLN:HB2	2.20	0.41
1:A:354:VAL:HG22	1:A:355:SER:H	1.86	0.41
1:A:457:ALA:HA	1:A:625:HIS:CD2	2.56	0.41
1:A:521:MET:HE3	1:A:600:MET:CB	2.51	0.41
1:B:677:ASP:OD1	1:B:690:ARG:NH1	2.43	0.41
1:C:672:LEU:HD21	1:C:679:LEU:HG	2.02	0.41
1:D:347:LEU:HD23	1:D:347:LEU:HA	1.95	0.41
1:D:539:TYR:HA	1:D:542:MET:HE3	2.02	0.41
1:E:641:LEU:HD23	1:E:641:LEU:HA	1.86	0.41
1:C:413:ILE:HA	1:C:414:PRO:HD3	1.91	0.40
1:D:354:VAL:HG21	1:D:370:ILE:HG13	2.02	0.40
1:E:427:LEU:HD22	1:E:432:TYR:CE2	2.56	0.40
1:E:501:MET:HE3	1:E:519:THR:CG2	2.51	0.40
1:F:593:VAL:HG12	1:F:627:ILE:HB	2.03	0.40
1:A:453:ILE:HD12	1:A:453:ILE:N	2.36	0.40
1:B:472:LYS:HE2	1:B:472:LYS:HB3	1.99	0.40
1:B:539:TYR:OH	1:B:621:ALA:HB3	2.21	0.40
1:C:648:THR:OG1	1:C:683:PRO:HD3	2.21	0.40
1:D:450:ARG:HH21	1:D:450:ARG:HG2	1.86	0.40
1:E:518:VAL:HG22	1:E:721:LEU:HD21	2.03	0.40
1:F:322:ASP:HA	1:F:323:PRO:HD3	1.79	0.40
1:A:440:PRO:O	1:A:482:SER:HB3	2.22	0.40
1:B:560:ALA:HB2	1:B:567:LEU:HG	2.03	0.40
1:C:488:THR:HG23	1:C:491:GLU:OE2	2.20	0.40
1:D:317:PRO:C	1:D:319:SER:N	2.79	0.40
1:D:612:ILE:HD12	1:D:628:LEU:HD11	2.04	0.40
1:E:457:ALA:HA	1:E:625:HIS:NE2	2.36	0.40
1:E:566:PRO:HB2	1:E:583:GLN:OE1	2.22	0.40
1:E:566:PRO:CB	1:E:583:GLN:OE1	2.70	0.40
1:E:657:LYS:HG2	1:E:670:GLU:OE1	2.21	0.40
1:F:639:THR:O	1:F:643:LYS:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:LEU:HD22	1:D:432:TYR:CZ	2.57	0.40
1:F:383:ASN:HD22	1:F:383:ASN:HA	1.63	0.40
1:A:320:LEU:O	1:A:703:ARG:NH2	2.44	0.40
1:E:418:ARG:NH2	1:E:675:HIS:HB2	2.36	0.40
1:F:593:VAL:O	1:F:593:VAL:HG23	2.20	0.40
1:F:711:ARG:HH21	1:F:711:ARG:CG	2.29	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ALA:O	1:D:434:GLU:OE2[4_554]	2.00	0.20

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	406/491 (83%)	373 (92%)	27 (7%)	6 (2%)	8	28
1	B	406/491 (83%)	376 (93%)	25 (6%)	5 (1%)	10	34
1	C	406/491 (83%)	377 (93%)	24 (6%)	5 (1%)	10	34
1	D	406/491 (83%)	380 (94%)	21 (5%)	5 (1%)	10	34
1	E	406/491 (83%)	375 (92%)	26 (6%)	5 (1%)	10	34
1	F	406/491 (83%)	375 (92%)	26 (6%)	5 (1%)	10	34
All	All	2436/2946 (83%)	2256 (93%)	149 (6%)	31 (1%)	9	32

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	MET
1	B	501	MET

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Mol	Chain	Res	Type
1	C	501	MET
1	D	501	MET
1	E	501	MET
1	F	501	MET
1	A	330	SER
1	A	564	GLY
1	A	718	GLU
1	B	330	SER
1	B	564	GLY
1	B	718	GLU
1	C	330	SER
1	C	564	GLY
1	C	718	GLU
1	D	330	SER
1	D	564	GLY
1	D	718	GLU
1	E	330	SER
1	E	718	GLU
1	F	330	SER
1	F	564	GLY
1	F	718	GLU
1	E	564	GLY
1	A	620	ARG
1	E	326	VAL
1	F	326	VAL
1	C	326	VAL
1	A	326	VAL
1	B	326	VAL
1	D	326	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/419 (83%)	324 (94%)	22 (6%)	16	44
1	B	346/419 (83%)	323 (93%)	23 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	346/419 (83%)	323 (93%)	23 (7%)	15	43
1	D	346/419 (83%)	324 (94%)	22 (6%)	16	44
1	E	346/419 (83%)	323 (93%)	23 (7%)	15	43
1	F	346/419 (83%)	325 (94%)	21 (6%)	17	46
All	All	2076/2514 (83%)	1942 (94%)	134 (6%)	15	44

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	LYS
1	A	337	GLU
1	A	342	LEU
1	A	343	LEU
1	A	365	ILE
1	A	370	ILE
1	A	376	VAL
1	A	378	VAL
1	A	384	LEU
1	A	397	VAL
1	A	402	VAL
1	A	456	LEU
1	A	502	LEU
1	A	506	ILE
1	A	519	THR
1	A	521	MET
1	A	541	LEU
1	A	626	LEU
1	A	650	ILE
1	A	658	ILE
1	A	663	ILE
1	A	696	VAL
1	B	329	LYS
1	B	337	GLU
1	B	342	LEU
1	B	343	LEU
1	B	352	VAL
1	B	365	ILE
1	B	370	ILE
1	B	376	VAL
1	B	378	VAL
1	B	384	LEU

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Mol	Chain	Res	Type
1	B	397	VAL
1	B	402	VAL
1	B	456	LEU
1	B	488	THR
1	B	502	LEU
1	B	506	ILE
1	B	519	THR
1	B	521	MET
1	B	541	LEU
1	B	626	LEU
1	B	650	ILE
1	B	663	ILE
1	B	696	VAL
1	C	329	LYS
1	C	337	GLU
1	C	342	LEU
1	C	343	LEU
1	C	352	VAL
1	C	365	ILE
1	C	370	ILE
1	C	376	VAL
1	C	378	VAL
1	C	384	LEU
1	C	397	VAL
1	C	402	VAL
1	C	456	LEU
1	C	488	THR
1	C	502	LEU
1	C	506	ILE
1	C	519	THR
1	C	521	MET
1	C	541	LEU
1	C	626	LEU
1	C	650	ILE
1	C	663	ILE
1	C	696	VAL
1	D	329	LYS
1	D	337	GLU
1	D	342	LEU
1	D	343	LEU
1	D	352	VAL
1	D	365	ILE

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Mol	Chain	Res	Type
1	D	370	ILE
1	D	376	VAL
1	D	378	VAL
1	D	384	LEU
1	D	402	VAL
1	D	456	LEU
1	D	488	THR
1	D	502	LEU
1	D	506	ILE
1	D	519	THR
1	D	521	MET
1	D	541	LEU
1	D	626	LEU
1	D	650	ILE
1	D	663	ILE
1	D	696	VAL
1	E	329	LYS
1	E	337	GLU
1	E	342	LEU
1	E	343	LEU
1	E	352	VAL
1	E	365	ILE
1	E	370	ILE
1	E	376	VAL
1	E	378	VAL
1	E	384	LEU
1	E	402	VAL
1	E	456	LEU
1	E	488	THR
1	E	502	LEU
1	E	506	ILE
1	E	519	THR
1	E	521	MET
1	E	541	LEU
1	E	626	LEU
1	E	650	ILE
1	E	658	ILE
1	E	663	ILE
1	E	696	VAL
1	F	329	LYS
1	F	337	GLU
1	F	342	LEU

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Mol	Chain	Res	Type
1	F	343	LEU
1	F	365	ILE
1	F	370	ILE
1	F	376	VAL
1	F	378	VAL
1	F	384	LEU
1	F	402	VAL
1	F	456	LEU
1	F	488	THR
1	F	502	LEU
1	F	506	ILE
1	F	519	THR
1	F	521	MET
1	F	541	LEU
1	F	626	LEU
1	F	650	ILE
1	F	663	ILE
1	F	696	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	383	ASN
1	A	415	ASN
1	A	554	ASN
1	A	631	GLN
1	A	645	ASN
1	A	666	GLN
1	A	692	HIS
1	B	328	GLN
1	B	383	ASN
1	B	415	ASN
1	B	554	ASN
1	B	631	GLN
1	B	645	ASN
1	B	692	HIS
1	C	328	GLN
1	C	383	ASN
1	C	554	ASN
1	C	631	GLN
1	C	692	HIS

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Mol	Chain	Res	Type
1	D	328	GLN
1	D	383	ASN
1	D	415	ASN
1	D	554	ASN
1	D	631	GLN
1	D	645	ASN
1	D	666	GLN
1	D	692	HIS
1	E	328	GLN
1	E	383	ASN
1	E	415	ASN
1	E	554	ASN
1	E	631	GLN
1	E	645	ASN
1	E	692	HIS
1	F	328	GLN
1	F	383	ASN
1	F	415	ASN
1	F	554	ASN
1	F	631	GLN
1	F	645	ASN
1	F	671	GLN
1	F	692	HIS

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](#)

6 ligands are modelled in this entry.

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	$\# Z > 2$
2	ADP	E	1723	-	28,29,29	1.24	2 (7%)	43,45,45	1.17	3 (6%)
2	ADP	F	1723	-	28,29,29	1.26	3 (10%)	43,45,45	1.18	3 (6%)
2	ADP	C	1723	-	28,29,29	1.22	3 (10%)	43,45,45	1.13	2 (4%)
2	ADP	A	1723	-	28,29,29	1.20	2 (7%)	43,45,45	1.16	3 (6%)
2	ADP	B	1723	-	28,29,29	1.20	4 (14%)	43,45,45	1.16	3 (6%)
2	ADP	D	1723	-	28,29,29	1.25	4 (14%)	43,45,45	1.18	3 (6%)

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
2	ADP	E	1723	-	-	2/16/32/32	0/3/3/3
2	ADP	F	1723	-	-	2/16/32/32	0/3/3/3
2	ADP	C	1723	-	-	2/16/32/32	0/3/3/3
2	ADP	A	1723	-	-	2/16/32/32	0/3/3/3
2	ADP	B	1723	-	-	3/16/32/32	0/3/3/3
2	ADP	D	1723	-	-	3/16/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1723	ADP	C2-N1	3.74	1.40	1.33
2	A	1723	ADP	C2-N1	3.63	1.40	1.33
2	E	1723	ADP	C2-N1	3.62	1.40	1.33
2	C	1723	ADP	C2-N1	3.52	1.40	1.33
2	D	1723	ADP	C2-N1	3.46	1.40	1.33
2	B	1723	ADP	C2-N1	3.39	1.39	1.33
2	E	1723	ADP	C1'-N9	2.42	1.53	1.46
2	C	1723	ADP	C1'-N9	2.42	1.53	1.46
2	D	1723	ADP	PA-O3A	-2.35	1.57	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1723	ADP	C8-N7	2.22	1.36	1.31
2	C	1723	ADP	C6-N6	-2.20	1.28	1.34
2	B	1723	ADP	C1'-N9	2.15	1.52	1.46
2	D	1723	ADP	C1'-N9	2.14	1.52	1.46
2	B	1723	ADP	C6-N6	-2.11	1.28	1.34
2	F	1723	ADP	C1'-N9	2.08	1.52	1.46
2	D	1723	ADP	C6-N6	-2.03	1.29	1.34
2	B	1723	ADP	C8-N7	2.02	1.35	1.31
2	A	1723	ADP	C1'-N9	2.00	1.51	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1723	ADP	N3-C2-N1	-3.56	123.19	128.58
2	A	1723	ADP	N3-C2-N1	-3.51	123.26	128.58
2	E	1723	ADP	N3-C2-N1	-3.48	123.31	128.58
2	C	1723	ADP	N3-C2-N1	-3.42	123.41	128.58
2	B	1723	ADP	N3-C2-N1	-3.35	123.51	128.58
2	F	1723	ADP	N3-C2-N1	-3.32	123.56	128.58
2	D	1723	ADP	C2-N1-C6	3.01	123.68	118.73
2	F	1723	ADP	C2-N1-C6	2.93	123.54	118.73
2	B	1723	ADP	C2-N1-C6	2.91	123.51	118.73
2	E	1723	ADP	C2-N1-C6	2.88	123.47	118.73
2	C	1723	ADP	C2-N1-C6	2.87	123.45	118.73
2	A	1723	ADP	C2-N1-C6	2.78	123.30	118.73
2	A	1723	ADP	C3'-C2'-C1'	2.31	105.84	101.46
2	B	1723	ADP	C3'-C2'-C1'	2.26	105.73	101.46
2	F	1723	ADP	C3'-C2'-C1'	2.24	105.71	101.46
2	D	1723	ADP	C3'-C2'-C1'	2.17	105.56	101.46
2	E	1723	ADP	C3'-C2'-C1'	2.14	105.50	101.46

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1723	ADP	PA-O3A-PB-O3B
2	B	1723	ADP	PA-O3A-PB-O3B
2	C	1723	ADP	PA-O3A-PB-O3B
2	D	1723	ADP	PA-O3A-PB-O3B
2	E	1723	ADP	PA-O3A-PB-O3B
2	F	1723	ADP	PA-O3A-PB-O3B
2	A	1723	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	B	1723	ADP	PA-O3A-PB-O2B
2	C	1723	ADP	PA-O3A-PB-O2B
2	D	1723	ADP	PA-O3A-PB-O2B
2	E	1723	ADP	PA-O3A-PB-O2B
2	F	1723	ADP	PA-O3A-PB-O2B
2	B	1723	ADP	PA-O3A-PB-O1B
2	D	1723	ADP	PA-O3A-PB-O1B

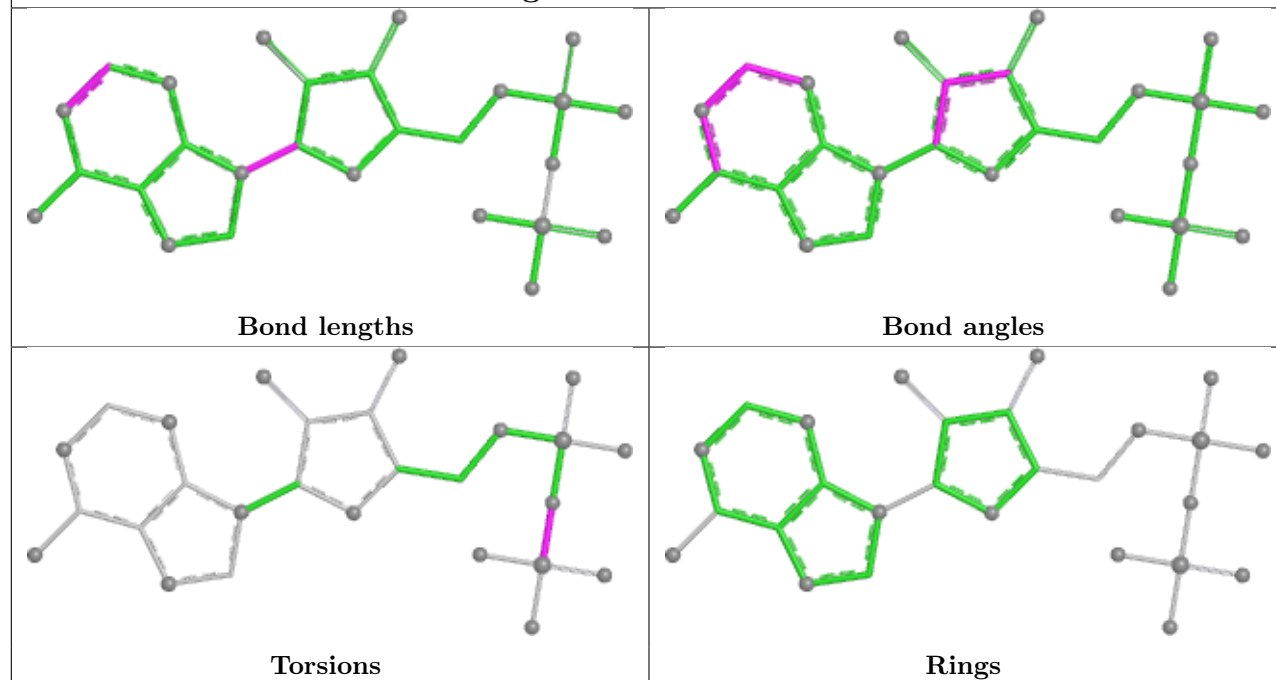
There are no ring outliers.

2 monomers are involved in 2 short contacts:

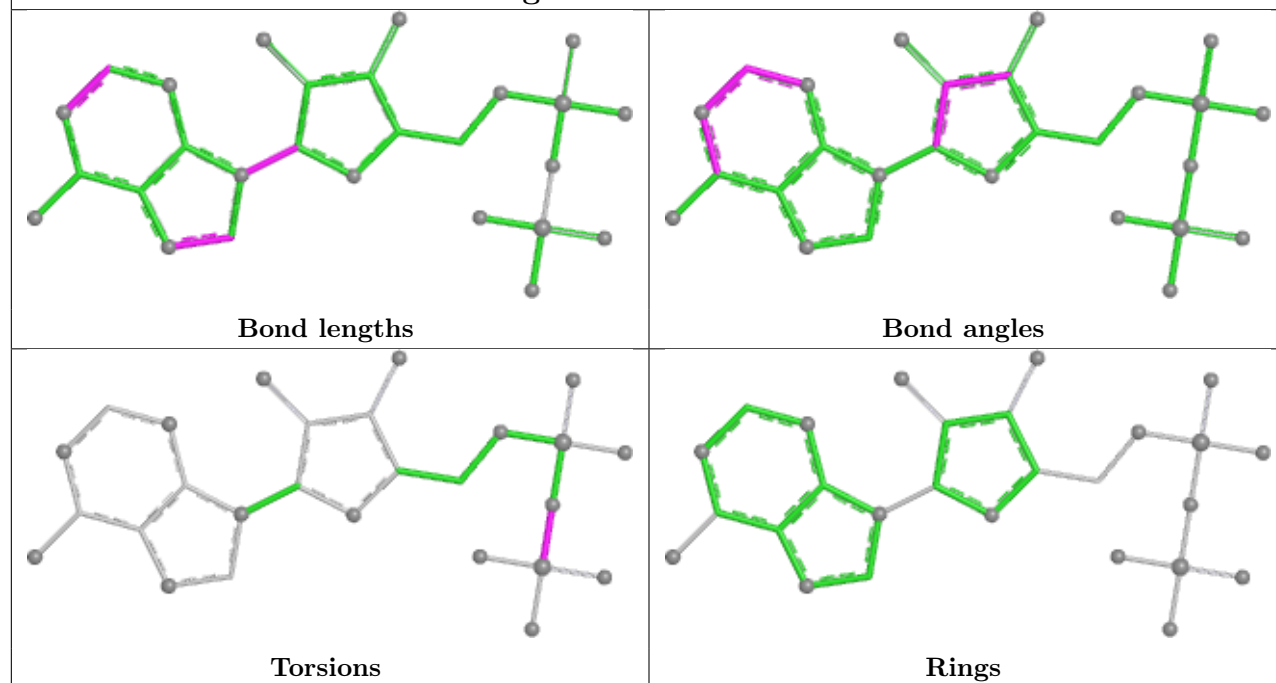
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1723	ADP	1	0
2	B	1723	ADP	1	0

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

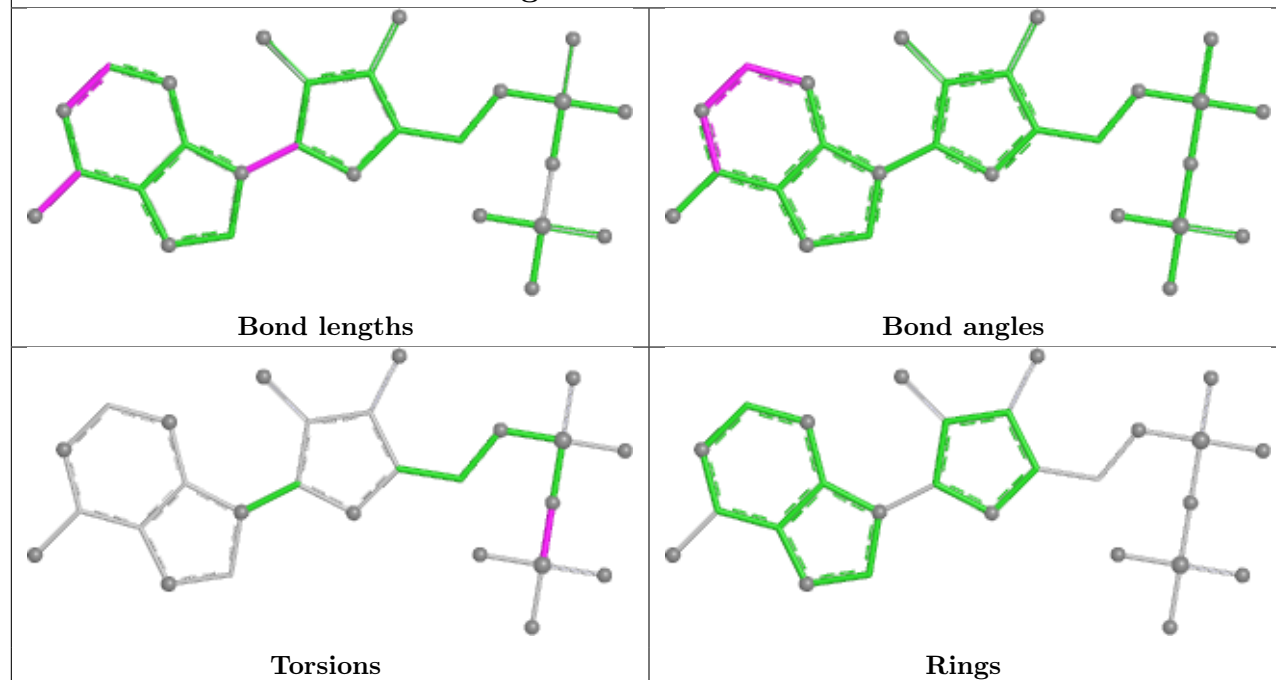
Ligand ADP E 1723



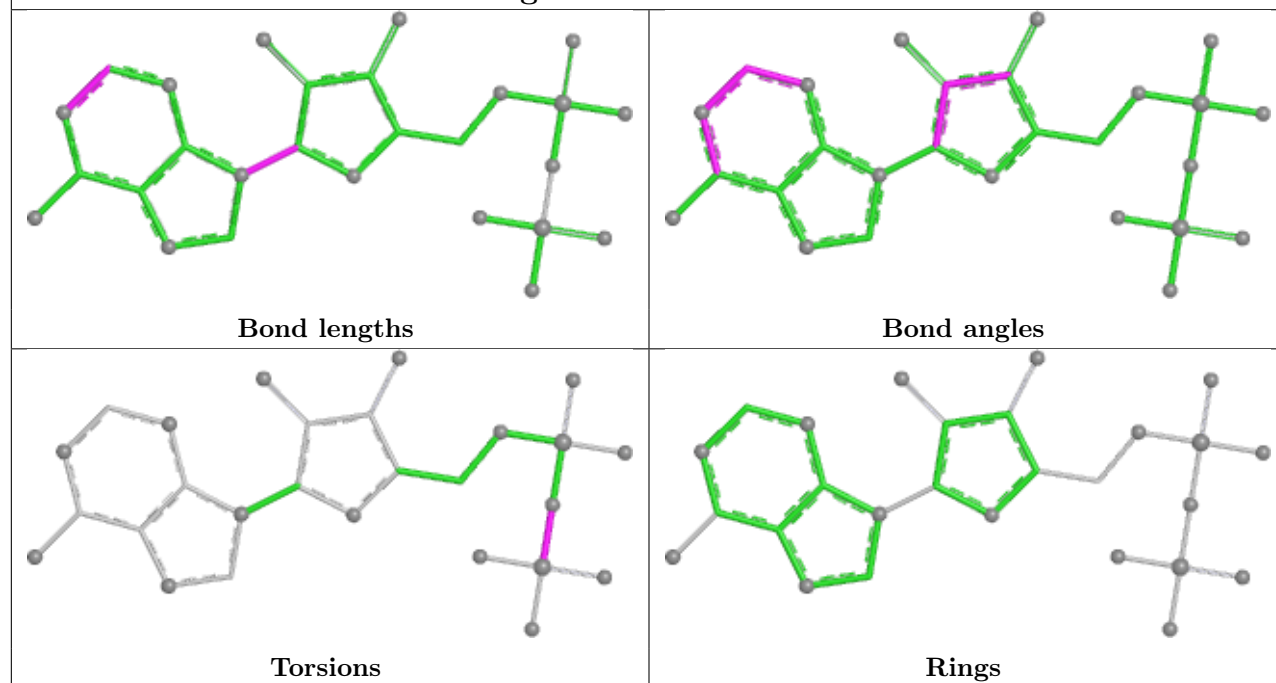
Ligand ADP F 1723

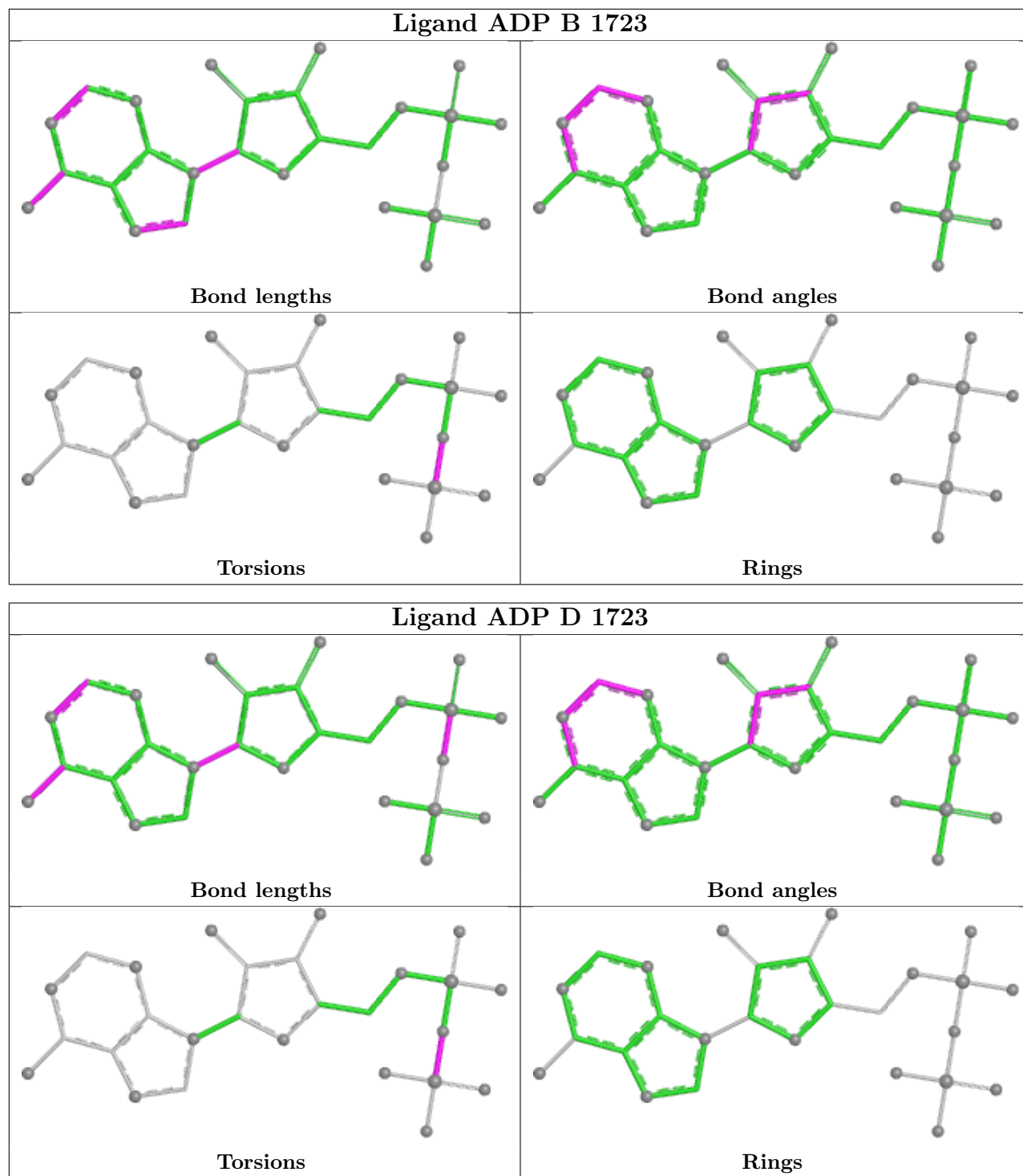


Ligand ADP C 1723



Ligand ADP A 1723





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	408/491 (83%)	0.62	16 (3%) 43 35	48, 72, 110, 136	0
1	B	408/491 (83%)	0.38	14 (3%) 48 39	37, 57, 97, 127	0
1	C	408/491 (83%)	0.16	13 (3%) 50 41	31, 51, 93, 140	0
1	D	408/491 (83%)	0.12	15 (3%) 45 37	32, 49, 85, 131	0
1	E	408/491 (83%)	0.42	20 (4%) 35 27	42, 65, 102, 142	0
1	F	408/491 (83%)	0.66	22 (5%) 31 24	47, 73, 108, 140	0
All	All	2448/2946 (83%)	0.39	100 (4%) 41 33	31, 62, 103, 142	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	331	TYR	6.2
1	C	331	TYR	5.4
1	B	331	TYR	5.4
1	D	331	TYR	5.4
1	B	326	VAL	5.0
1	F	331	TYR	4.6
1	A	326	VAL	4.4
1	B	328	GLN	4.1
1	C	341	ARG	3.9
1	A	331	TYR	3.8
1	E	329	LYS	3.7
1	E	328	GLN	3.6
1	D	431	GLU	3.5
1	D	719	ASP	3.4
1	A	501	MET	3.4
1	F	717	ILE	3.4
1	A	722	ALA	3.4
1	F	315	LEU	3.3
1	B	501	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	326	VAL	3.3
1	B	722	ALA	3.2
1	B	565	THR	3.2
1	F	329	LYS	3.1
1	E	717	ILE	3.1
1	A	714	PRO	3.1
1	D	687	LEU	3.1
1	E	710	LEU	3.1
1	D	434	GLU	3.0
1	A	315	LEU	3.0
1	E	714	PRO	3.0
1	F	327	LYS	2.9
1	A	719	ASP	2.9
1	D	501	MET	2.9
1	F	420	MET	2.9
1	A	324	ALA	2.9
1	C	326	VAL	2.8
1	A	694	ALA	2.8
1	F	324	ALA	2.8
1	F	323	PRO	2.8
1	B	330	SER	2.7
1	B	329	LYS	2.7
1	E	330	SER	2.7
1	C	503	GLU	2.7
1	E	573	ARG	2.6
1	E	323	PRO	2.6
1	B	324	ALA	2.6
1	A	354	VAL	2.5
1	F	720	ILE	2.5
1	C	573	ARG	2.5
1	C	685	THR	2.5
1	C	329	LYS	2.5
1	E	352	VAL	2.5
1	D	351	GLY	2.4
1	D	352	VAL	2.4
1	D	327	LYS	2.4
1	C	315	LEU	2.4
1	A	447	ILE	2.4
1	F	427	LEU	2.4
1	D	714	PRO	2.4
1	C	436	LYS	2.4
1	E	501	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	418	ARG	2.3
1	F	448	GLY	2.3
1	C	501	MET	2.3
1	E	418	ARG	2.3
1	D	503	GLU	2.3
1	E	687	LEU	2.3
1	F	695	PHE	2.3
1	B	325	GLU	2.2
1	B	717	ILE	2.2
1	B	450	ARG	2.2
1	F	418	ARG	2.2
1	E	685	THR	2.2
1	A	327	LYS	2.2
1	C	502	LEU	2.2
1	B	573	ARG	2.2
1	F	574	ARG	2.2
1	A	565	THR	2.2
1	F	326	VAL	2.2
1	D	718	GLU	2.2
1	F	501	MET	2.2
1	C	328	GLN	2.2
1	E	686	GLY	2.2
1	D	330	SER	2.2
1	F	316	PRO	2.1
1	F	696	VAL	2.1
1	C	722	ALA	2.1
1	F	719	ASP	2.1
1	E	572	PHE	2.1
1	A	546	GLY	2.1
1	A	567	LEU	2.1
1	F	351	GLY	2.1
1	E	502	LEU	2.1
1	D	685	THR	2.1
1	E	720	ILE	2.1
1	F	563	ALA	2.1
1	D	702	HIS	2.0
1	F	714	PRO	2.0
1	E	336	LEU	2.0
1	A	574	ARG	2.0

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](#)

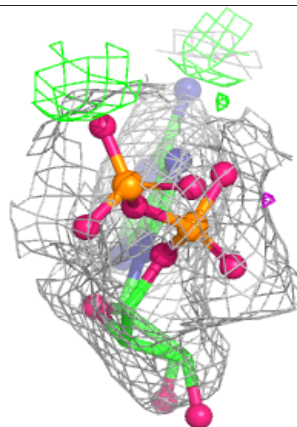
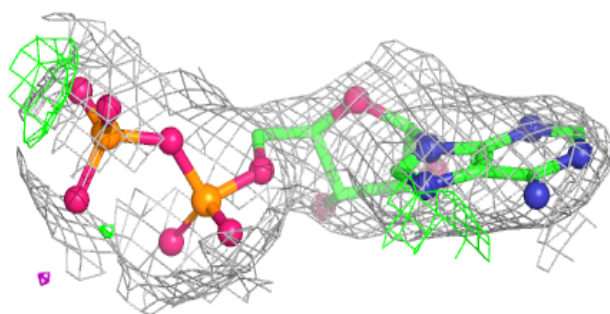
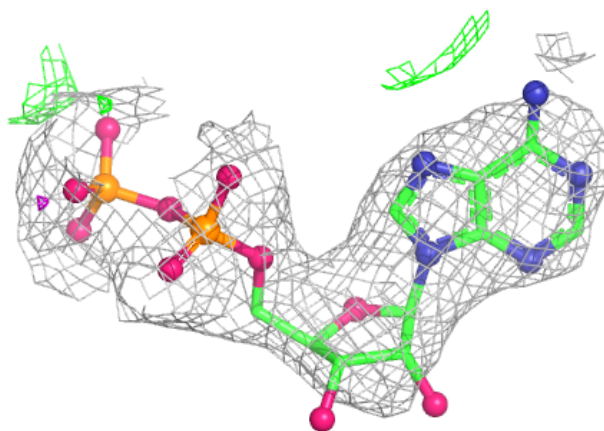
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	ADP	A	1723	27/27	0.85	0.12	93,96,103,104	0
2	ADP	F	1723	27/27	0.86	0.14	87,100,105,105	0
2	ADP	E	1723	27/27	0.89	0.12	87,90,91,91	0
2	ADP	C	1723	27/27	0.91	0.12	67,82,87,88	0
2	ADP	D	1723	27/27	0.91	0.11	62,72,76,81	0
2	ADP	B	1723	27/27	0.92	0.10	75,82,85,88	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.

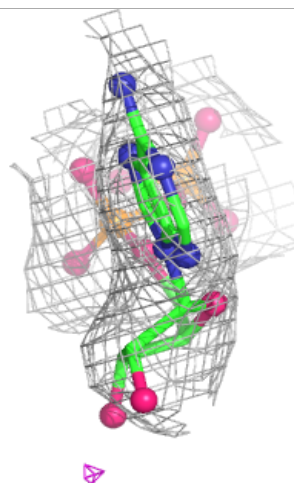
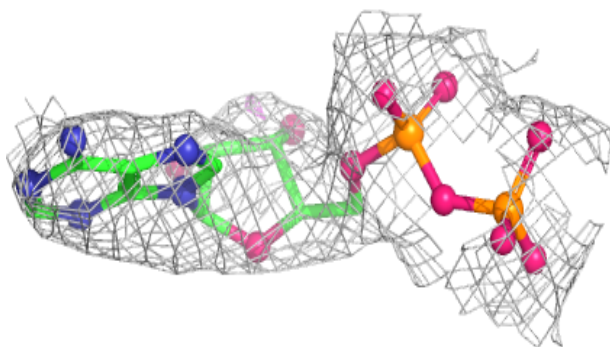
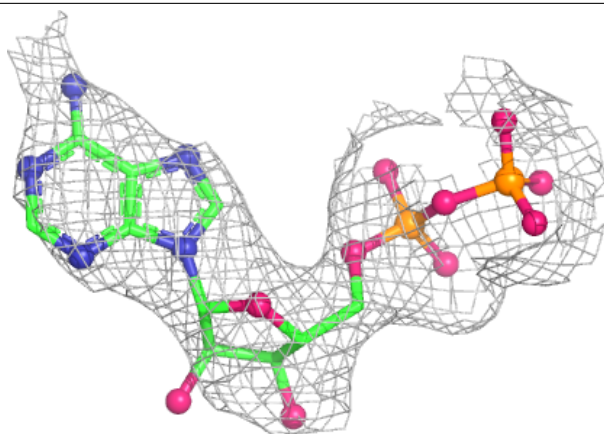
Electron density around ADP A 1723:

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



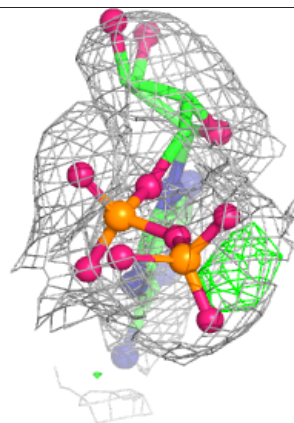
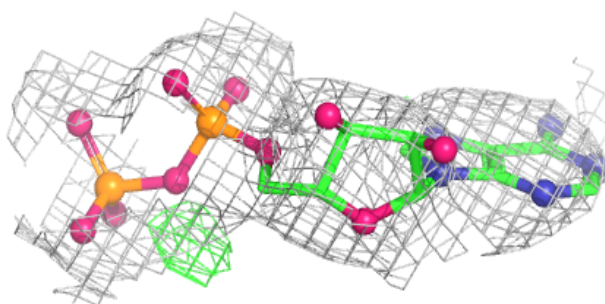
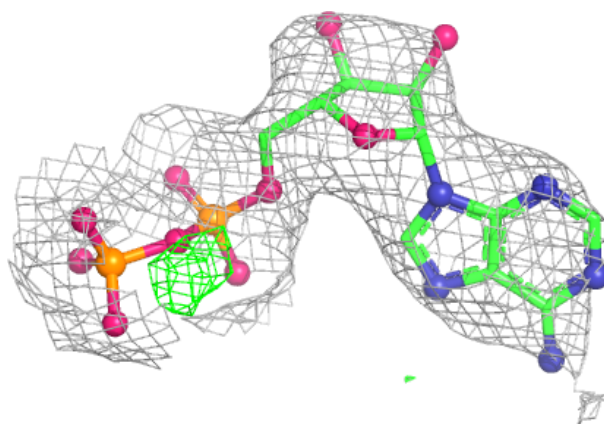
Electron density around ADP F 1723:

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

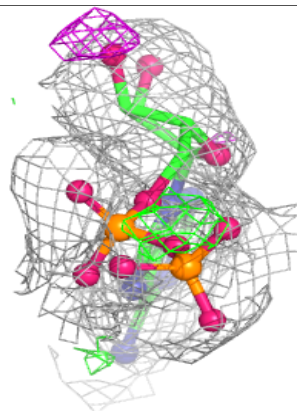
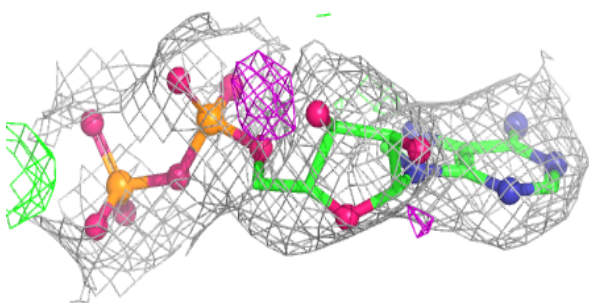
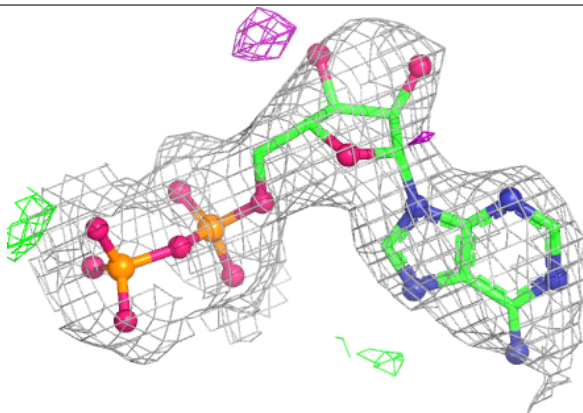


Electron density around ADP E 1723:

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

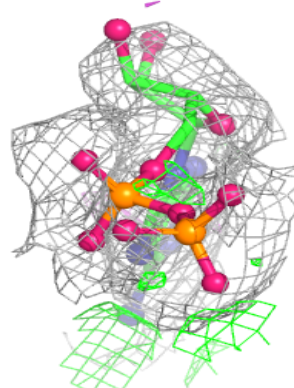
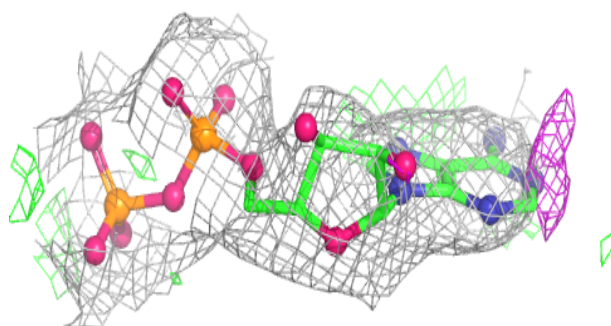
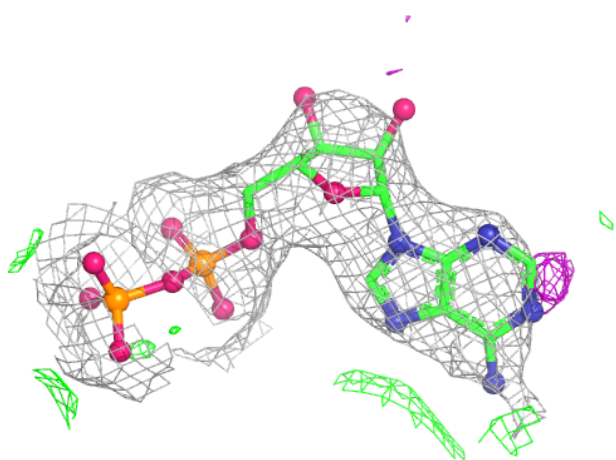
**Electron density around ADP C 1723:**

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



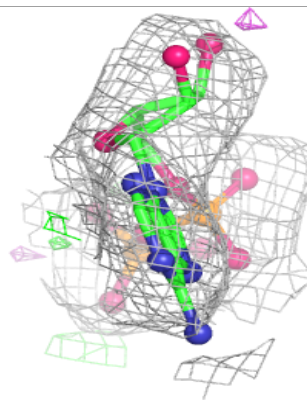
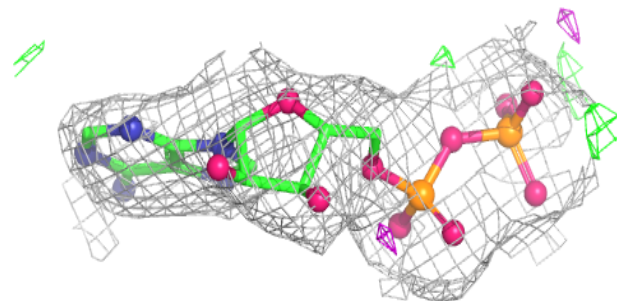
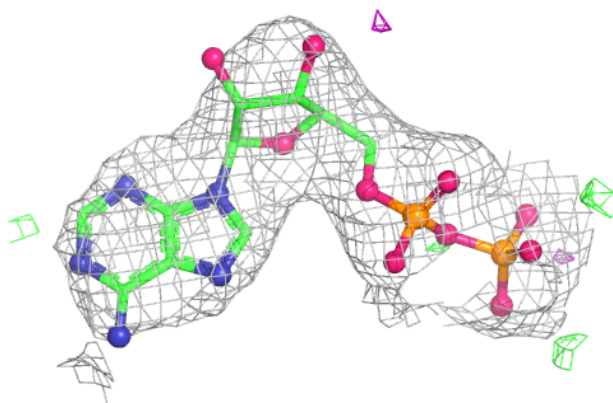
Electron density around ADP D 1723:

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



Electron density around ADP B 1723:

$2mF_o-DF_c$ (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.