



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:21 PM UTC

PDB ID : 6R72 / pdb_00006r72
Title : Crystal structure of BmrA-E504A in an outward-facing conformation
Authors : Chaptal, V.; Zampieri, V.; Kilburg, A.; Magnard, S.; Falson, P.
Deposited on : 2019-03-28
Resolution : 3.95 Å(reported)

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

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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

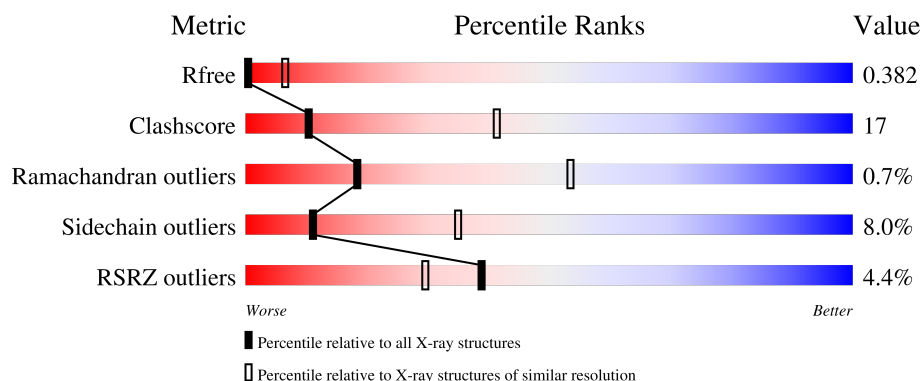
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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	599	4% 64% 27% • 5%
1	B	599	4% 62% 28% 5% 5%
1	C	599	3% 62% 29% • 6%
1	D	599	6% 64% 28% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17683 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 Multidrug exporter ATP-binding cassette.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4396	2822	734	823	17			
1	B	569	Total	C	N	O	S	0	0	0
			4392	2820	733	821	18			
1	C	565	Total	C	N	O	S	0	0	0
			4367	2806	728	816	17			
1	D	572	Total	C	N	O	S	0	0	0
			4400	2824	735	824	17			

There are 44 discrepancies between the modelled and reference sequences:

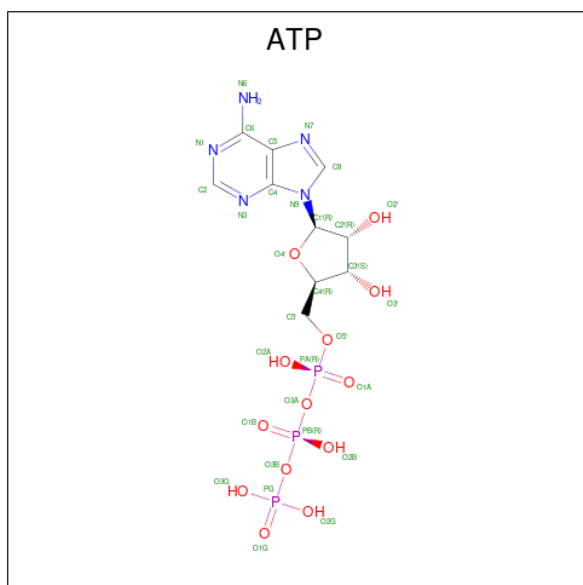
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP A0A164TVX9
A	-8	SER	-	expression tag	UNP A0A164TVX9
A	-7	SER	-	expression tag	UNP A0A164TVX9
A	-6	SER	-	expression tag	UNP A0A164TVX9
A	-5	HIS	-	expression tag	UNP A0A164TVX9
A	-4	HIS	-	expression tag	UNP A0A164TVX9
A	-3	HIS	-	expression tag	UNP A0A164TVX9
A	-2	HIS	-	expression tag	UNP A0A164TVX9
A	-1	HIS	-	expression tag	UNP A0A164TVX9
A	0	HIS	-	expression tag	UNP A0A164TVX9
A	504	ALA	GLU	engineered mutation	UNP A0A164TVX9
B	-9	MET	-	initiating methionine	UNP A0A164TVX9
B	-8	SER	-	expression tag	UNP A0A164TVX9
B	-7	SER	-	expression tag	UNP A0A164TVX9
B	-6	SER	-	expression tag	UNP A0A164TVX9
B	-5	HIS	-	expression tag	UNP A0A164TVX9
B	-4	HIS	-	expression tag	UNP A0A164TVX9
B	-3	HIS	-	expression tag	UNP A0A164TVX9
B	-2	HIS	-	expression tag	UNP A0A164TVX9
B	-1	HIS	-	expression tag	UNP A0A164TVX9
B	0	HIS	-	expression tag	UNP A0A164TVX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	504	ALA	GLU	engineered mutation	UNP A0A164TVX9
C	-9	MET	-	initiating methionine	UNP A0A164TVX9
C	-8	SER	-	expression tag	UNP A0A164TVX9
C	-7	SER	-	expression tag	UNP A0A164TVX9
C	-6	SER	-	expression tag	UNP A0A164TVX9
C	-5	HIS	-	expression tag	UNP A0A164TVX9
C	-4	HIS	-	expression tag	UNP A0A164TVX9
C	-3	HIS	-	expression tag	UNP A0A164TVX9
C	-2	HIS	-	expression tag	UNP A0A164TVX9
C	-1	HIS	-	expression tag	UNP A0A164TVX9
C	0	HIS	-	expression tag	UNP A0A164TVX9
C	504	ALA	GLU	engineered mutation	UNP A0A164TVX9
D	-9	MET	-	initiating methionine	UNP A0A164TVX9
D	-8	SER	-	expression tag	UNP A0A164TVX9
D	-7	SER	-	expression tag	UNP A0A164TVX9
D	-6	SER	-	expression tag	UNP A0A164TVX9
D	-5	HIS	-	expression tag	UNP A0A164TVX9
D	-4	HIS	-	expression tag	UNP A0A164TVX9
D	-3	HIS	-	expression tag	UNP A0A164TVX9
D	-2	HIS	-	expression tag	UNP A0A164TVX9
D	-1	HIS	-	expression tag	UNP A0A164TVX9
D	0	HIS	-	expression tag	UNP A0A164TVX9
D	504	ALA	GLU	engineered mutation	UNP A0A164TVX9

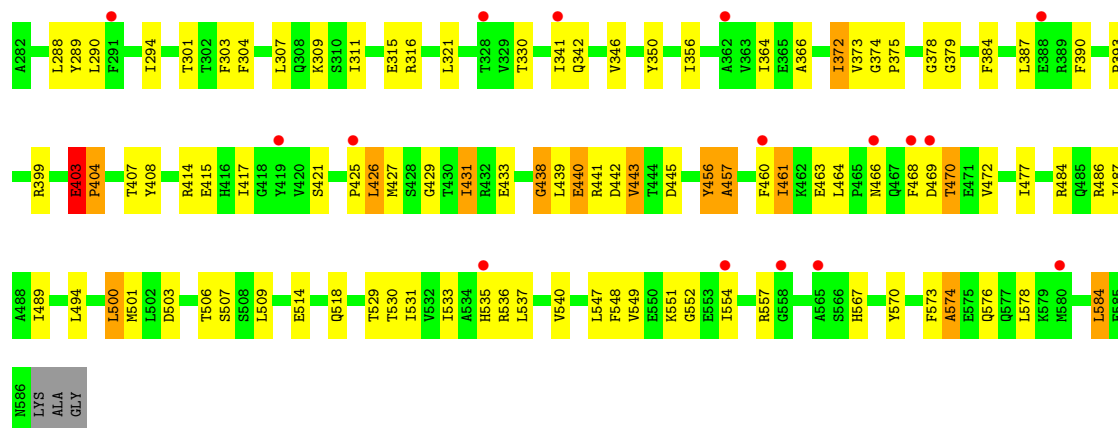
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



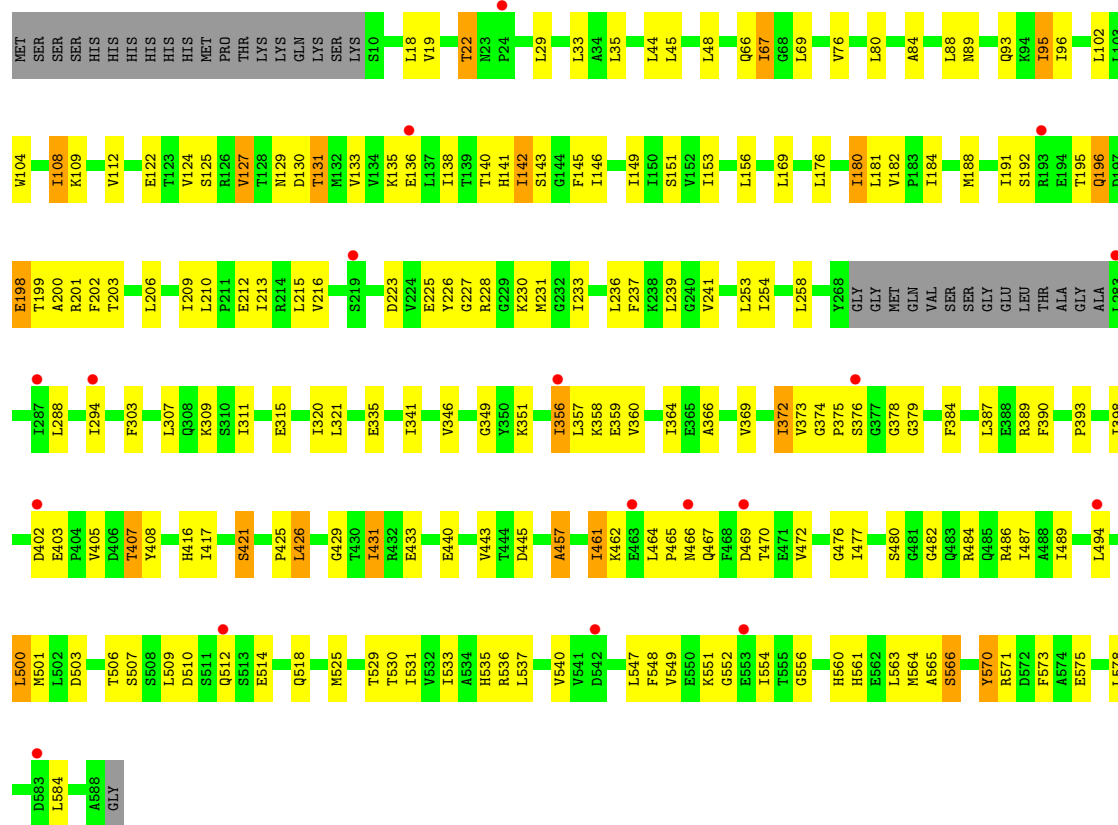
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

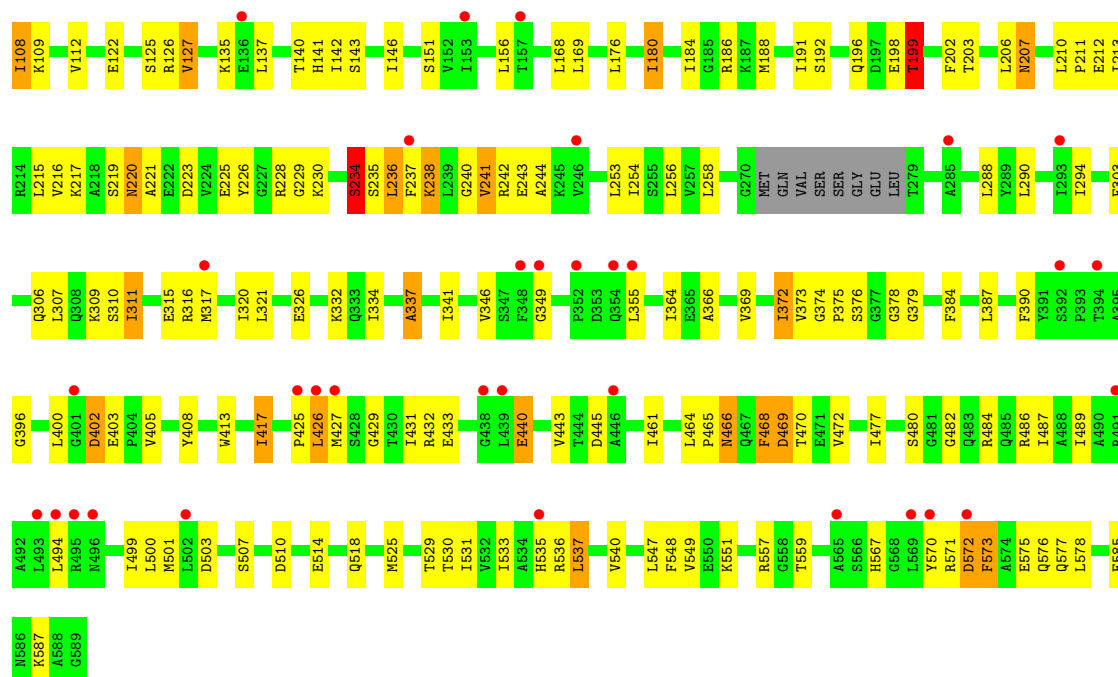


• Molecule 1: Multidrug exporter ATP-binding cassette



• Molecule 1: Multidrug exporter ATP-binding cassette





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.81Å 110.75Å 155.62Å 90.00° 93.23° 90.00°	Depositor
Resolution (Å)	28.42 – 3.95 28.42 – 3.95	Depositor EDS
% Data completeness (in resolution range)	92.0 (28.42-3.95) 57.7 (28.42-3.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.98Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.260 , 0.321 0.301 , 0.382	Depositor DCC
R_{free} test set	1019 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	198.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 112.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	17683	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.81	2/4462 (0.0%)	1.53	47/6038 (0.8%)
1	B	0.81	1/4458 (0.0%)	1.51	51/6031 (0.8%)
1	C	0.82	0/4433	1.54	42/5999 (0.7%)
1	D	0.81	0/4466	1.50	41/6043 (0.7%)
All	All	0.81	3/17819 (0.0%)	1.52	181/24111 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	316	ARG	CA-C	5.71	1.60	1.52
1	A	46	ILE	CA-CB	5.30	1.57	1.54
1	B	46	ILE	CA-CB	5.25	1.57	1.54

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	566	SER	N-CA-C	29.24	143.49	111.03
1	A	408	TYR	N-CA-C	-23.42	73.10	108.46
1	B	439	LEU	CB-CA-C	-15.78	87.78	111.77
1	B	438	GLY	N-CA-C	14.34	147.17	113.18
1	C	402	ASP	CB-CA-C	-13.37	90.22	111.48
1	D	236	LEU	N-CA-C	12.67	124.63	111.07
1	D	572	ASP	N-CA-C	-12.04	92.83	110.64
1	B	440	GLU	N-CA-CB	-11.74	91.63	109.71
1	D	572	ASP	CB-CA-C	11.68	124.17	109.80
1	A	402	ASP	CB-CA-C	-11.45	87.64	110.42
1	D	337	ALA	CB-CA-C	11.28	132.86	110.42
1	C	403	GLU	CA-C-N	11.23	131.64	120.52
1	C	403	GLU	C-N-CA	11.23	131.64	120.52
1	A	440	GLU	N-CA-CB	-10.95	93.95	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	LEU	CB-CA-C	-10.91	88.71	110.42
1	B	379	GLY	N-CA-C	10.87	131.41	115.32
1	C	565	ALA	N-CA-C	10.68	126.10	113.18
1	C	566	SER	N-CA-CB	-10.61	94.59	109.98
1	C	379	GLY	N-CA-C	10.58	131.37	115.08
1	A	379	GLY	N-CA-C	10.49	131.23	115.08
1	D	326	GLU	N-CA-C	10.43	126.07	112.72
1	B	218	ALA	N-CA-C	-10.41	94.75	108.19
1	D	379	GLY	N-CA-C	10.29	132.26	114.76
1	B	440	GLU	N-CA-C	10.18	124.56	109.59
1	A	334	ILE	N-CA-CB	-9.99	99.37	112.26
1	A	551	LYS	CB-CA-C	-9.91	90.70	110.42
1	D	238	LYS	N-CA-C	-9.82	100.65	111.36
1	A	409	SER	N-CA-CB	-9.70	96.49	110.45
1	D	551	LYS	CB-CA-C	-9.12	92.28	110.42
1	C	551	LYS	CB-CA-C	-8.94	92.63	110.42
1	D	402	ASP	CB-CA-C	-8.91	92.69	110.42
1	B	441	ARG	CB-CA-C	-8.69	95.16	111.06
1	B	203	THR	N-CA-C	-8.56	101.89	111.14
1	B	551	LYS	CB-CA-C	-8.43	93.65	110.42
1	D	203	THR	CB-CA-C	-8.38	97.72	110.88
1	C	565	ALA	CA-C-N	8.29	131.90	120.63
1	C	565	ALA	C-N-CA	8.29	131.90	120.63
1	D	199	THR	CB-CA-C	-8.15	98.03	110.90
1	A	334	ILE	N-CA-C	8.13	120.71	112.90
1	B	442	ASP	N-CA-C	-8.05	103.66	113.97
1	D	573	PHE	N-CA-CB	7.99	123.99	110.49
1	D	238	LYS	N-CA-CB	7.95	121.92	110.16
1	C	570	TYR	N-CA-C	7.94	121.78	108.20
1	B	443	VAL	N-CA-C	7.88	119.64	108.36
1	A	552	GLY	N-CA-C	7.76	126.22	115.27
1	D	219	SER	N-CA-C	7.75	127.30	110.80
1	B	439	LEU	N-CA-C	-7.66	89.94	107.48
1	A	317	MET	N-CA-CB	7.55	120.92	109.98
1	A	127	VAL	CA-C-N	7.52	130.69	120.38
1	A	127	VAL	C-N-CA	7.52	130.69	120.38
1	B	552	GLY	N-CA-C	7.30	124.86	114.64
1	C	552	GLY	N-CA-C	7.14	125.28	115.00
1	C	88	LEU	CA-C-N	7.05	129.73	120.28
1	C	88	LEU	C-N-CA	7.05	129.73	120.28
1	A	437	TYR	N-CA-C	6.99	120.69	111.75
1	B	15	PHE	CA-CB-CG	-6.98	106.82	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ARG	N-CA-C	-6.92	103.82	111.36
1	B	239	LEU	N-CA-C	-6.84	104.93	113.28
1	A	239	LEU	N-CA-C	-6.71	105.09	113.28
1	B	442	ASP	CB-CA-C	6.70	120.32	109.07
1	C	565	ALA	CB-CA-C	-6.59	96.83	109.95
1	B	230	LYS	N-CA-C	6.55	118.08	111.07
1	C	239	LEU	N-CA-C	-6.54	105.12	113.23
1	C	570	TYR	CB-CA-C	-6.53	100.34	110.78
1	C	131	THR	N-CA-C	-6.47	104.31	111.36
1	C	462	LYS	CA-C-N	6.45	129.25	120.54
1	C	462	LYS	C-N-CA	6.45	129.25	120.54
1	D	216	VAL	N-CA-C	-6.40	106.05	111.56
1	A	317	MET	N-CA-C	-6.35	103.98	111.03
1	D	469	ASP	CA-CB-CG	6.32	118.92	112.60
1	B	136	GLU	CB-CG-CD	6.11	122.99	112.60
1	C	403	GLU	N-CA-C	-6.09	98.83	109.48
1	B	205	LEU	N-CA-C	6.06	117.55	111.07
1	B	219	SER	N-CA-C	6.05	120.13	112.87
1	B	403	GLU	CB-CA-C	6.04	119.34	109.97
1	A	442	ASP	N-CA-C	-6.04	105.77	113.02
1	B	468	PHE	CA-CB-CG	5.95	119.75	113.80
1	D	202	PHE	CB-CA-C	5.94	122.08	110.67
1	A	439	LEU	N-CA-CB	5.92	120.50	110.49
1	C	131	THR	N-CA-CB	5.92	118.93	110.16
1	A	457	ALA	N-CA-C	-5.89	106.63	113.88
1	D	207	ASN	CA-C-N	5.88	128.16	120.28
1	D	207	ASN	C-N-CA	5.88	128.16	120.28
1	B	200	ALA	N-CA-C	-5.85	104.83	111.14
1	B	215	LEU	CA-C-N	5.84	128.14	120.60
1	B	215	LEU	C-N-CA	5.84	128.14	120.60
1	D	241	VAL	N-CA-C	-5.79	103.18	111.17
1	B	456	TYR	CA-C-N	5.79	128.03	120.28
1	B	456	TYR	C-N-CA	5.79	128.03	120.28
1	B	235	SER	CA-C-N	-5.78	113.08	122.26
1	B	235	SER	C-N-CA	-5.78	113.08	122.26
1	C	360	VAL	N-CA-CB	5.76	120.91	111.58
1	A	216	VAL	N-CA-C	-5.74	105.50	111.58
1	B	443	VAL	N-CA-CB	-5.71	104.14	110.99
1	B	217	LYS	N-CA-C	5.70	122.94	110.80
1	D	461	ILE	CA-C-N	5.68	127.89	120.28
1	D	461	ILE	C-N-CA	5.68	127.89	120.28
1	B	182	VAL	N-CA-CB	5.65	114.86	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	LEU	CA-C-N	5.62	124.83	120.33
1	B	45	LEU	C-N-CA	5.62	124.83	120.33
1	C	457	ALA	CA-C-N	5.62	128.08	120.38
1	C	457	ALA	C-N-CA	5.62	128.08	120.38
1	C	182	VAL	N-CA-CB	5.61	114.82	110.45
1	D	180	ILE	N-CA-C	-5.60	107.28	112.83
1	C	180	ILE	N-CA-C	-5.60	107.28	112.83
1	D	220	ASN	CA-CB-CG	5.59	118.19	112.60
1	D	559	THR	CA-C-N	5.57	129.18	120.82
1	D	559	THR	C-N-CA	5.57	129.18	120.82
1	A	440	GLU	N-CA-C	5.55	117.90	110.35
1	D	466	ASN	CA-CB-CG	5.53	118.13	112.60
1	D	45	LEU	CA-C-N	5.53	124.75	120.33
1	D	45	LEU	C-N-CA	5.53	124.75	120.33
1	A	45	LEU	CA-C-N	5.52	124.75	120.33
1	A	45	LEU	C-N-CA	5.52	124.75	120.33
1	C	129	ASN	N-CA-C	5.50	119.16	112.23
1	A	231	MET	CB-CA-C	5.49	122.23	110.21
1	C	45	LEU	CA-C-N	5.49	124.72	120.33
1	C	45	LEU	C-N-CA	5.49	124.72	120.33
1	B	440	GLU	CB-CA-C	-5.47	102.05	110.26
1	A	409	SER	CB-CA-C	5.46	125.66	113.33
1	A	436	CYS	CA-C-N	5.44	128.33	120.38
1	A	436	CYS	C-N-CA	5.44	128.33	120.38
1	A	182	VAL	N-CA-CB	5.44	114.69	110.45
1	D	337	ALA	CA-C-N	5.42	131.90	121.54
1	D	337	ALA	C-N-CA	5.42	131.90	121.54
1	A	180	ILE	N-CA-C	-5.41	107.48	112.83
1	A	88	LEU	CA-C-N	5.38	127.93	120.29
1	A	88	LEU	C-N-CA	5.38	127.93	120.29
1	D	403	GLU	N-CA-C	-5.38	98.06	108.45
1	A	197	ASP	CA-C-N	5.38	128.88	120.82
1	A	197	ASP	C-N-CA	5.38	128.88	120.82
1	A	136	GLU	CB-CG-CD	5.36	121.71	112.60
1	C	67	ILE	CB-CA-C	5.35	120.06	111.29
1	A	241	VAL	N-CA-C	-5.34	105.32	110.72
1	C	181	LEU	CA-C-N	5.34	124.60	120.33
1	C	181	LEU	C-N-CA	5.34	124.60	120.33
1	B	180	ILE	N-CA-C	-5.34	107.55	112.83
1	C	351	LYS	N-CA-C	-5.32	98.94	109.10
1	A	388	GLU	CA-C-N	5.31	130.86	122.78
1	A	388	GLU	C-N-CA	5.31	130.86	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	VAL	N-CA-C	-5.27	105.40	110.72
1	D	403	GLU	N-CA-CB	5.27	121.86	110.27
1	C	402	ASP	N-CA-C	5.22	118.94	112.47
1	C	153	ILE	CA-C-N	5.22	125.73	119.94
1	C	153	ILE	C-N-CA	5.22	125.73	119.94
1	D	234	SER	CA-C-N	-5.21	113.67	120.44
1	D	234	SER	C-N-CA	-5.21	113.67	120.44
1	C	241	VAL	N-CA-C	-5.20	105.46	110.72
1	A	461	ILE	CA-C-N	5.20	127.50	120.38
1	A	461	ILE	C-N-CA	5.20	127.50	120.38
1	A	197	ASP	N-CA-C	-5.17	99.78	110.80
1	C	461	ILE	CA-C-N	5.16	127.20	120.28
1	C	461	ILE	C-N-CA	5.16	127.20	120.28
1	D	573	PHE	N-CA-C	-5.16	99.81	110.80
1	A	457	ALA	CA-C-N	5.14	127.42	120.38
1	A	457	ALA	C-N-CA	5.14	127.42	120.38
1	B	181	LEU	CA-C-N	5.13	124.43	120.33
1	B	181	LEU	C-N-CA	5.13	124.43	120.33
1	B	457	ALA	CA-C-N	5.12	127.39	120.38
1	B	457	ALA	C-N-CA	5.12	127.39	120.38
1	C	421	SER	CA-C-N	5.11	128.48	120.82
1	C	421	SER	C-N-CA	5.11	128.48	120.82
1	B	219	SER	CB-CA-C	-5.10	99.03	110.21
1	D	85	THR	CA-C-N	5.09	127.11	120.28
1	D	85	THR	C-N-CA	5.09	127.11	120.28
1	B	116	ASP	N-CA-C	-5.09	106.76	113.12
1	A	226	TYR	N-CA-C	-5.08	105.44	111.69
1	B	442	ASP	N-CA-CB	5.07	117.72	110.67
1	A	197	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	306	GLN	CB-CG-CD	5.06	121.21	112.60
1	A	510	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	213	ILE	CA-C-N	5.05	127.55	120.28
1	B	213	ILE	C-N-CA	5.05	127.55	120.28
1	D	468	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	574	ALA	CA-C-N	5.04	127.28	120.38
1	B	574	ALA	C-N-CA	5.04	127.28	120.38
1	D	199	THR	N-CA-C	-5.03	105.71	111.14
1	A	421	SER	CA-C-N	5.02	128.34	120.82
1	A	421	SER	C-N-CA	5.02	128.34	120.82
1	B	421	SER	CA-C-N	5.01	128.34	120.82
1	B	421	SER	C-N-CA	5.01	128.34	120.82

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	4396	0	4566	189	0
1	B	4392	0	4562	147	0
1	C	4367	0	4539	176	0
1	D	4400	0	4568	163	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	17683	0	18283	610	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 17.

All (610) 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:D:141:HIS:CD2	1:D:303:PHE:CE1	1.93	1.53
1:C:141:HIS:CD2	1:C:303:PHE:CE1	2.13	1.35
1:A:217:LYS:HD2	1:B:414:ARG:NH1	1.40	1.35
1:A:141:HIS:CD2	1:A:303:PHE:CE1	2.15	1.33
1:D:99:LEU:HD22	1:D:317:MET:SD	1.68	1.33
1:A:99:LEU:HD22	1:A:317:MET:SD	1.69	1.33
1:D:198:GLU:HB3	1:D:236:LEU:CD1	1.60	1.32
1:D:141:HIS:HD2	1:D:303:PHE:CD1	1.48	1.30
1:C:198:GLU:OE2	1:C:236:LEU:HD13	1.30	1.29
1:A:217:LYS:HD3	1:A:222:GLU:OE2	1.21	1.28
1:C:141:HIS:CD2	1:C:303:PHE:HE1	1.50	1.26
1:C:104:TRP:CH2	1:D:206:LEU:HD21	1.75	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:HIS:CD2	1:B:303:PHE:CE1	2.27	1.21
1:D:141:HIS:CD2	1:D:303:PHE:HE1	1.38	1.21
1:B:188:MET:HE1	1:B:243:GLU:OE2	1.40	1.19
1:D:198:GLU:HB3	1:D:236:LEU:HD12	1.20	1.19
1:A:388:GLU:CG	1:A:419:TYR:CD2	2.27	1.17
1:D:198:GLU:CB	1:D:236:LEU:HD13	1.75	1.17
1:B:184:ILE:HD11	1:B:253:LEU:HD22	1.24	1.14
1:D:184:ILE:HD11	1:D:253:LEU:CD1	1.78	1.13
1:A:99:LEU:HD23	1:A:317:MET:HE1	1.31	1.12
1:A:141:HIS:HD2	1:A:303:PHE:CD1	1.66	1.12
1:B:141:HIS:CD2	1:B:303:PHE:HE1	1.65	1.11
1:C:184:ILE:HD11	1:C:253:LEU:CD1	1.79	1.10
1:A:99:LEU:CD2	1:A:317:MET:HE1	1.80	1.10
1:B:198:GLU:OE1	1:B:236:LEU:HD22	1.49	1.09
1:A:103:LEU:HD21	1:A:317:MET:HG3	1.32	1.09
1:D:19:VAL:CG2	1:D:95:ILE:HD11	1.81	1.09
1:A:35:LEU:HD12	1:A:84:ALA:HB2	1.31	1.09
1:D:141:HIS:NE2	1:D:303:PHE:CE1	2.21	1.08
1:C:141:HIS:HD2	1:C:303:PHE:CD1	1.72	1.07
1:D:198:GLU:CB	1:D:236:LEU:CD1	2.33	1.06
1:C:226:TYR:O	1:C:230:LYS:HB3	1.56	1.06
1:D:238:LYS:O	1:D:241:VAL:HG23	1.54	1.06
1:B:249:LEU:O	1:B:253:LEU:HD13	1.55	1.05
1:C:509:LEU:CD2	1:C:514:GLU:HB2	1.85	1.05
1:C:200:ALA:O	1:C:203:THR:OG1	1.75	1.04
1:C:563:LEU:HG	1:C:570:TYR:HE2	1.20	1.04
1:D:198:GLU:CG	1:D:236:LEU:HD13	1.88	1.04
1:A:388:GLU:HG2	1:A:419:TYR:CD2	1.90	1.04
1:A:509:LEU:CD2	1:A:514:GLU:HB2	1.87	1.04
1:B:35:LEU:HD12	1:B:84:ALA:HB2	1.34	1.04
1:C:195:THR:HG23	1:C:196:GLN:NE2	1.71	1.04
1:B:184:ILE:HD11	1:B:253:LEU:CD2	1.87	1.03
1:A:141:HIS:CD2	1:A:303:PHE:HE1	1.59	1.03
1:B:229:GLY:O	1:B:233:ILE:HG22	1.57	1.03
1:C:192:SER:C	1:C:195:THR:HG22	1.84	1.02
1:D:35:LEU:HD12	1:D:84:ALA:HB2	1.42	1.01
1:C:35:LEU:HD12	1:C:84:ALA:HB2	1.38	1.01
1:A:510:ASP:OD2	1:B:375:PRO:HA	1.58	1.01
1:C:141:HIS:HD2	1:C:303:PHE:CE1	1.66	1.01
1:A:99:LEU:CD2	1:A:317:MET:CE	2.38	1.00
1:D:19:VAL:HG22	1:D:95:ILE:CD1	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLU:OE2	1:A:419:TYR:HD2	1.44	0.99
1:D:184:ILE:HD11	1:D:253:LEU:HD13	1.44	0.99
1:A:367:GLY:H	1:A:529:THR:CG2	1.76	0.98
1:C:198:GLU:OE2	1:C:236:LEU:CD1	2.11	0.98
1:A:217:LYS:HD2	1:B:414:ARG:HH12	1.21	0.97
1:D:141:HIS:CD2	1:D:303:PHE:CD1	2.35	0.97
1:A:141:HIS:NE2	1:A:303:PHE:CE1	2.33	0.96
1:C:184:ILE:HD11	1:C:253:LEU:HD13	1.48	0.95
1:A:217:LYS:CD	1:A:222:GLU:OE2	2.15	0.95
1:D:199:THR:HG22	1:D:237:PHE:CE1	2.01	0.95
1:A:141:HIS:CD2	1:A:303:PHE:CD1	2.48	0.94
1:B:141:HIS:HD2	1:B:303:PHE:CE1	1.82	0.94
1:A:367:GLY:H	1:A:529:THR:HG23	1.30	0.94
1:C:226:TYR:CZ	1:C:230:LYS:HD3	2.01	0.94
1:C:237:PHE:HD1	1:D:93:GLN:HE22	0.97	0.93
1:C:93:GLN:NE2	1:D:237:PHE:O	2.01	0.93
1:D:19:VAL:HG22	1:D:95:ILE:HD11	0.93	0.93
1:C:226:TYR:CE2	1:C:230:LYS:HD3	2.02	0.93
1:D:465:PRO:O	1:D:470:THR:HG23	1.68	0.93
1:B:198:GLU:OE1	1:B:236:LEU:CD2	2.16	0.93
1:D:198:GLU:HG3	1:D:236:LEU:HD13	1.50	0.93
1:A:99:LEU:HD22	1:A:317:MET:CE	1.99	0.92
1:C:198:GLU:OE1	1:C:202:PHE:CE1	2.22	0.92
1:B:141:HIS:HD2	1:B:303:PHE:CD1	1.86	0.92
1:C:465:PRO:O	1:C:470:THR:HG23	1.69	0.92
1:A:509:LEU:HD22	1:A:514:GLU:HB2	1.49	0.92
1:A:217:LYS:HD2	1:B:414:ARG:HH11	1.27	0.92
1:D:141:HIS:NE2	1:D:303:PHE:HE1	1.64	0.91
1:A:99:LEU:HD23	1:A:317:MET:CE	1.99	0.91
1:C:192:SER:HA	1:C:195:THR:CG2	2.00	0.90
1:C:199:THR:O	1:C:203:THR:HG23	1.71	0.90
1:B:193:ARG:HD3	1:B:316:ARG:HH22	1.35	0.89
1:D:199:THR:HG22	1:D:237:PHE:CZ	2.08	0.88
1:D:238:LYS:O	1:D:241:VAL:CG2	2.20	0.88
1:A:99:LEU:CD2	1:A:317:MET:SD	2.61	0.88
1:B:193:ARG:HD3	1:B:316:ARG:NH2	1.89	0.88
1:A:217:LYS:CD	1:B:414:ARG:NH1	2.33	0.88
1:A:366:ALA:HA	1:A:529:THR:CG2	2.03	0.88
1:A:437:TYR:CE2	1:B:220:ASN:ND2	2.42	0.88
1:B:229:GLY:O	1:B:233:ILE:CG2	2.22	0.87
1:C:109:LYS:HA	1:D:217:LYS:HZ1	1.36	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD11	1:B:124:VAL:HG13	1.58	0.86
1:B:90:TYR:CZ	1:B:94:LYS:HD2	2.11	0.86
1:C:237:PHE:HD1	1:D:93:GLN:NE2	1.73	0.86
1:A:184:ILE:HD11	1:A:253:LEU:HD13	1.58	0.86
1:A:388:GLU:HG3	1:A:419:TYR:CD2	2.09	0.86
1:A:388:GLU:OE2	1:A:419:TYR:CD2	2.28	0.85
1:A:141:HIS:NE2	1:A:303:PHE:HE1	1.72	0.85
1:C:509:LEU:HD21	1:C:514:GLU:CA	2.06	0.85
1:C:563:LEU:HG	1:C:570:TYR:CE2	2.11	0.85
1:A:437:TYR:CD2	1:B:220:ASN:ND2	2.45	0.84
1:C:192:SER:CA	1:C:195:THR:HG22	2.07	0.84
1:C:198:GLU:O	1:C:202:PHE:HD1	1.61	0.84
1:C:104:TRP:CZ2	1:D:206:LEU:HD21	2.13	0.83
1:C:104:TRP:CH2	1:D:206:LEU:CD2	2.60	0.83
1:C:141:HIS:NE2	1:C:303:PHE:CE1	2.45	0.83
1:B:227:GLY:O	1:B:231:MET:HG2	1.79	0.83
1:C:509:LEU:CD2	1:C:514:GLU:CB	2.56	0.83
1:D:99:LEU:CD2	1:D:317:MET:SD	2.60	0.83
1:D:378:GLY:O	1:D:549:VAL:HG12	1.78	0.83
1:B:76:VAL:O	1:B:80:LEU:HG	1.79	0.82
1:B:125:SER:OG	1:B:203:THR:HG21	1.78	0.82
1:C:563:LEU:CG	1:C:570:TYR:HE2	1.92	0.82
1:C:192:SER:O	1:C:195:THR:CG2	2.27	0.82
1:A:76:VAL:O	1:A:80:LEU:HG	1.79	0.82
1:C:76:VAL:O	1:C:80:LEU:HG	1.79	0.81
1:C:509:LEU:HD22	1:C:514:GLU:HB2	1.62	0.81
1:D:400:LEU:CD1	1:D:413:TRP:HE1	1.93	0.81
1:A:217:LYS:CD	1:B:414:ARG:HH12	1.91	0.81
1:C:108:ILE:O	1:D:217:LYS:HD3	1.80	0.81
1:A:231:MET:O	1:A:235:SER:HB3	1.80	0.80
1:B:184:ILE:CD1	1:B:253:LEU:HD22	2.08	0.80
1:D:206:LEU:HD13	1:D:206:LEU:O	1.81	0.80
1:A:509:LEU:HD22	1:A:514:GLU:CB	2.12	0.80
1:A:388:GLU:CD	1:A:419:TYR:HD2	1.90	0.80
1:A:206:LEU:CD1	1:B:124:VAL:HG13	2.12	0.79
1:C:192:SER:O	1:C:195:THR:HG22	1.81	0.79
1:D:103:LEU:HD21	1:D:317:MET:HG3	1.63	0.79
1:A:509:LEU:CD2	1:A:514:GLU:CB	2.60	0.79
1:A:231:MET:O	1:A:235:SER:CB	2.31	0.79
1:C:192:SER:HA	1:C:195:THR:HG21	1.62	0.79
1:C:374:GLY:O	1:D:510:ASP:OD2	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:VAL:O	1:D:80:LEU:HG	1.82	0.79
1:C:510:ASP:OD2	1:D:375:PRO:HA	1.83	0.78
1:D:141:HIS:HD2	1:D:303:PHE:HD1	1.30	0.78
1:B:90:TYR:O	1:B:94:LYS:HG3	1.83	0.78
1:A:509:LEU:HD21	1:A:514:GLU:CA	2.12	0.78
1:A:509:LEU:HD21	1:A:514:GLU:N	1.97	0.78
1:A:201:ARG:O	1:A:205:LEU:HG	1.84	0.77
1:C:509:LEU:HD21	1:C:514:GLU:HA	1.66	0.77
1:A:378:GLY:O	1:A:549:VAL:HG12	1.83	0.77
1:C:506:THR:HG22	1:C:509:LEU:HD13	1.67	0.77
1:D:198:GLU:CG	1:D:236:LEU:CD1	2.62	0.76
1:C:426:LEU:HD11	1:C:484:ARG:HB2	1.67	0.76
1:B:440:GLU:O	1:B:440:GLU:HG3	1.86	0.75
1:D:225:GLU:OE1	1:D:228:ARG:HD2	1.86	0.75
1:C:466:ASN:HB2	1:C:469:ASP:HB2	1.66	0.75
1:A:103:LEU:CD2	1:A:317:MET:HG3	2.16	0.75
1:C:108:ILE:O	1:D:217:LYS:NZ	2.18	0.75
1:D:184:ILE:CD1	1:D:253:LEU:CD1	2.64	0.75
1:A:103:LEU:HD11	1:A:317:MET:SD	2.26	0.74
1:B:53:LEU:HB3	1:B:57:PHE:CZ	2.21	0.74
1:C:104:TRP:CZ3	1:D:206:LEU:HD21	2.22	0.74
1:A:388:GLU:HG2	1:A:419:TYR:CG	2.23	0.73
1:D:207:ASN:O	1:D:211:PRO:HD3	1.88	0.73
1:C:22:THR:HB	1:C:102:LEU:HD11	1.69	0.73
1:C:195:THR:CG2	1:C:196:GLN:NE2	2.50	0.73
1:A:388:GLU:CD	1:A:419:TYR:CD2	2.64	0.73
1:B:426:LEU:HD11	1:B:484:ARG:HB2	1.69	0.73
1:C:141:HIS:NE2	1:C:303:PHE:HE1	1.80	0.73
1:C:378:GLY:O	1:C:549:VAL:HG12	1.89	0.73
1:A:437:TYR:HD2	1:B:220:ASN:HD22	1.31	0.72
1:B:216:VAL:O	1:B:220:ASN:OD1	2.07	0.72
1:C:509:LEU:HD23	1:C:514:GLU:HB2	1.71	0.72
1:B:226:TYR:CZ	1:B:230:LYS:HD3	2.24	0.72
1:C:184:ILE:CD1	1:C:253:LEU:CD1	2.65	0.72
1:A:141:HIS:HD2	1:A:303:PHE:HD1	1.36	0.72
1:C:192:SER:HA	1:C:195:THR:HG22	1.67	0.72
1:C:209:ILE:HD11	1:C:228:ARG:HH22	1.54	0.72
1:A:388:GLU:HG3	1:A:419:TYR:CE2	2.26	0.71
1:B:25:SER:OG	1:B:94:LYS:HE2	1.89	0.71
1:B:378:GLY:O	1:B:549:VAL:HG12	1.91	0.71
1:B:141:HIS:NE2	1:B:303:PHE:CE1	2.59	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:O	1:A:206:LEU:HG	1.91	0.70
1:C:184:ILE:HD11	1:C:253:LEU:HD12	1.74	0.70
1:C:226:TYR:CZ	1:C:230:LYS:CD	2.74	0.70
1:D:11:LYS:HD2	1:D:186:ARG:HH12	1.57	0.70
1:C:509:LEU:HD22	1:C:514:GLU:CB	2.21	0.70
1:A:35:LEU:CD1	1:A:84:ALA:HB2	2.17	0.70
1:A:509:LEU:HD23	1:A:510:ASP:O	1.92	0.70
1:C:141:HIS:CD2	1:C:303:PHE:CD1	2.59	0.70
1:A:103:LEU:HG	1:A:317:MET:HE3	1.73	0.69
1:A:367:GLY:H	1:A:529:THR:HG22	1.57	0.69
1:C:196:GLN:OE1	1:C:196:GLN:HA	1.92	0.69
1:A:456:TYR:HE1	1:A:459:ASN:HD22	1.40	0.69
1:D:228:ARG:HG3	1:D:229:GLY:N	2.06	0.69
1:D:225:GLU:OE2	1:D:228:ARG:NE	2.25	0.69
1:D:184:ILE:HD11	1:D:253:LEU:HD12	1.73	0.69
1:A:388:GLU:CG	1:A:419:TYR:HD2	1.99	0.69
1:D:466:ASN:HB2	1:D:469:ASP:HB3	1.74	0.69
1:C:19:VAL:HG13	1:C:95:ILE:HD11	1.76	0.68
1:C:509:LEU:CD2	1:C:514:GLU:CA	2.71	0.68
1:A:509:LEU:CD2	1:A:514:GLU:CA	2.70	0.68
1:D:226:TYR:O	1:D:230:LYS:CB	2.41	0.68
1:A:103:LEU:HD21	1:A:317:MET:CG	2.19	0.68
1:C:109:LYS:HA	1:D:217:LYS:NZ	2.09	0.68
1:D:240:GLY:O	1:D:243:GLU:N	2.26	0.68
1:A:366:ALA:HA	1:A:529:THR:HG21	1.76	0.67
1:D:206:LEU:HD13	1:D:206:LEU:C	2.19	0.67
1:C:192:SER:C	1:C:195:THR:CG2	2.64	0.67
1:C:349:GLY:HA2	1:C:356:ILE:HG22	1.77	0.67
1:B:141:HIS:NE2	1:B:303:PHE:HE1	1.92	0.66
1:A:388:GLU:OE2	1:A:419:TYR:HB3	1.96	0.66
1:B:226:TYR:CE2	1:B:230:LYS:HD3	2.31	0.66
1:C:561:HIS:HB3	1:D:587:LYS:HE2	1.78	0.66
1:A:316:ARG:HA	1:A:319:GLU:HG2	1.78	0.66
1:C:226:TYR:O	1:C:230:LYS:CB	2.40	0.66
1:D:35:LEU:CD1	1:D:84:ALA:HB2	2.22	0.66
1:D:226:TYR:O	1:D:230:LYS:HB2	1.95	0.66
1:C:192:SER:CA	1:C:195:THR:CG2	2.69	0.66
1:A:207:ASN:OD1	1:B:124:VAL:HG21	1.96	0.65
1:A:284:VAL:HG11	1:B:57:PHE:CE1	2.31	0.65
1:C:407:THR:CG2	1:C:408:TYR:N	2.58	0.65
1:A:367:GLY:N	1:A:529:THR:CG2	2.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ILE:HD13	1:B:461:ILE:HG13	1.78	0.65
1:B:35:LEU:CD1	1:B:84:ALA:HB2	2.20	0.65
1:D:225:GLU:OE2	1:D:228:ARG:CZ	2.45	0.65
1:A:426:LEU:HD21	1:A:484:ARG:HB2	1.80	0.64
1:D:141:HIS:NE2	1:D:307:LEU:HD13	2.11	0.64
1:C:142:ILE:O	1:C:146:ILE:HG12	1.97	0.64
1:C:510:ASP:OD2	1:D:374:GLY:O	2.15	0.64
1:A:124:VAL:O	1:A:127:VAL:HG12	1.98	0.64
1:A:512:GLN:HG3	1:B:576:GLN:HG3	1.80	0.64
1:D:91:ASN:O	1:D:95:ILE:HG22	1.98	0.63
1:C:506:THR:HG21	1:C:514:GLU:HG2	1.81	0.63
1:A:406:ASP:O	1:A:408:TYR:O	2.16	0.63
1:C:461:ILE:HD13	1:C:467:GLN:HE21	1.64	0.63
1:C:507:SER:HB2	1:D:507:SER:HB2	1.81	0.62
1:C:500:LEU:HB2	1:C:525:MET:HE2	1.81	0.62
1:A:431:ILE:HD13	1:A:461:ILE:HG12	1.80	0.62
1:B:373:VAL:O	1:B:548:PHE:HA	2.00	0.62
1:D:341:ILE:HA	1:D:400:LEU:HD23	1.82	0.62
1:A:217:LYS:HG3	1:A:217:LYS:O	1.99	0.62
1:B:141:HIS:CD2	1:B:303:PHE:CD1	2.70	0.62
1:B:141:HIS:HE2	1:B:307:LEU:HD13	1.65	0.62
1:C:227:GLY:O	1:C:231:MET:HB2	1.99	0.61
1:C:198:GLU:OE2	1:C:236:LEU:HD22	2.00	0.61
1:B:138:ILE:HD12	1:B:141:HIS:ND1	2.15	0.61
1:C:509:LEU:HD21	1:C:514:GLU:N	2.16	0.61
1:A:389:ARG:NH1	1:A:405:VAL:HG22	2.16	0.61
1:A:184:ILE:CD1	1:A:253:LEU:HD13	2.30	0.61
1:D:571:ARG:O	1:D:572:ASP:C	2.44	0.61
1:A:367:GLY:N	1:A:529:THR:HG23	2.11	0.60
1:D:137:LEU:HD21	1:D:310:SER:HB3	1.83	0.60
1:D:184:ILE:CD1	1:D:253:LEU:HD12	2.29	0.60
1:C:104:TRP:CZ2	1:D:206:LEU:CD2	2.84	0.60
1:D:112:VAL:HG21	1:D:390:PHE:HB3	1.83	0.60
1:A:103:LEU:HD11	1:A:317:MET:HG3	1.82	0.60
1:A:206:LEU:HD23	1:A:233:ILE:CD1	2.32	0.60
1:C:198:GLU:OE1	1:C:202:PHE:HE1	1.77	0.60
1:B:567:HIS:HB2	1:B:570:TYR:HD1	1.67	0.60
1:B:112:VAL:HG21	1:B:390:PHE:HB3	1.83	0.59
1:C:112:VAL:HG21	1:C:390:PHE:HB3	1.84	0.59
1:D:99:LEU:HD22	1:D:317:MET:CE	2.31	0.59
1:A:509:LEU:HD23	1:A:514:GLU:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:GLY:HA3	1:B:433:GLU:OE1	2.01	0.59
1:C:35:LEU:CD1	1:C:84:ALA:HB2	2.22	0.59
1:D:24:PRO:HD2	1:D:94:LYS:HG2	1.83	0.59
1:C:184:ILE:CD1	1:C:253:LEU:HD12	2.30	0.59
1:C:141:HIS:HE2	1:C:307:LEU:HD13	1.67	0.59
1:C:192:SER:O	1:C:195:THR:HG23	2.01	0.59
1:D:199:THR:CG2	1:D:237:PHE:CE1	2.82	0.59
1:D:429:GLY:HA3	1:D:433:GLU:OE1	2.03	0.59
1:B:574:ALA:HB1	1:B:578:LEU:HD12	1.84	0.59
1:C:375:PRO:HA	1:D:510:ASP:OD2	2.03	0.58
1:A:509:LEU:HD21	1:A:514:GLU:HA	1.85	0.58
1:C:225:GLU:OE1	1:C:228:ARG:NH2	2.31	0.58
1:B:404:PRO:HD2	1:B:407:THR:OG1	2.04	0.58
1:C:210:LEU:O	1:C:213:ILE:HG23	2.02	0.58
1:A:499:ILE:HG12	1:A:529:THR:OG1	2.03	0.58
1:D:225:GLU:OE1	1:D:228:ARG:CD	2.51	0.58
1:A:509:LEU:HD21	1:A:513:SER:C	2.28	0.58
1:A:510:ASP:OD2	1:B:375:PRO:CA	2.43	0.58
1:C:122:GLU:HG3	1:C:201:ARG:HG3	1.86	0.58
1:C:206:LEU:HD21	1:C:233:ILE:HD11	1.84	0.58
1:B:403:GLU:HB3	1:B:408:TYR:HB2	1.84	0.57
1:B:464:LEU:HB3	1:B:470:THR:HG21	1.85	0.57
1:C:108:ILE:O	1:D:217:LYS:CD	2.50	0.57
1:C:512:GLN:HG3	1:D:576:GLN:HG3	1.86	0.57
1:A:367:GLY:N	1:A:529:THR:HG22	2.18	0.57
1:B:90:TYR:CE2	1:B:94:LYS:HD2	2.39	0.57
1:A:103:LEU:HD11	1:A:317:MET:CG	2.35	0.57
1:D:486:ARG:HA	1:D:489:ILE:HD12	1.87	0.57
1:A:220:ASN:HA	1:B:414:ARG:HH21	1.70	0.57
1:D:213:ILE:HG13	1:D:217:LYS:HG2	1.86	0.57
1:B:547:LEU:HD23	1:B:557:ARG:HG2	1.85	0.57
1:A:316:ARG:HA	1:A:319:GLU:CG	2.34	0.57
1:A:581:ASN:HB2	1:A:584:LEU:HD12	1.87	0.57
1:C:96:ILE:HD12	1:C:135:LYS:HB2	1.86	0.57
1:A:389:ARG:NH1	1:A:405:VAL:O	2.38	0.56
1:A:96:ILE:HD12	1:A:135:LYS:HB2	1.86	0.56
1:A:231:MET:O	1:A:235:SER:OG	2.24	0.56
1:B:466:ASN:HB2	1:B:469:ASP:HB2	1.86	0.56
1:A:25:SER:OG	1:A:95:ILE:HD11	2.05	0.56
1:C:198:GLU:OE1	1:C:202:PHE:CZ	2.57	0.56
1:C:372:ILE:HG13	1:C:547:LEU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:HE2	1:A:307:LEU:HD13	1.70	0.56
1:A:284:VAL:HG11	1:B:57:PHE:CD1	2.41	0.56
1:D:96:ILE:HD12	1:D:135:LYS:HB2	1.87	0.56
1:B:90:TYR:CE1	1:B:94:LYS:HD2	2.40	0.56
1:A:19:VAL:O	1:A:23:ASN:HB2	2.05	0.56
1:B:22:THR:HG21	1:B:99:LEU:HG	1.87	0.56
1:B:372:ILE:HG13	1:B:547:LEU:HB2	1.88	0.56
1:C:429:GLY:HA3	1:C:433:GLU:OE1	2.04	0.56
1:D:432:ARG:HD2	1:D:468:PHE:HB3	1.87	0.56
1:D:426:LEU:HD21	1:D:484:ARG:HB2	1.88	0.56
1:D:501:MET:HE1	1:D:503:ASP:HB2	1.87	0.56
1:B:230:LYS:HA	1:B:233:ILE:HG22	1.87	0.56
1:C:501:MET:HE1	1:C:503:ASP:HB2	1.88	0.56
1:C:570:TYR:O	1:C:570:TYR:CD2	2.58	0.56
1:D:18:LEU:HD23	1:D:317:MET:HE3	1.87	0.55
1:A:501:MET:HE1	1:A:503:ASP:HB2	1.87	0.55
1:C:138:ILE:HD12	1:C:141:HIS:ND1	2.21	0.55
1:C:198:GLU:CD	1:C:202:PHE:CE1	2.84	0.55
1:A:231:MET:C	1:A:235:SER:HB3	2.30	0.55
1:C:512:GLN:HA	1:D:576:GLN:HE21	1.72	0.55
1:A:431:ILE:CD1	1:A:470:THR:OG1	2.54	0.55
1:B:125:SER:OG	1:B:203:THR:CG2	2.54	0.55
1:C:563:LEU:CD2	1:C:570:TYR:CE2	2.89	0.55
1:A:104:TRP:NE1	1:B:229:GLY:HA3	2.21	0.55
1:C:130:ASP:HA	1:C:133:VAL:HG23	1.89	0.55
1:D:103:LEU:HD11	1:D:317:MET:HG3	1.88	0.55
1:B:229:GLY:O	1:B:233:ILE:CB	2.55	0.55
1:C:198:GLU:CD	1:C:236:LEU:HD13	2.23	0.55
1:A:372:ILE:HG13	1:A:547:LEU:HB2	1.89	0.55
1:B:96:ILE:HD12	1:B:135:LYS:HB2	1.89	0.55
1:D:234:SER:O	1:D:235:SER:C	2.46	0.55
1:B:501:MET:HE1	1:B:503:ASP:HB2	1.87	0.54
1:C:425:PRO:HG3	1:D:215:LEU:HD22	1.87	0.54
1:C:563:LEU:CD2	1:C:570:TYR:HE2	2.19	0.54
1:A:486:ARG:HA	1:A:489:ILE:HD12	1.90	0.54
1:D:547:LEU:HD23	1:D:557:ARG:HG2	1.90	0.54
1:C:472:VAL:HG12	1:C:476:GLY:HA2	1.90	0.54
1:D:228:ARG:CG	1:D:229:GLY:N	2.70	0.54
1:A:220:ASN:O	1:B:438:GLY:O	2.25	0.54
1:C:535:HIS:CD2	1:C:536:ARG:HG2	2.43	0.54
1:C:560:HIS:C	1:C:560:HIS:CD2	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ILE:HG13	1:D:547:LEU:HB2	1.88	0.54
1:C:141:HIS:NE2	1:C:307:LEU:HD13	2.22	0.54
1:C:358:LYS:O	1:C:359:GLU:C	2.51	0.53
1:A:438:GLY:HA3	1:A:495:ARG:HD3	1.90	0.53
1:A:535:HIS:CD2	1:A:536:ARG:HG2	2.43	0.53
1:A:141:HIS:NE2	1:A:307:LEU:HD13	2.24	0.53
1:B:32:ALA:HB2	1:B:87:ALA:HB3	1.90	0.53
1:B:535:HIS:CD2	1:B:536:ARG:HG2	2.44	0.53
1:C:457:ALA:HB2	1:C:486:ARG:HB3	1.89	0.53
1:A:578:LEU:HD21	1:B:584:LEU:HB2	1.92	0.53
1:B:503:ASP:HA	1:B:533:ILE:HB	1.91	0.53
1:B:141:HIS:NE2	1:B:307:LEU:HD13	2.24	0.52
1:C:564:MET:O	1:C:571:ARG:CA	2.57	0.52
1:D:225:GLU:CD	1:D:228:ARG:NE	2.68	0.52
1:C:431:ILE:HD13	1:C:461:ILE:HG12	1.92	0.52
1:D:503:ASP:HA	1:D:533:ILE:HB	1.91	0.52
1:A:32:ALA:HB2	1:A:87:ALA:HB3	1.91	0.52
1:D:141:HIS:HE2	1:D:307:LEU:HD13	1.72	0.52
1:A:387:LEU:C	1:A:389:ARG:H	2.17	0.52
1:D:238:LYS:O	1:D:241:VAL:CB	2.57	0.52
1:B:120:SER:O	1:B:123:THR:HG22	2.09	0.52
1:A:16:PHE:O	1:A:20:ARG:HG3	2.10	0.52
1:A:186:ARG:HH21	1:A:308:GLN:HE22	1.57	0.52
1:C:108:ILE:O	1:D:217:LYS:CE	2.58	0.52
1:A:206:LEU:HD23	1:A:233:ILE:HD13	1.92	0.52
1:C:500:LEU:HB3	1:C:530:THR:HG23	1.91	0.52
1:C:564:MET:O	1:C:571:ARG:HB2	2.10	0.52
1:D:198:GLU:HG3	1:D:236:LEU:CD1	2.32	0.52
1:D:571:ARG:O	1:D:573:PHE:HD1	1.92	0.52
1:A:503:ASP:HA	1:A:533:ILE:HB	1.91	0.52
1:D:99:LEU:CD2	1:D:317:MET:CE	2.88	0.52
1:D:535:HIS:CD2	1:D:536:ARG:HG2	2.45	0.51
1:A:499:ILE:CG1	1:A:529:THR:OG1	2.58	0.51
1:C:503:ASP:HA	1:C:533:ILE:HB	1.92	0.51
1:C:563:LEU:CG	1:C:570:TYR:CE2	2.82	0.51
1:A:220:ASN:HB3	1:B:438:GLY:O	2.10	0.51
1:C:198:GLU:OE2	1:C:236:LEU:CD2	2.59	0.51
1:D:236:LEU:HD23	1:D:236:LEU:N	2.26	0.51
1:D:341:ILE:HB	1:D:364:ILE:HB	1.93	0.51
1:D:500:LEU:HB2	1:D:525:MET:HE2	1.91	0.51
1:A:417:ILE:HG12	1:A:499:ILE:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ILE:HB	1:B:364:ILE:HB	1.93	0.51
1:C:563:LEU:O	1:C:566:SER:OG	2.27	0.51
1:C:198:GLU:OE2	1:C:236:LEU:CG	2.58	0.51
1:C:556:GLY:HA3	1:C:563:LEU:HD11	1.93	0.51
1:B:342:GLN:HB2	1:B:399:ARG:HB2	1.92	0.51
1:C:509:LEU:HD23	1:C:510:ASP:O	2.10	0.51
1:A:341:ILE:HB	1:A:364:ILE:HB	1.93	0.50
1:B:125:SER:C	1:B:127:VAL:H	2.19	0.50
1:B:188:MET:HE3	1:B:309:LYS:HG3	1.93	0.50
1:C:341:ILE:HB	1:C:364:ILE:HB	1.92	0.50
1:C:560:HIS:NE2	1:C:564:MET:SD	2.84	0.50
2:C:700:ATP:H5'1	1:D:480:SER:HB3	1.93	0.50
1:A:500:LEU:HB2	1:A:525:MET:HE2	1.91	0.50
1:A:500:LEU:HD23	1:A:501:MET:N	2.26	0.50
1:B:122:GLU:HG3	1:B:201:ARG:HG3	1.92	0.50
1:B:466:ASN:CG	1:B:469:ASP:OD2	2.54	0.50
1:C:125:SER:C	1:C:127:VAL:H	2.18	0.50
1:A:12:LEU:HD23	1:A:311:ILE:HD13	1.93	0.50
1:A:334:ILE:HG13	1:A:337:ALA:HB3	1.94	0.50
1:A:414:ARG:HD3	1:B:218:ALA:HA	1.93	0.50
1:B:231:MET:HG3	1:B:232:GLY:N	2.26	0.50
1:D:217:LYS:HD2	1:D:221:ALA:HB2	1.91	0.50
1:A:456:TYR:O	1:A:456:TYR:CG	2.65	0.50
1:A:316:ARG:HA	1:A:319:GLU:CD	2.37	0.50
1:A:507:SER:HB2	1:B:507:SER:HB2	1.93	0.50
1:C:407:THR:HG22	1:C:408:TYR:N	2.24	0.50
1:B:18:LEU:HD11	1:B:321:LEU:HD13	1.94	0.49
1:C:407:THR:HG22	1:C:408:TYR:H	1.77	0.49
1:D:141:HIS:CE1	1:D:307:LEU:HD13	2.47	0.49
1:D:225:GLU:OE2	1:D:228:ARG:NH1	2.45	0.49
1:A:456:TYR:O	1:A:456:TYR:CD2	2.66	0.49
1:B:500:LEU:HB3	1:B:530:THR:HG23	1.94	0.49
1:D:500:LEU:HD23	1:D:501:MET:N	2.27	0.49
1:A:107:LEU:HB3	1:B:210:LEU:HD21	1.94	0.49
1:B:460:PHE:HD1	1:B:463:GLU:HG3	1.77	0.49
1:A:103:LEU:CG	1:A:317:MET:HE3	2.40	0.49
1:C:421:SER:HB2	1:D:215:LEU:HD21	1.94	0.49
1:C:509:LEU:CD2	1:C:514:GLU:HA	2.38	0.49
1:D:44:LEU:HD11	1:D:151:SER:HA	1.95	0.49
1:B:108:ILE:HD12	1:B:109:LYS:HG3	1.95	0.48
1:B:236:LEU:HD23	1:B:239:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:ARG:HA	1:B:489:ILE:HD12	1.95	0.48
1:C:564:MET:O	1:C:571:ARG:CB	2.61	0.48
1:A:366:ALA:HA	1:A:529:THR:HG22	1.90	0.48
1:A:48:LEU:HA	1:A:51:LYS:HE3	1.95	0.48
1:A:203:THR:HA	1:A:206:LEU:CD2	2.43	0.48
1:D:464:LEU:HB3	1:D:470:THR:HG21	1.95	0.48
1:A:546:LEU:HD12	1:A:559:THR:HA	1.96	0.48
1:B:159:LEU:HD11	1:B:289:TYR:HB3	1.95	0.48
1:D:427:MET:O	1:D:472:VAL:CG2	2.62	0.48
1:A:166:LEU:HD22	1:A:265:VAL:HA	1.95	0.48
1:A:461:ILE:HD13	1:A:467:GLN:HE21	1.78	0.48
1:B:25:SER:CB	1:B:94:LYS:HE2	2.44	0.48
1:B:229:GLY:O	1:B:233:ILE:HB	2.13	0.48
1:C:564:MET:O	1:C:571:ARG:HA	2.14	0.48
1:B:216:VAL:HG12	1:B:221:ALA:HB2	1.95	0.48
1:C:124:VAL:HG22	1:D:210:LEU:HD13	1.94	0.48
1:C:570:TYR:CD1	1:C:573:PHE:HB2	2.48	0.48
1:D:369:VAL:HG13	1:D:530:THR:HB	1.96	0.48
1:B:12:LEU:HD22	1:B:307:LEU:HD23	1.96	0.47
1:D:93:GLN:O	1:D:93:GLN:HG3	2.13	0.47
1:A:425:PRO:HG3	1:B:215:LEU:HD22	1.95	0.47
1:A:437:TYR:HE2	1:B:220:ASN:ND2	2.04	0.47
1:D:466:ASN:HB2	1:D:469:ASP:CB	2.41	0.47
1:A:389:ARG:HH11	1:A:405:VAL:HG22	1.79	0.47
1:B:217:LYS:HA	1:B:221:ALA:HB3	1.96	0.47
1:C:398:ILE:O	1:C:405:VAL:HG13	2.15	0.47
1:D:220:ASN:HB3	1:D:223:ASP:HB3	1.96	0.47
1:B:12:LEU:HD22	1:B:307:LEU:CD2	2.44	0.47
1:C:44:LEU:HD11	1:C:151:SER:HA	1.96	0.47
1:C:124:VAL:HG21	1:D:207:ASN:ND2	2.29	0.47
1:C:215:LEU:HG	1:D:425:PRO:HG3	1.96	0.47
1:C:226:TYR:CE2	1:C:230:LYS:CD	2.89	0.47
1:A:127:VAL:HG13	1:A:128:THR:N	2.30	0.47
1:A:207:ASN:HB2	1:B:124:VAL:HG11	1.96	0.47
1:C:366:ALA:HA	1:C:529:THR:OG1	2.14	0.47
1:A:466:ASN:HB2	1:A:469:ASP:HB2	1.96	0.47
1:B:366:ALA:HA	1:B:529:THR:OG1	2.15	0.47
1:C:369:VAL:HG13	1:C:530:THR:HB	1.98	0.47
1:C:195:THR:CG2	1:C:196:GLN:HE22	2.28	0.46
1:A:198:GLU:HB3	1:A:236:LEU:HD13	1.97	0.46
1:B:537:LEU:HD13	1:B:573:PHE:HB3	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:SER:HB3	2:D:700:ATP:H5'1	1.97	0.46
1:A:44:LEU:HD11	1:A:151:SER:HA	1.97	0.46
1:D:206:LEU:C	1:D:206:LEU:CD1	2.85	0.46
1:D:366:ALA:HA	1:D:529:THR:OG1	2.15	0.46
1:D:108:ILE:HD12	1:D:109:LYS:HG3	1.97	0.46
1:A:500:LEU:HB3	1:A:530:THR:HG23	1.98	0.46
1:B:15:PHE:CZ	1:B:18:LEU:HD22	2.50	0.46
1:D:500:LEU:HB3	1:D:530:THR:HG23	1.98	0.46
1:A:564:MET:HA	1:A:571:ARG:HG2	1.97	0.46
1:C:89:ASN:HB3	1:D:244:ALA:HB1	1.97	0.46
1:A:217:LYS:O	1:A:217:LYS:CG	2.64	0.46
1:A:369:VAL:HG13	1:A:530:THR:HB	1.97	0.46
1:A:466:ASN:O	1:A:470:THR:CG2	2.64	0.46
1:C:29:LEU:O	1:C:33:LEU:HG	2.15	0.46
1:D:537:LEU:H	1:D:577:GLN:HE22	1.64	0.46
1:B:427:MET:O	1:B:472:VAL:CG2	2.64	0.46
1:D:188:MET:HE3	1:D:309:LYS:HG3	1.97	0.45
1:D:230:LYS:HD3	1:D:230:LYS:C	2.41	0.45
1:A:456:TYR:HE1	1:A:459:ASN:ND2	2.10	0.45
1:C:108:ILE:HD12	1:C:109:LYS:HG3	1.97	0.45
1:C:373:VAL:O	1:C:548:PHE:HA	2.16	0.45
1:D:417:ILE:HG13	1:D:499:ILE:HB	1.98	0.45
1:A:342:GLN:HB2	1:A:399:ARG:HB2	1.98	0.45
1:C:188:MET:HE3	1:C:309:LYS:HG3	1.99	0.45
1:B:125:SER:CB	1:B:203:THR:HG21	2.46	0.45
1:C:335:GLU:HA	1:C:416:HIS:HD2	1.82	0.45
1:A:127:VAL:HG13	1:A:128:THR:H	1.82	0.45
1:D:93:GLN:HA	1:D:96:ILE:HG22	1.99	0.45
1:D:92:GLY:HA2	1:D:95:ILE:HG22	1.98	0.45
1:C:443:VAL:HG11	1:C:494:LEU:HD11	1.98	0.45
1:C:482:GLY:HA3	1:D:376:SER:HB2	1.97	0.45
1:D:88:LEU:HD13	1:D:143:SER:HB2	1.99	0.45
1:A:215:LEU:HD13	1:B:425:PRO:HB3	1.98	0.45
1:A:510:ASP:OD2	1:B:374:GLY:O	2.34	0.45
1:B:350:TYR:HD1	1:B:356:ILE:HD13	1.82	0.45
1:B:537:LEU:O	1:B:537:LEU:HD23	2.17	0.45
1:C:547:LEU:HD22	1:C:554:ILE:HD13	1.98	0.45
1:A:140:THR:HA	1:A:143:SER:HB3	1.98	0.45
1:B:140:THR:HA	1:B:143:SER:HB3	1.99	0.45
1:B:198:GLU:OE1	1:B:236:LEU:HD21	2.11	0.45
1:C:384:PHE:HA	1:C:387:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:LEU:HB3	1:C:470:THR:HG21	1.99	0.44
1:A:85:THR:HA	1:A:88:LEU:HD12	1.99	0.44
1:B:25:SER:OG	1:B:94:LYS:CE	2.61	0.44
1:B:44:LEU:HD11	1:B:151:SER:HA	1.98	0.44
1:C:104:TRP:CZ3	1:D:206:LEU:HD11	2.53	0.44
1:D:226:TYR:O	1:D:230:LYS:HB3	2.16	0.44
1:C:140:THR:HA	1:C:143:SER:HB3	1.98	0.44
1:D:373:VAL:O	1:D:548:PHE:HA	2.18	0.44
1:A:108:ILE:HD12	1:A:109:LYS:HG3	1.99	0.44
1:C:230:LYS:O	1:C:231:MET:C	2.58	0.44
1:A:384:PHE:HA	1:A:387:LEU:HB2	1.99	0.44
1:D:140:THR:HA	1:D:143:SER:HB3	1.98	0.44
1:A:103:LEU:CD1	1:A:317:MET:HE3	2.47	0.44
1:A:431:ILE:HD12	1:A:470:THR:OG1	2.16	0.44
1:D:349:GLY:HA3	1:D:355:LEU:HA	1.99	0.44
1:B:209:ILE:HD11	1:B:228:ARG:HH12	1.83	0.44
1:C:195:THR:HG23	1:C:196:GLN:N	2.32	0.44
1:C:376:SER:HB2	1:D:482:GLY:HA3	2.00	0.44
1:A:357:LEU:HD11	1:A:383:LEU:HD12	1.99	0.43
1:D:24:PRO:HB2	1:D:94:LYS:HE3	1.99	0.43
1:D:125:SER:C	1:D:127:VAL:H	2.26	0.43
1:A:506:THR:HG21	1:A:514:GLU:HG2	1.99	0.43
1:A:509:LEU:CD2	1:A:514:GLU:HA	2.43	0.43
1:B:209:ILE:HD11	1:B:228:ARG:NH1	2.33	0.43
1:C:407:THR:HG23	1:C:408:TYR:N	2.33	0.43
1:A:584:LEU:HD21	1:B:537:LEU:CD2	2.48	0.43
1:D:346:VAL:HA	1:D:396:GLY:HA3	2.00	0.43
1:C:108:ILE:C	1:D:217:LYS:HZ3	2.23	0.43
1:A:414:ARG:HH21	1:A:417:ILE:HG22	1.83	0.43
1:A:456:TYR:CE1	1:A:459:ASN:ND2	2.87	0.43
1:B:202:PHE:N	1:B:202:PHE:CD1	2.86	0.43
1:D:575:GLU:HA	1:D:578:LEU:HD12	2.00	0.43
1:A:373:VAL:O	1:A:548:PHE:HA	2.19	0.43
1:B:384:PHE:HA	1:B:387:LEU:HB2	2.00	0.43
1:C:584:LEU:HB2	1:D:578:LEU:HD21	1.99	0.43
1:D:15:PHE:CG	1:D:311:ILE:HG13	2.54	0.43
1:D:431:ILE:HD11	1:D:470:THR:OG1	2.19	0.43
1:A:578:LEU:O	1:A:582:ALA:HB2	2.19	0.43
1:D:384:PHE:HA	1:D:387:LEU:HB2	2.00	0.43
1:C:33:LEU:HD23	1:C:146:ILE:HD13	2.00	0.43
1:A:127:VAL:HG13	1:A:128:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ALA:HB1	1:B:461:ILE:HD13	2.00	0.43
1:C:18:LEU:HD11	1:C:321:LEU:HD13	2.01	0.43
1:A:547:LEU:HD22	1:A:554:ILE:HD13	2.00	0.42
1:B:440:GLU:O	1:B:440:GLU:CG	2.56	0.42
1:B:484:ARG:HA	1:B:487:ILE:HD12	2.01	0.42
1:B:547:LEU:HD22	1:B:554:ILE:HD13	2.01	0.42
1:B:15:PHE:O	1:B:19:VAL:HG23	2.18	0.42
1:C:486:ARG:HA	1:C:489:ILE:HD12	2.01	0.42
1:C:506:THR:CG2	1:C:514:GLU:HG2	2.48	0.42
1:D:225:GLU:HA	1:D:228:ARG:HG2	2.01	0.42
1:A:512:GLN:HE21	1:B:576:GLN:HB2	1.85	0.42
1:B:183:PRO:HA	1:B:186:ARG:HG2	2.01	0.42
1:B:197:ASP:O	1:B:201:ARG:HB2	2.19	0.42
1:C:346:VAL:HG13	1:C:393:PRO:HB3	2.01	0.42
1:A:197:ASP:OD2	1:A:316:ARG:NH2	2.52	0.42
1:D:405:VAL:HA	1:D:408:TYR:HD2	1.85	0.42
1:A:414:ARG:NH2	1:A:417:ILE:HG22	2.33	0.42
1:D:18:LEU:HD21	1:D:321:LEU:HD13	2.02	0.42
1:D:192:SER:O	1:D:196:GLN:HB2	2.19	0.42
1:D:443:VAL:HG11	1:D:494:LEU:HD11	2.00	0.42
1:B:202:PHE:N	1:B:202:PHE:HD1	2.18	0.42
1:A:207:ASN:O	1:A:211:PRO:HD3	2.19	0.42
1:C:563:LEU:HD21	1:C:570:TYR:CE2	2.54	0.42
1:A:537:LEU:H	1:A:577:GLN:NE2	2.17	0.42
1:B:138:ILE:HA	1:B:141:HIS:HB2	2.01	0.42
1:C:564:MET:HE2	1:C:564:MET:HB3	1.68	0.42
1:D:238:LYS:O	1:D:241:VAL:HB	2.20	0.42
1:B:506:THR:HA	1:B:509:LEU:HB2	2.03	0.41
1:C:195:THR:HG23	1:C:196:GLN:HE22	1.73	0.41
1:D:484:ARG:HA	1:D:487:ILE:HD12	2.01	0.41
1:A:213:ILE:C	1:A:215:LEU:H	2.28	0.41
1:A:346:VAL:HG13	1:A:393:PRO:HB3	2.01	0.41
1:A:50:THR:HG22	1:A:53:LEU:HD13	2.03	0.41
1:A:138:ILE:HD12	1:A:141:HIS:ND1	2.35	0.41
1:D:18:LEU:HA	1:D:21:ARG:HG3	2.03	0.41
1:A:203:THR:C	1:A:206:LEU:HG	2.44	0.41
1:D:240:GLY:C	1:D:242:ARG:N	2.77	0.41
1:D:400:LEU:HD11	1:D:413:TRP:HE1	1.78	0.41
1:A:203:THR:HA	1:A:206:LEU:HG	2.01	0.41
1:A:389:ARG:HH22	1:A:406:ASP:HA	1.85	0.41
1:B:185:GLY:HA3	1:B:304:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LYS:HA	1:B:221:ALA:CB	2.51	0.41
1:B:182:VAL:HG12	1:B:186:ARG:HE	1.86	0.41
1:B:456:TYR:O	1:B:456:TYR:CG	2.74	0.41
1:D:126:ARG:NH2	1:D:316:ARG:HH21	2.18	0.41
1:A:25:SER:OG	1:A:95:ILE:CD1	2.69	0.41
1:B:122:GLU:CG	1:B:201:ARG:HG3	2.51	0.41
1:C:145:PHE:O	1:C:149:ILE:HG12	2.21	0.41
1:A:99:LEU:CB	1:A:317:MET:HE1	2.50	0.41
1:A:484:ARG:HA	1:A:487:ILE:HD12	2.02	0.41
1:B:226:TYR:OH	1:B:230:LYS:HD3	2.21	0.41
1:B:234:SER:C	1:B:236:LEU:N	2.77	0.41
1:C:484:ARG:HA	1:C:487:ILE:HD12	2.03	0.41
1:B:443:VAL:HG11	1:B:494:LEU:HD11	2.03	0.41
1:D:217:LYS:HZ2	1:D:221:ALA:HB3	1.86	0.40
1:D:332:LYS:HB3	1:D:334:ILE:HD12	2.02	0.40
1:A:104:TRP:CZ3	1:B:206:LEU:HD22	2.56	0.40
1:A:387:LEU:C	1:A:389:ARG:N	2.79	0.40
1:B:346:VAL:HG13	1:B:393:PRO:HB3	2.03	0.40
1:D:217:LYS:HZ2	1:D:221:ALA:CB	2.34	0.40
1:D:567:HIS:CE1	1:D:570:TYR:HB2	2.56	0.40
1:A:68:GLY:HA2	1:A:72:LEU:HD13	2.03	0.40
1:A:166:LEU:HA	1:A:169:LEU:HD12	2.03	0.40
1:C:213:ILE:HA	1:C:216:VAL:HB	2.03	0.40
1:B:254:ILE:HD11	1:B:301:THR:HG21	2.04	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	567/599 (95%)	499 (88%)	64 (11%)	4 (1%)	18 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	565/599 (94%)	528 (94%)	33 (6%)	4 (1%)	18	53
1	C	561/599 (94%)	510 (91%)	49 (9%)	2 (0%)	30	65
1	D	568/599 (95%)	525 (92%)	38 (7%)	5 (1%)	14	48
All	All	2261/2396 (94%)	2062 (91%)	184 (8%)	15 (1%)	18	53

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	404	PRO
1	A	428	SER
1	A	560	HIS
1	D	337	ALA
1	B	222	GLU
1	C	389	ARG
1	D	21	ARG
1	A	121	GLY
1	B	217	LYS
1	D	402	ASP
1	D	440	GLU
1	A	540	VAL
1	B	540	VAL
1	C	540	VAL
1	D	540	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	480/506 (95%)	443 (92%)	37 (8%)	12	36
1	B	481/506 (95%)	443 (92%)	38 (8%)	11	35
1	C	479/506 (95%)	436 (91%)	43 (9%)	9	31
1	D	480/506 (95%)	444 (92%)	36 (8%)	12	37
All	All	1920/2024 (95%)	1766 (92%)	154 (8%)	11	35

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	48	LEU
1	A	69	LEU
1	A	108	ILE
1	A	118	ASN
1	A	123	THR
1	A	142	ILE
1	A	146	ILE
1	A	156	LEU
1	A	169	LEU
1	A	176	LEU
1	A	180	ILE
1	A	186	ARG
1	A	196	GLN
1	A	233	ILE
1	A	256	LEU
1	A	258	LEU
1	A	288	LEU
1	A	290	LEU
1	A	294	ILE
1	A	311	ILE
1	A	315	GLU
1	A	320	ILE
1	A	325	GLU
1	A	326	GLU
1	A	357	LEU
1	A	372	ILE
1	A	410	LEU
1	A	414	ARG
1	A	416	HIS
1	A	431	ILE
1	A	440	GLU
1	A	445	ASP
1	A	477	ILE
1	A	518	GLN
1	A	531	ILE
1	A	537	LEU
1	B	21	ARG
1	B	48	LEU
1	B	67	ILE
1	B	95	ILE
1	B	108	ILE

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Mol	Chain	Res	Type
1	B	123	THR
1	B	127	VAL
1	B	142	ILE
1	B	146	ILE
1	B	156	LEU
1	B	169	LEU
1	B	176	LEU
1	B	180	ILE
1	B	191	ILE
1	B	212	GLU
1	B	254	ILE
1	B	258	LEU
1	B	288	LEU
1	B	290	LEU
1	B	294	ILE
1	B	311	ILE
1	B	315	GLU
1	B	330	THR
1	B	372	ILE
1	B	403	GLU
1	B	415	GLU
1	B	417	ILE
1	B	426	LEU
1	B	431	ILE
1	B	445	ASP
1	B	461	ILE
1	B	470	THR
1	B	477	ILE
1	B	500	LEU
1	B	514	GLU
1	B	518	GLN
1	B	531	ILE
1	B	584	LEU
1	C	22	THR
1	C	48	LEU
1	C	66	GLN
1	C	67	ILE
1	C	69	LEU
1	C	95	ILE
1	C	108	ILE
1	C	127	VAL
1	C	131	THR

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Mol	Chain	Res	Type
1	C	136	GLU
1	C	142	ILE
1	C	156	LEU
1	C	169	LEU
1	C	176	LEU
1	C	180	ILE
1	C	191	ILE
1	C	196	GLN
1	C	198	GLU
1	C	212	GLU
1	C	223	ASP
1	C	254	ILE
1	C	258	LEU
1	C	288	LEU
1	C	294	ILE
1	C	311	ILE
1	C	315	GLU
1	C	320	ILE
1	C	356	ILE
1	C	357	LEU
1	C	372	ILE
1	C	407	THR
1	C	417	ILE
1	C	426	LEU
1	C	431	ILE
1	C	440	GLU
1	C	445	ASP
1	C	477	ILE
1	C	500	LEU
1	C	518	GLN
1	C	531	ILE
1	C	537	LEU
1	C	575	GLU
1	C	578	LEU
1	D	48	LEU
1	D	51	LYS
1	D	108	ILE
1	D	122	GLU
1	D	127	VAL
1	D	142	ILE
1	D	146	ILE
1	D	156	LEU

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Mol	Chain	Res	Type
1	D	168	LEU
1	D	169	LEU
1	D	176	LEU
1	D	180	ILE
1	D	191	ILE
1	D	199	THR
1	D	212	GLU
1	D	234	SER
1	D	254	ILE
1	D	256	LEU
1	D	258	LEU
1	D	288	LEU
1	D	290	LEU
1	D	294	ILE
1	D	311	ILE
1	D	315	GLU
1	D	320	ILE
1	D	372	ILE
1	D	417	ILE
1	D	426	LEU
1	D	440	GLU
1	D	445	ASP
1	D	477	ILE
1	D	514	GLU
1	D	518	GLN
1	D	531	ILE
1	D	537	LEU
1	D	585	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	61	ASN
1	A	91	ASN
1	A	93	GLN
1	A	141	HIS
1	A	196	GLN
1	A	308	GLN
1	A	416	HIS
1	A	434	ASN
1	A	459	ASN

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Mol	Chain	Res	Type
1	A	467	GLN
1	A	496	ASN
1	A	512	GLN
1	A	518	GLN
1	A	567	HIS
1	A	577	GLN
1	B	61	ASN
1	B	93	GLN
1	B	141	HIS
1	B	207	ASN
1	B	306	GLN
1	B	416	HIS
1	B	422	GLN
1	B	434	ASN
1	B	467	GLN
1	B	496	ASN
1	B	512	GLN
1	B	518	GLN
1	B	576	GLN
1	C	52	GLN
1	C	93	GLN
1	C	141	HIS
1	C	207	ASN
1	C	306	GLN
1	C	416	HIS
1	C	467	GLN
1	C	496	ASN
1	C	512	GLN
1	C	518	GLN
1	C	561	HIS
1	D	141	HIS
1	D	207	ASN
1	D	220	ASN
1	D	247	GLN
1	D	336	ASN
1	D	483	GLN
1	D	496	ASN
1	D	512	GLN
1	D	518	GLN
1	D	576	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
2	ATP	D	700	3	32,33,33	0.30	0	48,52,52	0.46	0
2	ATP	C	700	3	32,33,33	0.27	0	48,52,52	0.46	0
2	ATP	A	700	3	32,33,33	0.35	0	48,52,52	0.44	0
2	ATP	B	700	3	32,33,33	0.29	0	48,52,52	0.49	0

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	ATP	D	700	3	-	4/22/38/38	0/3/3/3
2	ATP	C	700	3	-	4/22/38/38	0/3/3/3
2	ATP	A	700	3	-	7/22/38/38	0/3/3/3
2	ATP	B	700	3	-	4/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	700	ATP	O4'-C1'-N9-C8
2	B	700	ATP	O4'-C1'-N9-C4
2	C	700	ATP	O4'-C1'-N9-C8
2	C	700	ATP	O4'-C1'-N9-C4
2	D	700	ATP	O4'-C1'-N9-C8
2	D	700	ATP	O4'-C1'-N9-C4
2	A	700	ATP	PA-O3A-PB-O2B
2	A	700	ATP	C5'-O5'-PA-O3A
2	A	700	ATP	PG-O3B-PB-O2B
2	B	700	ATP	PG-O3B-PB-O1B
2	D	700	ATP	PG-O3B-PB-O1B
2	A	700	ATP	O4'-C1'-N9-C8
2	C	700	ATP	PG-O3B-PB-O1B
2	A	700	ATP	O4'-C1'-N9-C4
2	B	700	ATP	PB-O3B-PG-O2G
2	C	700	ATP	PB-O3B-PG-O2G
2	D	700	ATP	PB-O3B-PG-O2G
2	A	700	ATP	PG-O3B-PB-O1B
2	A	700	ATP	PA-O3A-PB-O1B

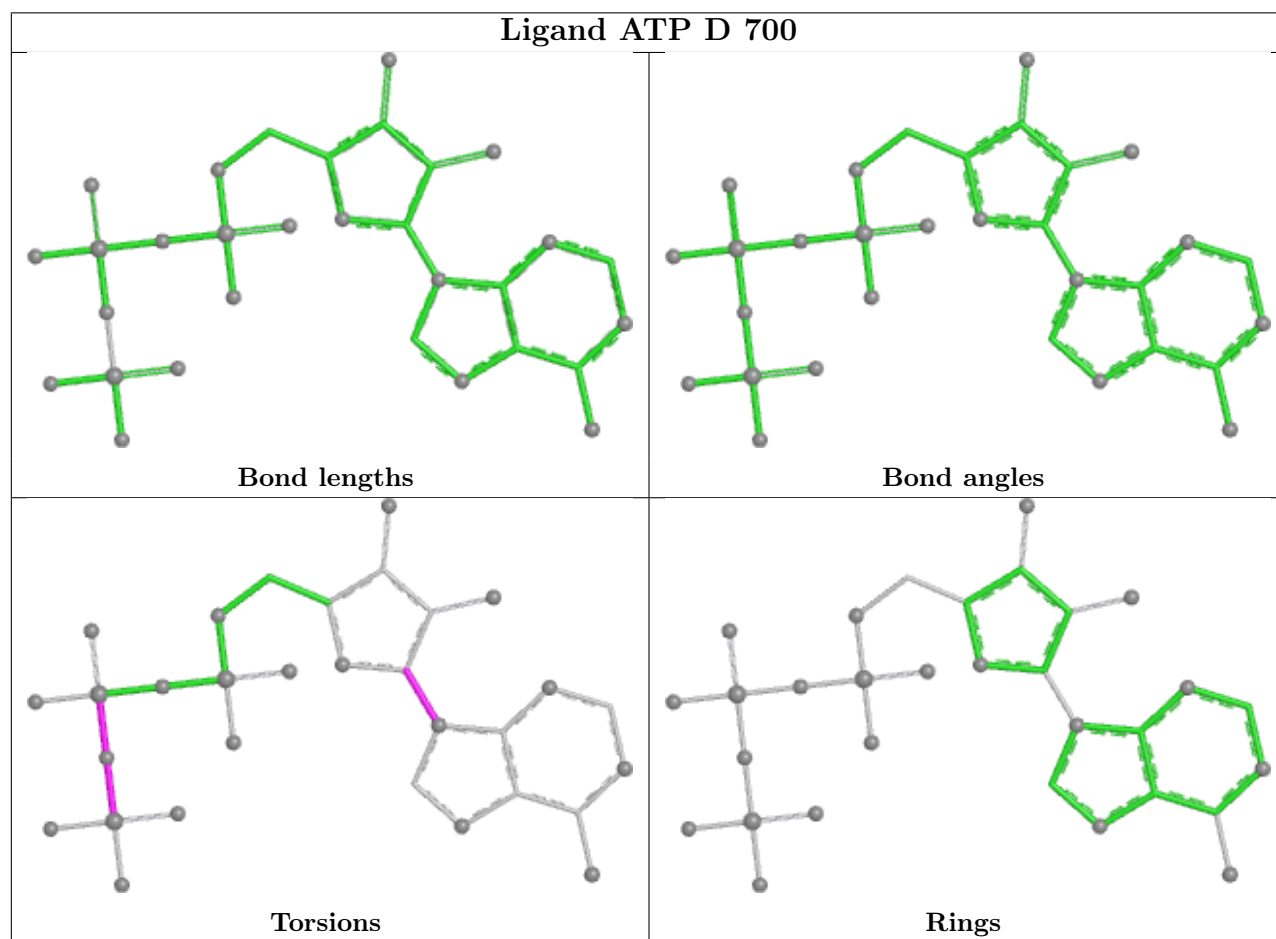
There are no ring outliers.

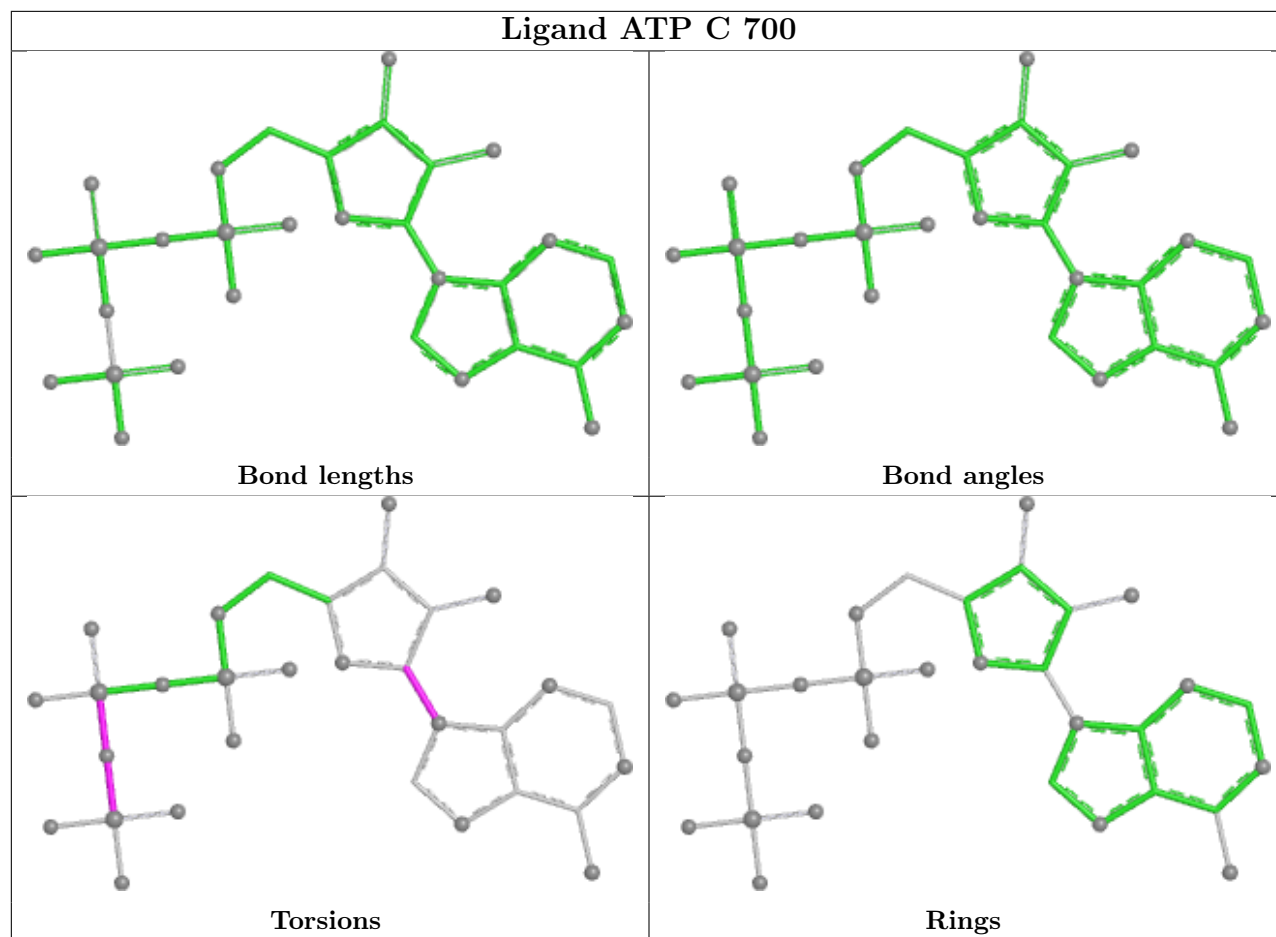
2 monomers are involved in 2 short contacts:

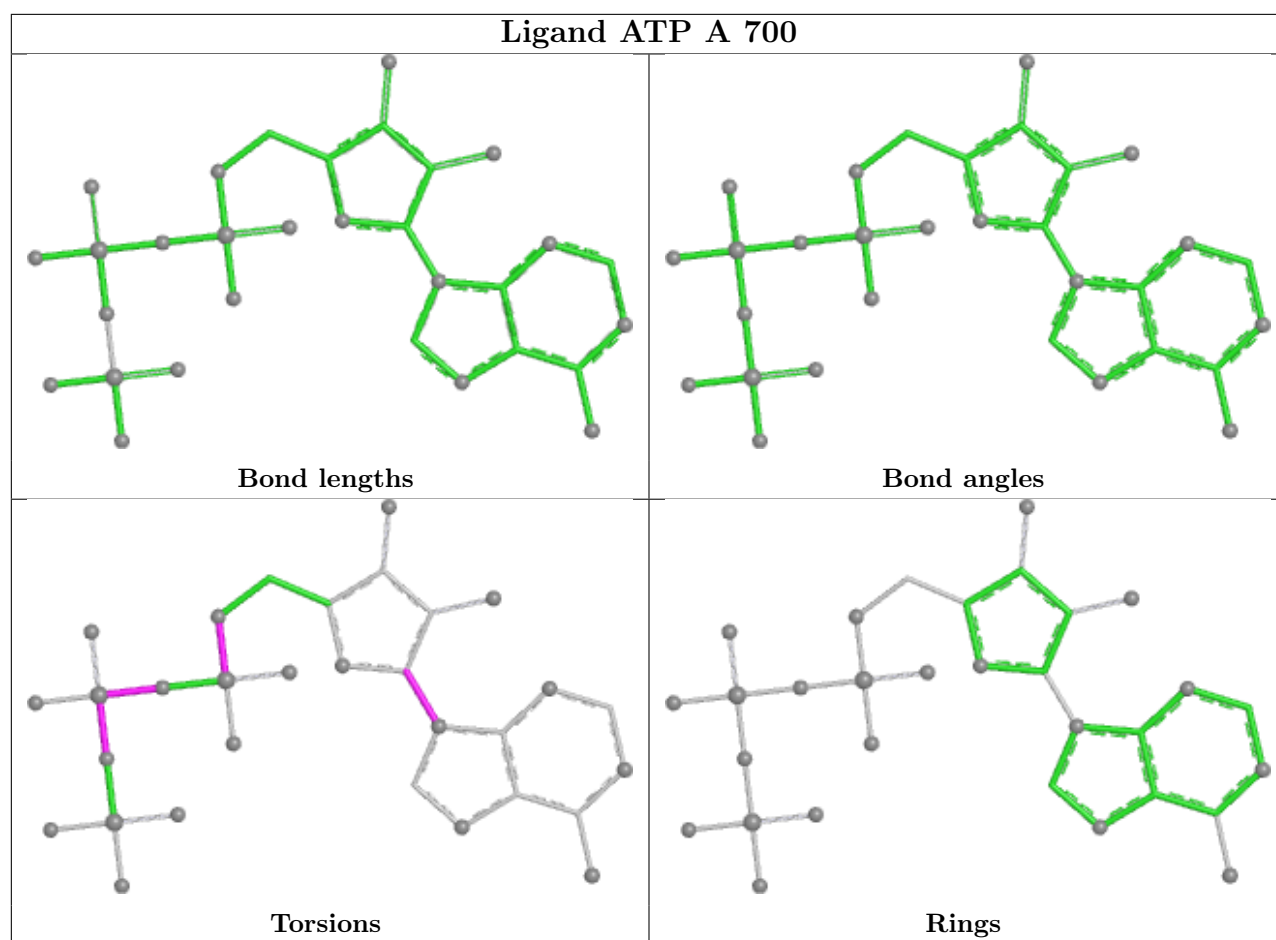
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	700	ATP	1	0
2	C	700	ATP	1	0

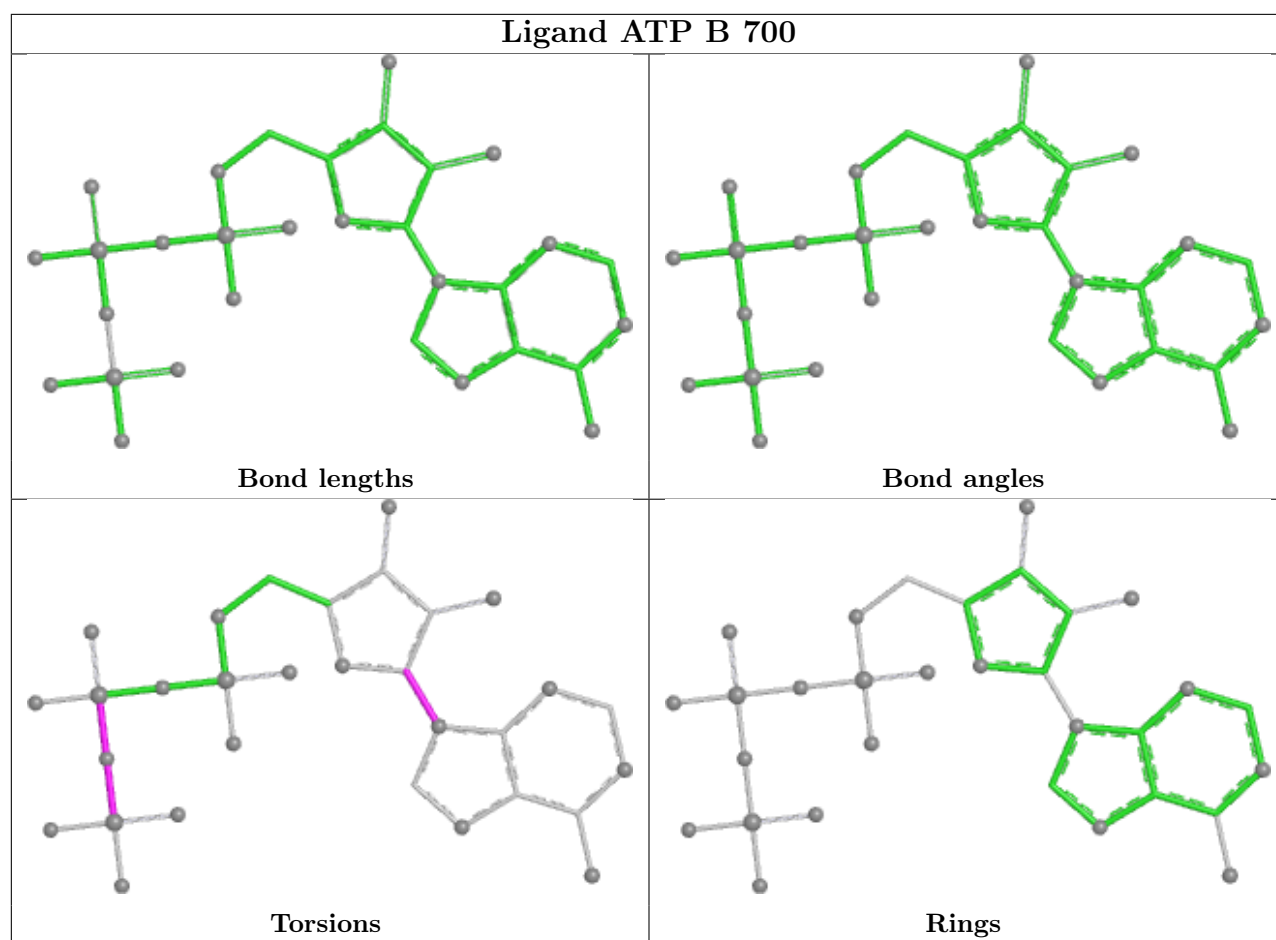
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	571/599 (95%)	0.10	25 (4%)	39	29	9, 75, 294, 300	0
1	B	569/599 (94%)	0.07	23 (4%)	42	31	18, 83, 295, 300	0
1	C	565/599 (94%)	-0.08	18 (3%)	50	36	24, 75, 289, 300	0
1	D	572/599 (95%)	0.12	34 (5%)	28	24	21, 82, 300, 300	0
All	All	2277/2396 (95%)	0.05	100 (4%)	39	29	9, 79, 296, 300	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	GLU	8.1
1	A	436	CYS	6.7
1	A	293	ILE	6.5
1	D	425	PRO	5.7
1	A	378	GLY	5.6
1	A	136	GLU	5.3
1	D	572	ASP	5.2
1	D	349	GLY	4.9
1	C	512	GLN	4.8
1	D	565	ALA	4.7
1	D	426	LEU	4.5
1	B	172	VAL	4.4
1	D	348	PHE	4.2
1	D	317	MET	4.2
1	A	440	GLU	4.2
1	A	535	HIS	4.2
1	D	535	HIS	4.2
1	D	494	LEU	4.1
1	A	549	VAL	4.0
1	C	283	LEU	4.0
1	D	285	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	379	GLY	3.9
1	D	153	ILE	3.9
1	C	294	ILE	3.8
1	D	439	LEU	3.8
1	A	479	LEU	3.7
1	D	354	GLN	3.7
1	C	376	SER	3.7
1	A	55	ASP	3.6
1	D	394	THR	3.5
1	B	291	PHE	3.5
1	A	290	LEU	3.5
1	B	425	PRO	3.5
1	A	294	ILE	3.5
1	D	401	GLY	3.5
1	B	341	ILE	3.4
1	D	392	SER	3.2
1	C	136	GLU	3.2
1	A	141	HIS	3.1
1	D	157	THR	3.1
1	D	491	ARG	3.1
1	A	514	GLU	3.0
1	B	210	LEU	3.0
1	A	509	LEU	3.0
1	D	570	TYR	3.0
1	C	553	GLU	3.0
1	B	468	PHE	3.0
1	B	419	TYR	3.0
1	D	355	LEU	3.0
1	C	24	PRO	2.8
1	B	191	ILE	2.8
1	A	291	PHE	2.8
1	D	569	LEU	2.7
1	C	463	GLU	2.7
1	D	493	LEU	2.7
1	B	580	MET	2.7
1	D	15	PHE	2.7
1	A	523	VAL	2.6
1	B	75	PHE	2.6
1	D	427	MET	2.6
1	C	287	ILE	2.6
1	C	466	ASN	2.5
1	D	237	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	438	GLY	2.5
1	D	502	LEU	2.5
1	D	496	ASN	2.5
1	B	535	HIS	2.5
1	B	362	ALA	2.4
1	C	469	ASP	2.4
1	C	542	ASP	2.4
1	A	536	ARG	2.4
1	C	356	ILE	2.4
1	D	495	ARG	2.4
1	B	466	ASN	2.4
1	A	578	LEU	2.4
1	B	469	ASP	2.4
1	A	388	GLU	2.4
1	A	534	ALA	2.4
1	C	402	ASP	2.3
1	C	193	ARG	2.3
1	C	219	SER	2.3
1	D	352	PRO	2.3
1	B	328	THR	2.2
1	B	554	ILE	2.2
1	B	565	ALA	2.2
1	A	427	MET	2.2
1	B	388	GLU	2.1
1	A	162	MET	2.1
1	D	446	ALA	2.1
1	B	141	HIS	2.1
1	D	136	GLU	2.1
1	A	218	ALA	2.1
1	D	293	ILE	2.1
1	A	26	TYR	2.0
1	B	558	GLY	2.0
1	C	494	LEU	2.0
1	D	246	VAL	2.0
1	B	15	PHE	2.0
1	B	460	PHE	2.0
1	C	583	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

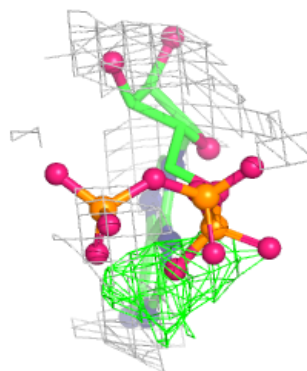
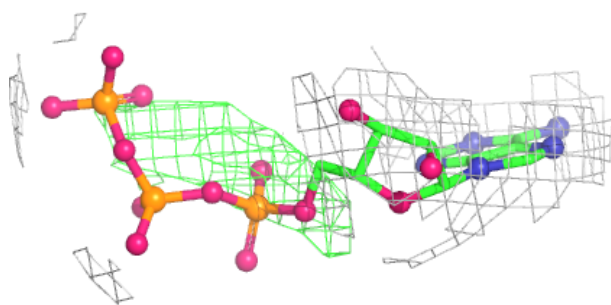
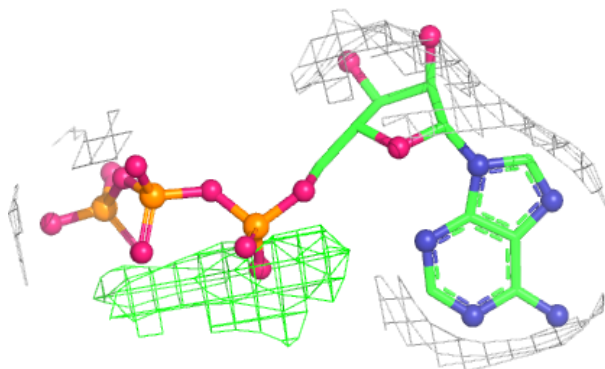
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ATP	D	700	31/31	0.92	0.08	43,55,65,70	0
2	ATP	B	700	31/31	0.93	0.10	39,54,62,63	0
2	ATP	A	700	31/31	0.95	0.06	33,41,49,50	0
2	ATP	C	700	31/31	0.97	0.05	30,37,43,48	0
3	MG	D	701	1/1	0.97	0.17	41,41,41,41	0
3	MG	B	701	1/1	0.98	0.12	43,43,43,43	0
3	MG	C	701	1/1	0.99	0.04	31,31,31,31	0
3	MG	A	701	1/1	1.00	0.09	34,34,34,34	0

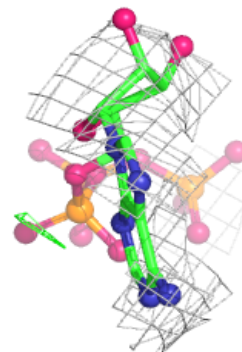
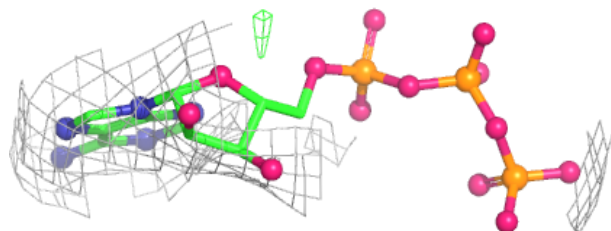
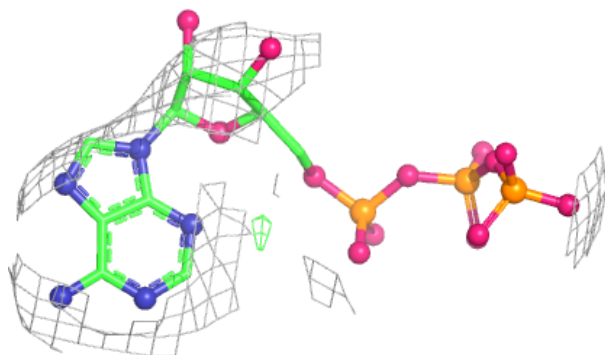
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP D 700:

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

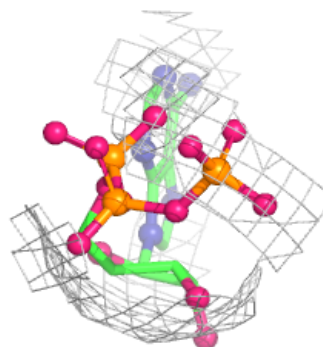
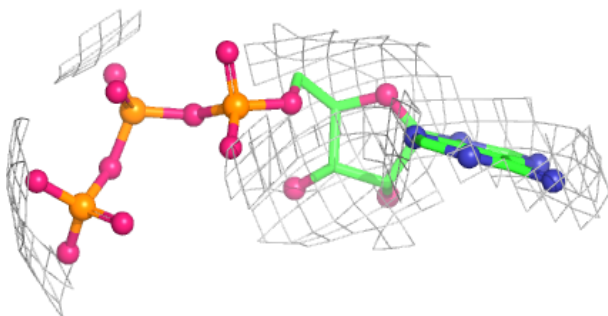
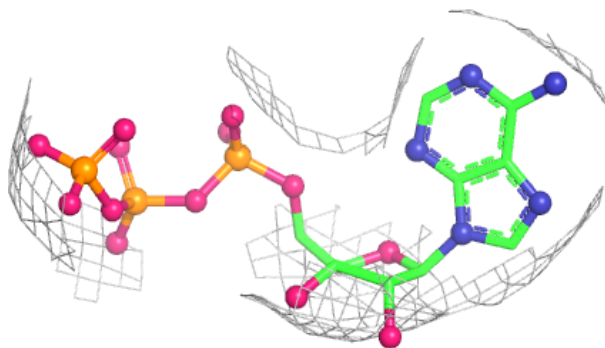
**Electron density around ATP B 700:**

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

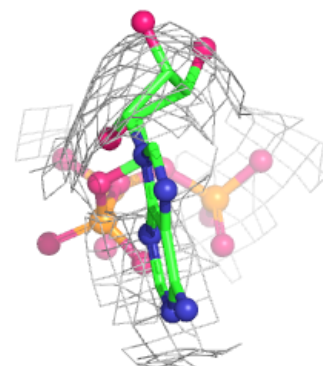
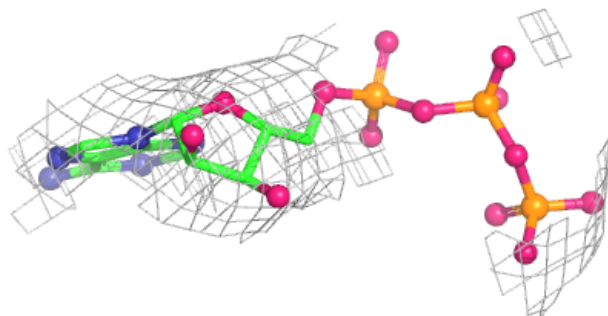
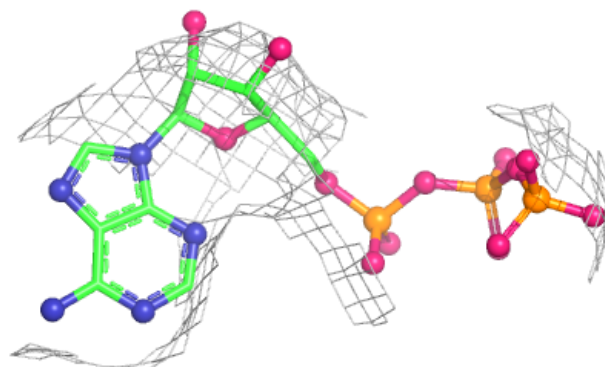


Electron density around ATP A 700:

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

**Electron density around ATP C 700:**

$2mF_o-DF_c$ (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.