



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:54 PM UTC

PDB ID : 7CM9 / pdb_00007cm9
Title : DMSP lyase DddX
Authors : Li, C.Y.; Zhang, Y.Z.
Deposited on : 2020-07-25
Resolution : 2.25 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

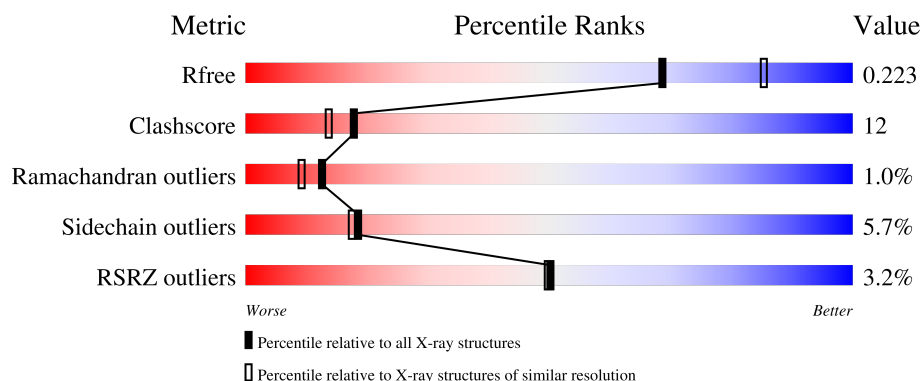
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	748	3% 72% 18% • 7%
1	B	748	3% 71% 18% • 7%
1	C	748	2% 74% 14% • 7%
1	D	748	4% 70% 20% • 7%

2 Entry composition [i](#)

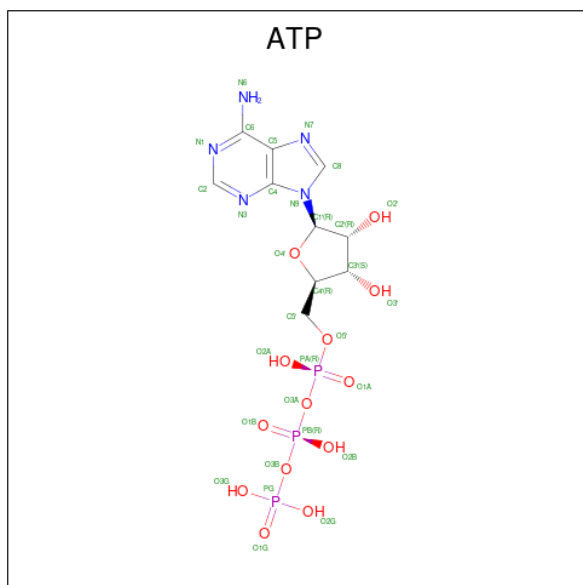
There are 4 unique types of molecules in this entry. The entry contains 22513 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DMSP lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5312	3396	881	1016	19			
1	B	693	Total	C	N	O	S	0	0	0
			5312	3396	881	1016	19			
1	C	693	Total	C	N	O	S	0	0	0
			5312	3396	881	1016	19			
1	D	692	Total	C	N	O	S	0	0	0
			5307	3393	880	1015	19			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



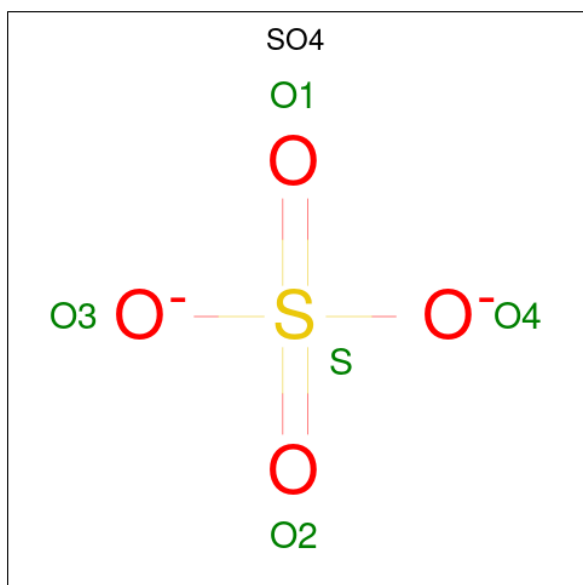
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

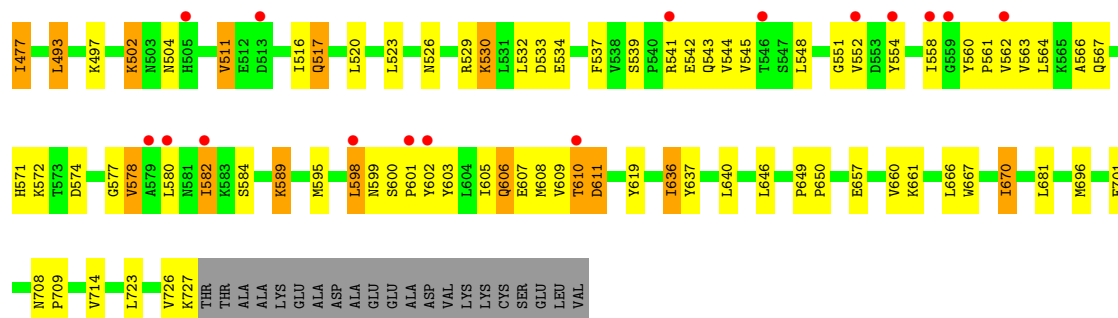
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	255	Total	O	0	0
			255	255		
4	B	247	Total	O	0	0
			247	247		
4	C	321	Total	O	0	0
			321	321		

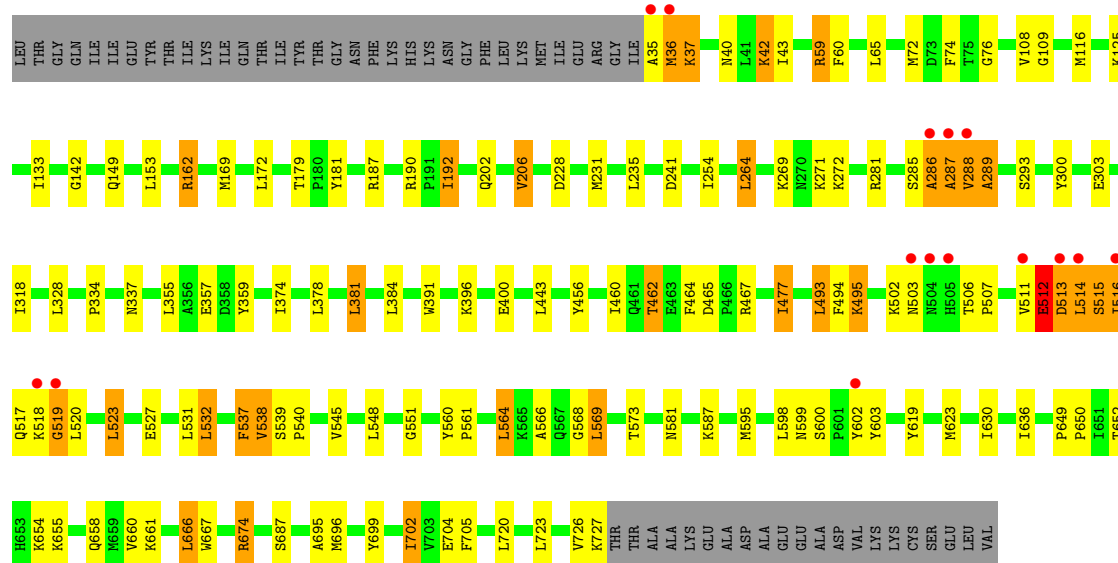
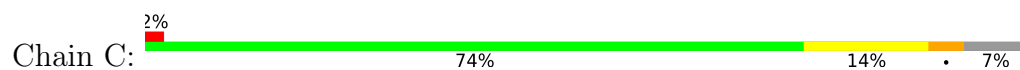
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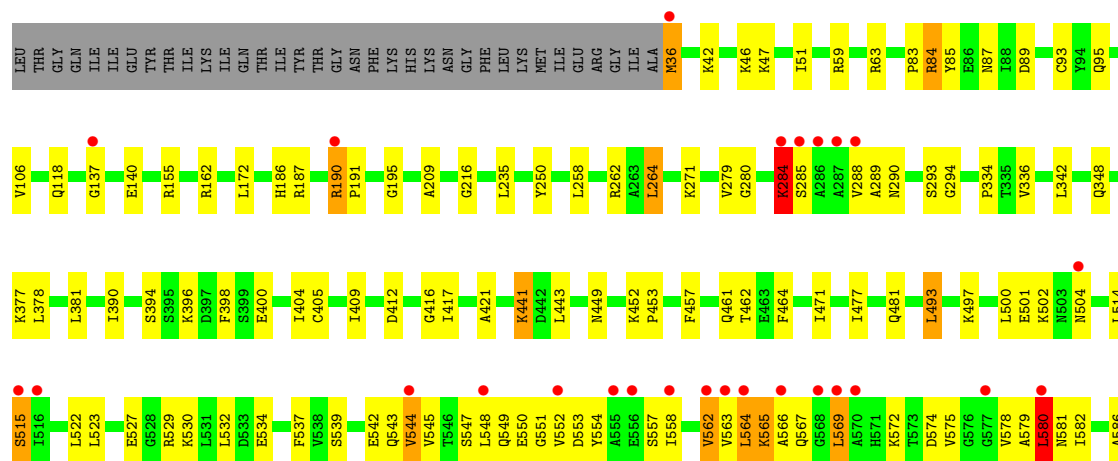
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	303	Total 303	O 303	0	0

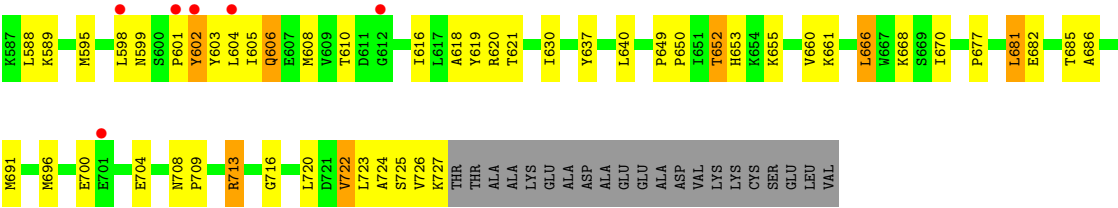


• Molecule 1: DMSP lyase



• Molecule 1: DMSP lyase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.56Å 88.80Å 273.26Å 90.00° 99.94° 90.00°	Depositor
Resolution (Å)	30.68 – 2.25 30.68 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.5 (30.68-2.25) 97.0 (30.68-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.184 , 0.230 0.181 , 0.223	Depositor DCC
R_{free} test set	7847 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22513	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: ATP, SO4

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	0.49	1/5407 (0.0%)	0.82	3/7333 (0.0%)
1	B	0.48	1/5407 (0.0%)	0.80	5/7333 (0.1%)
1	C	0.52	0/5407	0.83	1/7333 (0.0%)
1	D	0.50	1/5402 (0.0%)	0.82	3/7326 (0.0%)
All	All	0.50	3/21623 (0.0%)	0.82	12/29325 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	PRO	N-CD	5.35	1.55	1.47
1	D	191	PRO	N-CD	5.15	1.54	1.47
1	A	134	PRO	N-CD	5.12	1.54	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	LYS	N-CA-C	6.97	118.57	110.97
1	B	182	ILE	CB-CA-C	-5.78	106.75	113.22
1	D	290	ASN	N-CA-C	-5.59	107.00	113.88
1	B	187	ARG	CA-C-N	-5.55	113.00	119.32
1	B	187	ARG	C-N-CA	-5.55	113.00	119.32
1	B	610	THR	N-CA-C	5.40	122.30	110.80
1	D	190	ARG	CA-C-N	-5.30	113.21	119.84
1	D	190	ARG	C-N-CA	-5.30	113.21	119.84
1	A	133	ILE	CA-C-N	-5.25	113.27	119.84
1	A	133	ILE	C-N-CA	-5.25	113.27	119.84
1	C	537	PHE	N-CA-C	5.19	119.66	112.45
1	B	182	ILE	N-CA-C	5.14	111.71	106.21

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	5312	0	5392	144	0
1	B	5312	0	5392	121	0
1	C	5312	0	5392	114	0
1	D	5307	0	5387	152	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	3	0
2	D	31	0	12	6	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	255	0	0	8	0
4	B	247	0	0	3	0
4	C	321	0	0	10	0
4	D	303	0	0	15	0
All	All	22513	0	21611	529	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 12.

All (529) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:VAL:HB	1:A:564:LEU:HA	1.29	1.13
1:A:563:VAL:HG11	1:A:605:ILE:HA	1.12	1.11
1:D:652:THR:HG22	1:D:655:LYS:H	1.17	1.06
1:A:563:VAL:CG1	1:A:605:ILE:HA	1.86	1.03
1:A:563:VAL:HG13	1:A:606:GLN:H	1.19	1.03
1:C:702:ILE:HD11	1:C:705:PHE:HB2	1.37	1.02
1:C:288:VAL:HG22	1:C:289:ALA:H	1.21	1.01
1:A:563:VAL:HB	1:A:564:LEU:CA	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ARG:HB2	1:D:190:ARG:O	1.63	0.98
1:B:284:LYS:H	1:B:284:LYS:HD2	1.26	0.97
1:A:563:VAL:CB	1:A:564:LEU:HA	1.95	0.96
2:D:801:ATP:H5'1	2:D:801:ATP:H8	1.31	0.95
1:A:562:VAL:HG12	1:A:607:GLU:HA	1.52	0.92
1:B:562:VAL:HG23	1:B:582:ILE:HD11	1.52	0.90
1:A:302:ILE:HD12	1:A:628:VAL:HG11	1.51	0.90
1:D:579:ALA:O	1:D:580:LEU:HB2	1.72	0.89
1:B:36:MET:HG3	1:B:37:LYS:H	1.37	0.87
1:A:570:ALA:HB1	1:A:571:HIS:HB2	1.57	0.87
1:A:570:ALA:CB	1:A:571:HIS:HB2	2.05	0.86
1:A:652:THR:HG23	1:A:655:LYS:H	1.41	0.86
1:A:564:LEU:H	1:A:579:ALA:HB3	1.39	0.84
1:B:726:VAL:O	1:B:727:LYS:HB2	1.76	0.84
1:D:563:VAL:CG2	1:D:606:GLN:HG3	2.08	0.84
1:B:517:GLN:OE1	1:B:727:LYS:HD3	1.78	0.83
2:C:801:ATP:H5'1	2:C:801:ATP:H8	1.45	0.82
1:A:524:HIS:HB2	4:A:908:HOH:O	1.78	0.81
1:A:206:VAL:HG21	1:A:250:TYR:CE2	2.15	0.81
1:A:72:MET:HG3	1:A:179:THR:HG21	1.63	0.81
1:C:652:THR:HG23	1:C:655:LYS:H	1.45	0.81
1:C:566:ALA:HB2	1:C:595:MET:HE3	1.62	0.80
1:A:595:MET:HE2	1:A:603:TYR:HE2	1.47	0.80
2:D:801:ATP:H5'1	2:D:801:ATP:C8	2.16	0.80
1:C:59:ARG:HG3	1:C:60:PHE:N	1.99	0.78
1:D:563:VAL:HG21	1:D:606:GLN:HG3	1.65	0.78
1:D:461:GLN:NE2	4:D:905:HOH:O	2.15	0.78
1:B:541:ARG:HH22	1:B:558:ILE:HG23	1.49	0.78
1:A:636:ILE:HD13	1:A:637:TYR:CD1	2.20	0.76
1:D:652:THR:CG2	1:D:655:LYS:H	1.98	0.75
1:B:562:VAL:CG2	1:B:582:ILE:HD11	2.15	0.75
1:D:284:LYS:CD	1:D:285:SER:H	1.99	0.75
1:B:566:ALA:HB2	1:B:595:MET:HE3	1.68	0.75
1:D:548:LEU:O	1:D:552:VAL:HG23	1.86	0.75
1:D:36:MET:HE3	1:D:36:MET:N	2.03	0.74
1:D:542:GLU:HB3	1:D:606:GLN:HB3	1.68	0.74
1:D:700:GLU:O	4:D:901:HOH:O	2.04	0.73
1:D:522:LEU:HD23	1:D:569:LEU:HD13	1.69	0.73
1:A:563:VAL:HG13	1:A:606:GLN:N	2.00	0.73
1:D:566:ALA:HB2	1:D:595:MET:HE3	1.70	0.73
1:C:566:ALA:HB2	1:C:595:MET:CE	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:704:GLU:HB2	1:D:725:SER:HB2	1.72	0.71
1:A:206:VAL:HG22	1:A:318:ILE:HD11	1.73	0.71
1:A:570:ALA:HB3	1:A:571:HIS:O	1.91	0.70
1:B:284:LYS:HD2	1:B:284:LYS:N	2.01	0.70
1:C:288:VAL:HG22	1:C:289:ALA:N	2.02	0.70
1:D:47:LYS:NZ	4:D:908:HOH:O	2.24	0.70
1:B:334:PRO:HD3	1:B:493:LEU:HD13	1.73	0.70
2:C:801:ATP:H5'1	2:C:801:ATP:C8	2.25	0.70
1:D:342:LEU:HD11	1:D:409:ILE:HD12	1.75	0.69
1:C:598:LEU:O	4:C:901:HOH:O	2.08	0.69
1:C:59:ARG:HG3	1:C:60:PHE:H	1.56	0.69
1:D:653:HIS:ND1	4:D:911:HOH:O	2.26	0.69
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.59	0.68
1:C:378:LEU:HD23	1:C:396:LYS:HE2	1.75	0.68
1:C:511:VAL:O	1:C:512:GLU:HB2	1.93	0.68
1:C:467:ARG:HG3	1:C:467:ARG:HH11	1.58	0.68
1:D:285:SER:O	4:D:902:HOH:O	2.13	0.67
1:B:582:ILE:HG12	1:B:582:ILE:O	1.94	0.67
1:A:172:LEU:C	1:A:172:LEU:HD12	2.20	0.67
1:A:481:GLN:NE2	4:A:903:HOH:O	2.28	0.67
1:A:562:VAL:HB	1:A:563:VAL:HG22	1.78	0.66
1:A:342:LEU:HD21	1:A:390:ILE:CD1	2.25	0.66
1:D:564:LEU:HD23	1:D:605:ILE:HG22	1.76	0.66
1:C:573:THR:HG22	2:C:801:ATP:O2B	1.95	0.66
1:D:652:THR:HG22	1:D:655:LYS:N	2.01	0.66
1:D:294:GLY:HA2	1:D:620:ARG:NH1	2.11	0.66
1:C:162:ARG:HH12	1:C:228:ASP:CG	2.04	0.65
1:B:562:VAL:O	1:B:582:ILE:HD13	1.95	0.65
1:C:595:MET:HE2	1:C:603:TYR:HE1	1.60	0.65
1:B:554:TYR:CZ	1:B:558:ILE:HD11	2.31	0.65
1:D:677:PRO:O	4:D:903:HOH:O	2.14	0.65
1:D:579:ALA:O	1:D:580:LEU:CB	2.45	0.65
1:D:545:VAL:HG11	1:D:551:GLY:HA2	1.78	0.65
1:D:660:VAL:HG13	1:D:666:LEU:HD13	1.79	0.65
1:C:36:MET:O	1:C:37:LYS:HB2	1.97	0.64
1:D:87:ASN:OD1	4:D:904:HOH:O	2.15	0.64
1:A:569:LEU:CD1	1:A:575:VAL:HG21	2.28	0.64
1:A:544:VAL:HG11	1:A:602:TYR:CD2	2.33	0.64
1:C:162:ARG:NH1	1:C:228:ASP:OD2	2.31	0.64
1:D:162:ARG:NH2	4:D:914:HOH:O	2.30	0.64
1:D:527:GLU:HA	1:D:530:LYS:HE3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:LYS:HE3	2:D:801:ATP:O1A	1.99	0.63
1:C:661:LYS:HE2	1:C:667:TRP:CH2	2.34	0.63
1:D:567:GLN:HE21	1:D:604:LEU:HB2	1.63	0.63
1:B:714:VAL:O	4:B:901:HOH:O	2.16	0.63
1:D:271:LYS:NZ	1:D:500:LEU:HD22	2.13	0.63
1:C:661:LYS:HG2	1:C:667:TRP:CZ3	2.34	0.63
1:B:417:ILE:HG12	1:B:453:PRO:HG2	1.80	0.63
1:C:674:ARG:HD2	1:D:574:ASP:OD1	1.99	0.63
1:D:564:LEU:H	1:D:579:ALA:HB3	1.64	0.62
1:B:36:MET:CG	1:B:37:LYS:H	2.08	0.62
1:B:657:GLU:HG2	1:B:661:LYS:HE3	1.81	0.62
1:B:548:LEU:O	1:B:552:VAL:HG23	1.99	0.62
1:D:554:TYR:CD2	1:D:605:ILE:HD11	2.34	0.62
1:C:465:ASP:OD1	1:C:467:ARG:NH1	2.32	0.62
1:C:514:LEU:O	1:C:515:SER:C	2.41	0.62
1:D:190:ARG:NH1	4:D:916:HOH:O	2.32	0.62
1:D:542:GLU:CB	1:D:606:GLN:HB3	2.29	0.62
1:D:334:PRO:HD3	1:D:493:LEU:HD13	1.82	0.62
1:B:541:ARG:NH2	1:B:558:ILE:HG23	2.14	0.62
1:D:284:LYS:HD2	1:D:285:SER:H	1.64	0.62
1:D:601:PRO:HD2	1:D:602:TYR:CE1	2.34	0.62
1:A:134:PRO:HD2	4:A:990:HOH:O	1.99	0.61
1:A:636:ILE:CD1	1:A:637:TYR:HD1	2.12	0.61
1:A:334:PRO:HD3	1:A:493:LEU:HD13	1.82	0.61
1:A:595:MET:HE2	1:A:603:TYR:CE2	2.34	0.61
1:D:137:GLY:N	1:D:140:GLU:OE1	2.33	0.61
1:A:187:ARG:NH2	1:A:208:ASP:OD1	2.33	0.61
1:A:284:LYS:HE2	1:A:285:SER:H	1.65	0.61
1:A:134:PRO:CB	1:A:168:CYS:O	2.48	0.61
1:B:681:LEU:C	1:B:681:LEU:HD23	2.26	0.61
1:C:271:LYS:HE2	4:C:930:HOH:O	2.00	0.61
1:D:250:TYR:OH	1:D:279:VAL:HG21	2.00	0.61
1:A:563:VAL:CG2	1:A:605:ILE:HG23	2.31	0.60
1:D:187:ARG:CB	1:D:190:ARG:O	2.44	0.60
1:A:284:LYS:HD3	1:A:284:LYS:N	2.15	0.60
1:B:140:GLU:OE2	1:B:225:ASN:ND2	2.30	0.60
1:C:515:SER:O	1:C:516:ILE:HG23	2.01	0.60
1:D:84:ARG:HG2	1:D:85:TYR:CE1	2.37	0.60
1:A:563:VAL:CG1	1:A:564:LEU:HA	2.31	0.60
1:B:637:TYR:HD1	1:B:640:LEU:HD12	1.66	0.59
1:A:692:GLY:O	1:A:696:MET:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:TYR:OH	1:C:702:ILE:HG13	2.02	0.59
1:A:596:GLU:HG3	1:A:597:HIS:N	2.17	0.59
1:D:186:HIS:ND1	4:D:915:HOH:O	2.32	0.59
1:A:58:TYR:O	1:A:63:ARG:HD3	2.03	0.59
1:C:661:LYS:HG2	1:C:667:TRP:CE3	2.37	0.59
1:A:541:ARG:HB3	1:A:607:GLU:HG2	1.84	0.59
1:B:548:LEU:HD21	1:B:589:LYS:HG3	1.84	0.59
1:A:502:LYS:HE3	1:A:505:HIS:CD2	2.38	0.59
1:C:573:THR:HG21	1:C:636:ILE:HD12	1.84	0.59
1:D:562:VAL:C	1:D:563:VAL:HG13	2.28	0.59
1:B:255:ARG:HG3	4:B:1040:HOH:O	2.03	0.59
1:D:726:VAL:O	1:D:727:LYS:HB3	2.03	0.59
1:C:460:ILE:HG13	1:C:462:THR:HG23	1.84	0.58
1:B:554:TYR:CZ	1:B:558:ILE:CD1	2.86	0.58
1:D:481:GLN:OE1	4:D:906:HOH:O	2.17	0.58
1:A:570:ALA:HB3	1:A:571:HIS:HB2	1.81	0.58
1:B:526:ASN:HD22	1:B:529:ARG:NH1	2.02	0.58
1:D:235:LEU:HD21	1:D:264:LEU:HD13	1.84	0.58
1:A:137:GLY:HA2	1:A:141:SER:HB2	1.87	0.57
1:D:610:THR:O	1:D:713:ARG:NH2	2.38	0.57
1:A:636:ILE:HD13	1:A:637:TYR:HD1	1.63	0.57
1:C:702:ILE:CD1	1:C:705:PHE:HB2	2.24	0.57
1:A:190:ARG:O	1:A:190:ARG:HG3	2.05	0.57
1:C:334:PRO:HD3	1:C:493:LEU:HD13	1.86	0.57
1:D:378:LEU:HD21	1:D:404:ILE:HD12	1.86	0.57
1:D:566:ALA:HB2	1:D:595:MET:CE	2.34	0.57
1:D:713:ARG:HG2	1:D:716:GLY:O	2.04	0.57
1:D:704:GLU:O	1:D:724:ALA:HA	2.05	0.57
1:B:348:GLN:HB3	1:B:459:HIS:CE1	2.40	0.57
1:A:284:LYS:CD	1:A:285:SER:H	2.17	0.56
1:B:378:LEU:HB3	1:B:381:LEU:HD13	1.86	0.56
1:B:701:GLU:O	1:B:726:VAL:HG23	2.06	0.56
1:B:564:LEU:HD11	1:B:603:TYR:HD2	1.70	0.56
1:A:291:ALA:HB1	1:A:706:GLU:CD	2.31	0.56
1:D:293:SER:HB2	1:D:630:ILE:HD13	1.88	0.56
1:A:284:LYS:CE	1:A:285:SER:H	2.19	0.55
1:B:284:LYS:O	1:B:285:SER:HB3	2.06	0.55
1:B:562:VAL:O	1:B:582:ILE:CD1	2.54	0.55
1:D:258:LEU:HD21	1:D:262:ARG:NH2	2.22	0.55
1:B:467:ARG:NH1	4:B:905:HOH:O	2.38	0.55
1:A:519:GLY:O	1:A:727:LYS:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:LYS:NZ	4:C:913:HOH:O	2.40	0.55
1:C:511:VAL:O	1:C:512:GLU:CB	2.55	0.55
1:D:59:ARG:O	1:D:63:ARG:HG2	2.06	0.55
1:A:532:LEU:HD11	1:A:722:VAL:HG22	1.88	0.55
1:D:514:LEU:HD11	1:D:621:THR:HG21	1.89	0.55
1:B:530:LYS:O	1:B:534:GLU:HG3	2.06	0.55
1:C:537:PHE:O	1:C:538:VAL:HB	2.07	0.55
1:C:568:GLY:O	1:C:569:LEU:HD23	2.08	0.54
1:A:502:LYS:HE3	1:A:505:HIS:HD2	1.71	0.54
1:D:502:LYS:O	1:D:504:ASN:ND2	2.41	0.54
1:A:235:LEU:HD21	1:A:264:LEU:HD13	1.90	0.54
1:A:571:HIS:HB3	1:A:574:ASP:OD2	2.07	0.54
1:A:162:ARG:HD2	1:A:228:ASP:OD2	2.08	0.54
1:C:36:MET:O	1:C:37:LYS:CB	2.55	0.54
1:C:42:LYS:HB3	1:C:42:LYS:HZ2	1.73	0.54
1:D:417:ILE:HG12	1:D:453:PRO:HG2	1.90	0.54
1:A:563:VAL:HG21	1:A:605:ILE:HG23	1.88	0.54
1:C:514:LEU:HD12	1:C:514:LEU:H	1.72	0.54
1:B:542:GLU:HB3	1:B:606:GLN:HB3	1.90	0.53
1:C:162:ARG:NH1	1:C:228:ASP:CG	2.66	0.53
1:C:513:ASP:OD1	1:C:513:ASP:N	2.36	0.53
1:D:532:LEU:HG	1:D:722:VAL:HG11	1.89	0.53
1:B:563:VAL:O	1:B:605:ILE:HA	2.08	0.53
1:A:419:THR:HA	1:A:455:LEU:O	2.09	0.53
1:D:661:LYS:O	1:D:661:LYS:HG3	2.07	0.53
1:A:284:LYS:HD3	1:A:284:LYS:H	1.73	0.53
1:A:560:TYR:HB3	1:A:561:PRO:HA	1.90	0.53
1:B:235:LEU:HD21	1:B:264:LEU:HD13	1.90	0.53
1:A:569:LEU:HD11	1:A:575:VAL:HG21	1.91	0.53
1:D:271:LYS:HZ2	1:D:500:LEU:HD22	1.71	0.53
1:B:563:VAL:HG13	1:B:580:LEU:HD23	1.91	0.53
1:D:412:ASP:O	1:D:452:LYS:NZ	2.42	0.53
1:C:206:VAL:HG22	1:C:318:ILE:HD11	1.91	0.53
1:D:42:LYS:O	1:D:46:LYS:HD2	2.09	0.53
1:D:649:PRO:HA	1:D:650:PRO:C	2.34	0.53
1:C:192:ILE:HG13	4:C:943:HOH:O	2.08	0.52
1:B:342:LEU:HD21	1:B:390:ILE:CD1	2.39	0.52
1:A:524:HIS:CG	4:A:908:HOH:O	2.62	0.52
1:B:637:TYR:CD1	1:B:640:LEU:HD12	2.45	0.52
1:C:460:ILE:CG1	1:C:462:THR:HG23	2.39	0.52
1:A:548:LEU:CD1	1:A:589:LYS:HG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LYS:HD2	1:D:285:SER:N	2.24	0.52
1:D:681:LEU:HD23	1:D:682:GLU:N	2.25	0.52
1:A:206:VAL:HG21	1:A:250:TYR:CZ	2.45	0.52
1:D:618:ALA:HA	1:D:691:MET:HE3	1.92	0.52
1:C:727:LYS:HA	4:C:902:HOH:O	2.10	0.52
1:C:443:LEU:HB3	1:C:477:ILE:HD12	1.92	0.52
1:A:638:THR:HG23	1:A:639:GLU:N	2.26	0.51
1:D:723:LEU:C	1:D:723:LEU:HD23	2.35	0.51
1:A:579:ALA:O	1:A:580:LEU:HB2	2.10	0.51
1:B:610:THR:O	1:B:611:ASP:OD1	2.27	0.51
1:B:636:ILE:HD13	1:B:637:TYR:CE2	2.45	0.51
1:D:563:VAL:HG22	1:D:606:GLN:H	1.76	0.51
1:D:601:PRO:C	1:D:602:TYR:CG	2.88	0.51
1:A:548:LEU:HD22	1:A:552:VAL:HG23	1.92	0.51
1:B:72:MET:HG3	1:B:179:THR:HG21	1.91	0.51
1:D:599:ASN:O	1:D:601:PRO:HD3	2.11	0.51
1:B:189:LEU:N	1:B:189:LEU:HD23	2.25	0.51
1:C:288:VAL:CG2	1:C:289:ALA:H	2.02	0.51
1:D:443:LEU:HB3	1:D:477:ILE:HD13	1.91	0.51
1:D:532:LEU:HD11	1:D:722:VAL:HG13	1.92	0.51
1:A:661:LYS:HG2	1:A:667:TRP:CE3	2.46	0.51
1:B:284:LYS:H	1:B:284:LYS:CD	2.01	0.51
1:C:502:LYS:HG3	1:C:503:ASN:N	2.24	0.51
1:A:305:LEU:HD22	1:A:646:LEU:HB2	1.93	0.51
1:C:289:ALA:HA	1:C:704:GLU:OE2	2.11	0.51
1:D:681:LEU:HD23	1:D:682:GLU:HG2	1.93	0.51
1:A:566:ALA:HB2	1:A:595:MET:HE3	1.92	0.51
1:D:562:VAL:O	1:D:580:LEU:O	2.28	0.51
1:A:592:TRP:O	1:A:592:TRP:CD1	2.63	0.51
1:D:390:ILE:HG13	1:D:398:PHE:HE1	1.76	0.50
1:D:553:ASP:O	1:D:557:SER:HB3	2.11	0.50
1:A:569:LEU:HD22	1:A:570:ALA:H	1.76	0.50
1:C:460:ILE:HG21	1:D:209:ALA:HB1	1.92	0.50
1:A:155:ARG:HH11	1:A:155:ARG:HG3	1.75	0.50
1:A:563:VAL:HG21	1:A:605:ILE:HG12	1.93	0.50
1:C:286:ALA:HB1	1:C:288:VAL:CG1	2.41	0.50
1:C:514:LEU:O	1:C:515:SER:O	2.29	0.50
1:D:649:PRO:HB2	1:D:696:MET:HG3	1.94	0.50
1:A:202:GLN:CD	1:A:231:MET:CE	2.84	0.50
1:D:504:ASN:ND2	4:D:930:HOH:O	2.45	0.50
1:A:537:PHE:O	1:A:538:VAL:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ALA:O	1:C:287:ALA:HB3	2.12	0.50
1:C:649:PRO:HA	1:C:650:PRO:C	2.36	0.50
1:C:702:ILE:HG13	1:C:702:ILE:O	2.12	0.50
1:B:336:VAL:O	1:B:416:GLY:HA3	2.12	0.50
1:B:511:VAL:HG13	1:B:511:VAL:O	2.11	0.50
1:A:193:LYS:HG3	1:A:216:GLY:HA2	1.94	0.50
1:A:570:ALA:CB	1:A:571:HIS:CB	2.83	0.50
1:B:58:TYR:CE2	1:C:400:GLU:HG3	2.47	0.50
1:C:285:SER:O	1:C:287:ALA:N	2.37	0.50
1:D:284:LYS:CG	1:D:285:SER:H	2.25	0.50
1:B:726:VAL:O	1:B:727:LYS:CB	2.56	0.50
1:B:173:ASN:ND2	1:B:219:LYS:HE3	2.27	0.49
1:B:598:LEU:O	1:B:600:SER:N	2.45	0.49
1:A:202:GLN:CD	1:A:231:MET:HE1	2.37	0.49
1:A:284:LYS:CG	1:A:285:SER:N	2.75	0.49
1:A:649:PRO:HA	1:A:650:PRO:C	2.37	0.49
1:C:72:MET:HG3	1:C:179:THR:HG21	1.94	0.49
1:D:46:LYS:HE3	4:D:1145:HOH:O	2.12	0.49
1:D:84:ARG:O	1:D:84:ARG:HG3	2.10	0.49
1:C:374:ILE:HB	1:C:384:LEU:HD11	1.94	0.49
1:C:467:ARG:HG3	1:C:467:ARG:NH1	2.26	0.49
1:C:660:VAL:HG13	1:C:666:LEU:HD13	1.93	0.49
1:D:522:LEU:CD2	1:D:569:LEU:HD13	2.38	0.49
1:C:202:GLN:HG3	1:C:231:MET:CE	2.43	0.49
1:A:133:ILE:O	1:A:166:PRO:HA	2.13	0.49
1:A:586:ALA:HA	1:A:589:LYS:NZ	2.27	0.49
1:B:666:LEU:O	1:B:670:ILE:HD12	2.12	0.49
1:C:573:THR:HG21	1:C:636:ILE:CD1	2.42	0.49
1:A:570:ALA:HB3	1:A:571:HIS:C	2.37	0.49
1:D:563:VAL:O	1:D:605:ILE:HA	2.12	0.49
1:B:140:GLU:HG3	1:B:167:ASN:ND2	2.28	0.48
1:B:281:ARG:HA	1:B:300:TYR:CD2	2.48	0.48
1:A:36:MET:HG2	1:A:160:GLY:HA3	1.94	0.48
1:B:649:PRO:HA	1:B:650:PRO:C	2.37	0.48
1:C:35:ALA:HB1	4:C:1099:HOH:O	2.12	0.48
1:D:279:VAL:CG1	1:D:280:GLY:N	2.75	0.48
1:D:567:GLN:NE2	1:D:604:LEU:CB	2.76	0.48
1:A:563:VAL:HB	1:A:564:LEU:CB	2.43	0.48
1:B:192:ILE:HG12	1:B:211:ILE:HG23	1.95	0.48
1:A:84:ARG:HD2	1:A:84:ARG:O	2.13	0.48
1:B:470:SER:O	1:B:474:GLU:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:HB2	1:A:155:ARG:HD3	1.94	0.48
1:B:660:VAL:HG13	1:B:666:LEU:CD2	2.44	0.48
1:C:378:LEU:HB3	1:C:381:LEU:HD23	1.95	0.48
1:D:579:ALA:CB	1:D:582:ILE:HD11	2.44	0.48
1:D:666:LEU:O	1:D:670:ILE:HG12	2.14	0.48
1:A:172:LEU:HD12	1:A:172:LEU:O	2.13	0.48
1:A:511:VAL:O	1:A:514:LEU:HB3	2.13	0.48
1:C:286:ALA:HB1	1:C:288:VAL:HG12	1.96	0.48
1:A:563:VAL:HG11	1:A:605:ILE:CA	2.08	0.48
1:C:281:ARG:HA	1:C:300:TYR:CD2	2.49	0.48
1:A:630:ILE:HG13	1:A:646:LEU:HD22	1.96	0.47
1:B:288:VAL:HG23	1:B:289:ALA:N	2.28	0.47
1:B:561:PRO:HB2	1:B:608:MET:HG3	1.95	0.47
1:C:116:MET:HE3	1:C:133:ILE:HG23	1.96	0.47
1:D:567:GLN:NE2	1:D:604:LEU:HB2	2.26	0.47
1:A:241:ASP:O	1:A:272:LYS:NZ	2.45	0.47
1:A:427:GLY:O	1:B:187:ARG:HG2	2.15	0.47
1:B:139:GLY:HA2	1:B:146:GLN:HA	1.96	0.47
1:D:558:ILE:O	1:D:558:ILE:HG13	2.14	0.47
1:D:575:VAL:O	1:D:598:LEU:HD11	2.15	0.47
1:A:564:LEU:HD22	1:A:565:LYS:N	2.29	0.47
1:D:562:VAL:O	1:D:563:VAL:CG1	2.63	0.47
1:A:393:LYS:HE3	4:A:1032:HOH:O	2.14	0.47
1:B:636:ILE:HD13	1:B:637:TYR:CD2	2.49	0.47
1:A:284:LYS:HG2	1:A:285:SER:N	2.29	0.47
1:B:121:SER:HB2	1:B:155:ARG:HD3	1.97	0.47
1:B:595:MET:HE2	1:B:603:TYR:HE2	1.80	0.47
1:B:667:TRP:HZ3	1:B:681:LEU:HD12	1.80	0.47
1:C:539:SER:HB3	1:C:540:PRO:HD2	1.95	0.47
1:C:660:VAL:HG13	1:C:666:LEU:CD1	2.45	0.47
1:D:279:VAL:HG12	1:D:280:GLY:N	2.29	0.47
1:A:150:ASN:O	1:A:154:GLU:HB2	2.15	0.47
1:C:142:GLY:CA	4:C:923:HOH:O	2.62	0.47
1:A:569:LEU:HD22	1:A:570:ALA:N	2.30	0.47
1:B:456:TYR:CD1	1:B:464:PHE:HZ	2.33	0.47
1:D:549:GLN:HG3	1:D:549:GLN:O	2.15	0.47
1:A:318:ILE:HD12	1:B:348:GLN:HE22	1.80	0.46
1:B:385:SER:O	1:B:388:LEU:HB2	2.16	0.46
1:C:598:LEU:O	1:C:600:SER:N	2.48	0.46
1:D:562:VAL:C	1:D:563:VAL:CG1	2.88	0.46
1:D:580:LEU:CD2	1:D:608:MET:HE1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:LEU:HD11	1:A:589:LYS:HG2	1.97	0.46
1:C:74:PHE:CZ	1:C:76:GLY:HA3	2.50	0.46
1:C:702:ILE:HD12	1:C:704:GLU:O	2.15	0.46
1:B:370:THR:HG23	1:B:408:SER:OG	2.16	0.46
1:A:40:ASN:ND2	1:A:160:GLY:O	2.36	0.46
1:C:514:LEU:HB2	1:C:515:SER:H	1.53	0.46
1:C:619:TYR:CD1	1:C:619:TYR:C	2.93	0.46
1:D:378:LEU:HB3	1:D:381:LEU:HD13	1.97	0.46
1:D:547:SER:HB3	1:D:550:GLU:HB2	1.97	0.46
1:A:569:LEU:HD23	1:A:569:LEU:HA	1.67	0.46
1:C:337:ASN:HA	1:C:494:PHE:CE1	2.51	0.46
1:D:497:LYS:O	1:D:501:GLU:HG3	2.16	0.46
1:D:580:LEU:HD23	1:D:608:MET:HE1	1.98	0.46
1:B:526:ASN:ND2	1:B:529:ARG:HH12	2.14	0.46
1:B:391:TRP:O	1:B:393:LYS:HG2	2.16	0.45
1:C:271:LYS:NZ	4:C:930:HOH:O	2.49	0.45
1:C:695:ALA:O	1:C:699:TYR:HB3	2.15	0.45
1:D:637:TYR:HD2	1:D:640:LEU:HD12	1.81	0.45
1:B:288:VAL:HG23	1:B:289:ALA:H	1.82	0.45
1:C:172:LEU:C	1:C:172:LEU:HD12	2.41	0.45
1:D:514:LEU:O	1:D:515:SER:CB	2.64	0.45
1:A:524:HIS:ND1	4:A:908:HOH:O	2.36	0.45
1:B:203:SER:HB3	1:B:206:VAL:HG22	1.98	0.45
1:C:495:LYS:HA	1:C:495:LYS:HD2	1.85	0.45
1:A:460:ILE:HD12	1:A:462:THR:OG1	2.16	0.45
1:B:520:LEU:HD23	1:B:520:LEU:HA	1.82	0.45
1:B:564:LEU:HD11	1:B:603:TYR:CD2	2.50	0.45
1:B:636:ILE:O	1:B:636:ILE:HG12	2.13	0.45
1:C:190:ARG:O	1:C:190:ARG:HG3	2.17	0.45
1:C:560:TYR:HB3	1:C:561:PRO:HA	1.98	0.45
1:A:570:ALA:HB1	1:A:571:HIS:CB	2.37	0.45
1:B:554:TYR:CE2	1:B:558:ILE:HD12	2.52	0.45
1:B:563:VAL:CG1	1:B:580:LEU:HD23	2.47	0.45
1:B:619:TYR:CD1	1:B:619:TYR:C	2.94	0.45
1:D:682:GLU:O	1:D:685:THR:HG22	2.17	0.45
1:A:610:THR:HB	1:A:611:ASP:H	1.50	0.45
1:B:610:THR:OG1	1:B:611:ASP:N	2.50	0.45
1:D:572:LYS:HE3	2:D:801:ATP:O3A	2.17	0.45
1:D:588:LEU:HD23	1:D:588:LEU:O	2.17	0.45
1:D:605:ILE:C	1:D:605:ILE:HD12	2.42	0.45
1:A:554:TYR:HE2	1:A:605:ILE:HG22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ASP:O	1:B:272:LYS:NZ	2.50	0.44
1:B:545:VAL:HG11	1:B:551:GLY:HA2	1.98	0.44
1:A:279:VAL:HG12	1:A:280:GLY:N	2.32	0.44
1:B:36:MET:CG	1:B:37:LYS:N	2.79	0.44
1:C:149:GLN:O	1:C:153:LEU:HG	2.17	0.44
1:D:288:VAL:O	1:D:289:ALA:HB2	2.16	0.44
1:A:564:LEU:HD23	1:A:604:LEU:O	2.17	0.44
1:B:666:LEU:HD23	1:B:670:ILE:CD1	2.48	0.44
1:A:316:GLU:OE1	4:A:901:HOH:O	2.21	0.44
1:B:567:GLN:HB2	1:B:602:TYR:O	2.17	0.44
1:C:513:ASP:CB	1:C:514:LEU:HA	2.47	0.44
1:D:567:GLN:HA	1:D:567:GLN:OE1	2.17	0.44
1:A:343:THR:HB	4:A:987:HOH:O	2.17	0.44
1:A:661:LYS:HG2	1:A:667:TRP:CD2	2.52	0.44
1:B:526:ASN:HD22	1:B:529:ARG:HH12	1.65	0.44
1:C:271:LYS:CE	4:C:930:HOH:O	2.61	0.44
1:C:328:LEU:HD21	1:C:493:LEU:HD23	1.99	0.44
1:D:284:LYS:CE	1:D:285:SER:H	2.31	0.44
1:D:396:LYS:NZ	1:D:400:GLU:OE2	2.50	0.44
1:A:134:PRO:HB2	1:A:168:CYS:O	2.18	0.44
1:A:461:GLN:HB3	1:B:319:ASP:OD2	2.18	0.44
1:A:636:ILE:HD13	1:A:637:TYR:CE1	2.52	0.44
1:B:342:LEU:HD21	1:B:390:ILE:HD13	2.00	0.44
1:C:649:PRO:HB2	1:C:696:MET:HG3	2.00	0.44
1:D:63:ARG:NH1	1:D:89:ASP:OD2	2.51	0.44
1:B:548:LEU:O	1:B:548:LEU:HD12	2.18	0.44
1:C:235:LEU:HD21	1:C:264:LEU:HD13	1.99	0.44
1:C:520:LEU:HD23	1:C:520:LEU:HA	1.86	0.44
1:D:85:TYR:O	1:D:93:CYS:HB2	2.18	0.44
1:D:563:VAL:HG22	1:D:606:GLN:O	2.18	0.44
1:A:306:PHE:CD1	1:A:625:TYR:HB3	2.53	0.44
1:B:284:LYS:N	1:B:284:LYS:CD	2.71	0.44
1:C:293:SER:HB3	1:C:630:ILE:HD13	2.00	0.44
1:B:36:MET:HG3	1:B:37:LYS:N	2.20	0.44
1:C:523:LEU:HD12	1:C:523:LEU:HA	1.74	0.44
1:D:396:LYS:HZ3	1:D:400:GLU:CB	2.30	0.44
1:D:685:THR:HG23	1:D:686:ALA:N	2.33	0.44
1:B:35:ALA:O	1:B:36:MET:HB2	2.17	0.43
1:B:373:GLU:HG2	1:B:377:LYS:HZ2	1.83	0.43
1:C:65:LEU:HD11	1:C:108:VAL:HG11	2.00	0.43
1:C:723:LEU:HD23	1:C:723:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:LYS:O	1:D:378:LEU:HD23	2.18	0.43
1:A:592:TRP:CD1	1:A:592:TRP:C	2.96	0.43
1:B:305:LEU:HD22	1:B:646:LEU:HB2	2.00	0.43
1:B:443:LEU:HB3	1:B:477:ILE:HD12	2.00	0.43
1:B:511:VAL:O	1:B:511:VAL:CG1	2.65	0.43
1:C:162:ARG:NH1	1:C:228:ASP:OD1	2.45	0.43
1:B:288:VAL:HB	1:B:520:LEU:HG	2.00	0.43
1:B:566:ALA:C	1:B:567:GLN:HG2	2.43	0.43
1:C:456:TYR:CE1	1:C:464:PHE:HZ	2.36	0.43
1:B:497:LYS:HA	1:B:497:LYS:HD2	1.84	0.43
1:B:577:GLY:C	1:B:578:VAL:HG23	2.43	0.43
1:A:284:LYS:HE2	1:A:285:SER:HA	2.01	0.43
1:C:519:GLY:O	4:C:902:HOH:O	2.21	0.43
1:D:84:ARG:HG2	1:D:85:TYR:CZ	2.53	0.43
1:D:336:VAL:O	1:D:416:GLY:HA3	2.19	0.43
1:D:580:LEU:O	1:D:582:ILE:N	2.52	0.43
1:B:342:LEU:HD13	1:B:406:LEU:CD2	2.49	0.43
1:D:195:GLY:HA3	1:D:216:GLY:C	2.44	0.43
1:D:529:ARG:HH21	1:D:567:GLN:NE2	2.17	0.43
1:D:530:LYS:O	1:D:534:GLU:HG3	2.18	0.43
1:D:586:ALA:O	1:D:589:LYS:HB3	2.19	0.43
1:B:411:LYS:HB2	1:B:411:LYS:HE2	1.77	0.43
1:A:40:ASN:O	1:A:43:ILE:HG22	2.19	0.43
1:A:563:VAL:HG22	1:A:605:ILE:HG23	1.98	0.43
1:B:40:ASN:O	1:B:43:ILE:HG22	2.19	0.43
1:D:443:LEU:HD23	1:D:443:LEU:HA	1.81	0.43
1:D:543:GLN:HG2	1:D:544:VAL:N	2.33	0.43
1:D:532:LEU:HD11	1:D:722:VAL:CG1	2.49	0.43
1:D:660:VAL:HG13	1:D:666:LEU:CD1	2.47	0.43
1:A:43:ILE:HD12	1:A:43:ILE:HA	1.85	0.43
1:A:532:LEU:HD11	1:A:722:VAL:CG2	2.48	0.43
1:A:554:TYR:O	1:A:557:SER:HB3	2.19	0.43
1:A:619:TYR:CD1	1:A:619:TYR:C	2.96	0.43
1:C:241:ASP:O	1:C:272:LYS:NZ	2.47	0.43
1:D:619:TYR:CD1	1:D:619:TYR:C	2.97	0.43
1:A:493:LEU:HA	1:A:493:LEU:HD23	1.62	0.42
1:B:502:LYS:C	1:B:504:ASN:H	2.26	0.42
1:B:532:LEU:HD22	1:B:537:PHE:CB	2.49	0.42
1:B:649:PRO:HB2	1:B:696:MET:HG3	2.01	0.42
1:B:304:LYS:O	1:B:308:GLU:HG3	2.20	0.42
1:B:582:ILE:O	1:B:582:ILE:CG1	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:HE2	1:A:285:SER:N	2.31	0.42
1:A:287:ALA:C	1:A:288:VAL:HG23	2.44	0.42
1:C:381:LEU:HA	1:C:381:LEU:HD13	1.81	0.42
1:C:654:LYS:O	1:C:658:GLN:HG3	2.19	0.42
1:B:193:LYS:CG	1:B:216:GLY:HA2	2.49	0.42
1:C:202:GLN:CG	1:C:231:MET:HE3	2.49	0.42
1:D:578:VAL:HG11	2:D:801:ATP:H5'2	2.01	0.42
1:A:36:MET:HE3	1:A:36:MET:HB3	1.80	0.42
1:A:342:LEU:HD21	1:A:390:ILE:HG12	2.01	0.42
1:A:529:ARG:NH2	1:A:567:GLN:OE1	2.45	0.42
1:B:571:HIS:HB3	1:B:574:ASP:OD1	2.18	0.42
1:C:40:ASN:O	1:C:43:ILE:HG22	2.19	0.42
1:C:511:VAL:HG12	1:C:512:GLU:N	2.34	0.42
1:C:623:MET:HE2	1:C:623:MET:HB3	1.93	0.42
1:D:190:ARG:HA	1:D:190:ARG:HD3	1.84	0.42
1:B:193:LYS:HG3	1:B:216:GLY:HA2	2.00	0.42
1:B:723:LEU:C	1:B:723:LEU:HD23	2.44	0.42
1:C:564:LEU:HD13	1:C:595:MET:SD	2.59	0.42
1:D:83:PRO:HA	1:D:95:GLN:NE2	2.34	0.42
1:D:334:PRO:HA	4:D:925:HOH:O	2.20	0.42
1:A:542:GLU:HA	1:A:605:ILE:O	2.20	0.42
1:C:254:ILE:HD12	1:C:303:GLU:OE1	2.20	0.42
1:A:289:ALA:HA	1:A:704:GLU:OE2	2.20	0.42
1:C:391:TRP:HA	1:C:391:TRP:CE3	2.54	0.42
1:D:342:LEU:HD11	1:D:409:ILE:CD1	2.46	0.42
1:A:517:GLN:HE21	1:A:517:GLN:CA	2.25	0.42
1:A:638:THR:CG2	1:A:639:GLU:N	2.82	0.42
1:B:200:ILE:HG21	1:B:231:MET:HG3	2.02	0.42
1:A:564:LEU:HD22	1:A:565:LYS:H	1.85	0.41
1:B:516:ILE:HD12	1:B:517:GLN:N	2.34	0.41
1:B:572:LYS:HB2	1:B:578:VAL:HG23	2.01	0.41
1:D:685:THR:CG2	1:D:686:ALA:N	2.83	0.41
1:A:564:LEU:N	1:A:579:ALA:HB3	2.20	0.41
1:B:560:TYR:HA	1:B:561:PRO:C	2.45	0.41
1:C:532:LEU:HD22	1:C:537:PHE:HB2	2.02	0.41
1:D:348:GLN:HG3	4:D:938:HOH:O	2.20	0.41
1:A:687:SER:OG	1:A:717:VAL:HG21	2.20	0.41
1:D:441:LYS:HD2	1:D:471:ILE:HD13	2.01	0.41
1:D:720:LEU:N	1:D:720:LEU:HD23	2.34	0.41
1:C:545:VAL:HG11	1:C:551:GLY:HA2	2.02	0.41
1:D:708:ASN:HA	1:D:709:PRO:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:HD12	1:A:523:LEU:HA	1.85	0.41
1:A:204:GLY:C	1:A:206:VAL:H	2.29	0.41
1:D:51:ILE:HA	1:D:106:VAL:O	2.21	0.41
1:D:421:ALA:HA	1:D:457:PHE:O	2.20	0.41
1:D:405:CYS:O	1:D:409:ILE:HG13	2.21	0.41
1:A:465:ASP:HA	1:A:466:PRO:HD2	1.91	0.41
1:D:682:GLU:HA	1:D:685:THR:HG22	2.03	0.41
1:C:506:THR:HA	1:C:507:PRO:HD3	1.94	0.41
1:C:566:ALA:N	1:C:595:MET:HE1	2.36	0.41
1:D:532:LEU:HD22	1:D:537:PHE:HB2	2.01	0.41
1:A:578:VAL:HG12	1:A:580:LEU:HG	2.03	0.41
1:A:696:MET:HE2	1:A:696:MET:HB3	1.98	0.41
1:B:681:LEU:C	1:B:681:LEU:CD2	2.94	0.41
1:D:640:LEU:HD23	1:D:640:LEU:HA	1.90	0.41
2:D:801:ATP:C8	2:D:801:ATP:C5'	2.95	0.41
1:B:708:ASN:HA	1:B:709:PRO:HA	1.73	0.40
1:D:595:MET:HE2	1:D:603:TYR:CE1	2.56	0.40
1:A:205:SER:HB2	1:B:345:SER:HB2	2.02	0.40
1:A:386:ASN:HA	1:A:387:PRO:C	2.45	0.40
1:B:542:GLU:HA	1:B:605:ILE:O	2.22	0.40
1:C:355:LEU:O	1:C:359:TYR:HD2	2.05	0.40
1:C:460:ILE:HD12	1:C:462:THR:CG2	2.52	0.40
1:D:36:MET:N	1:D:36:MET:CE	2.80	0.40
1:D:294:GLY:HA2	1:D:620:ARG:HH11	1.85	0.40
1:D:580:LEU:HB3	1:D:581:ASN:H	1.52	0.40
1:D:616:ILE:HG13	1:D:708:ASN:HB2	2.04	0.40
1:C:109:GLY:C	1:C:116:MET:HE1	2.47	0.40
1:C:169:MET:HE2	1:C:181:TYR:CZ	2.57	0.40
1:C:531:LEU:HD23	1:C:531:LEU:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	691/748 (92%)	644 (93%)	41 (6%)	6 (1%)	14	11
1	B	691/748 (92%)	658 (95%)	25 (4%)	8 (1%)	10	6
1	C	691/748 (92%)	657 (95%)	23 (3%)	11 (2%)	7	4
1	D	690/748 (92%)	652 (94%)	34 (5%)	4 (1%)	21	20
All	All	2763/2992 (92%)	2611 (94%)	123 (4%)	29 (1%)	12	9

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	563	VAL
1	A	570	ALA
1	A	610	THR
1	C	37	LYS
1	C	286	ALA
1	C	289	ALA
1	C	512	GLU
1	C	515	SER
1	D	284	LYS
1	D	580	LEU
1	A	288	VAL
1	B	584	SER
1	C	288	VAL
1	C	519	GLY
1	A	36	MET
1	B	599	ASN
1	B	609	VAL
1	C	518	LYS
1	D	515	SER
1	B	36	MET
1	B	288	VAL
1	B	601	PRO
1	C	287	ALA
1	C	538	VAL
1	A	538	VAL
1	B	284	LYS
1	C	599	ASN
1	D	562	VAL
1	B	578	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	578/624 (93%)	545 (94%)	33 (6%)	18	17
1	B	578/624 (93%)	543 (94%)	35 (6%)	17	15
1	C	578/624 (93%)	543 (94%)	35 (6%)	17	15
1	D	578/624 (93%)	550 (95%)	28 (5%)	23	23
All	All	2312/2496 (93%)	2181 (94%)	131 (6%)	18	17

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	MET
1	A	49	GLN
1	A	143	VAL
1	A	144	GLU
1	A	172	LEU
1	A	206	VAL
1	A	231	MET
1	A	264	LEU
1	A	284	LYS
1	A	288	VAL
1	A	376	SER
1	A	381	LEU
1	A	464	PHE
1	A	493	LEU
1	A	498	GLU
1	A	512	GLU
1	A	514	LEU
1	A	515	SER
1	A	517	GLN
1	A	518	LYS
1	A	546	THR
1	A	548	LEU
1	A	556	GLU
1	A	563	VAL

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Mol	Chain	Res	Type
1	A	564	LEU
1	A	569	LEU
1	A	590	LYS
1	A	598	LEU
1	A	610	THR
1	A	636	ILE
1	A	643	GLU
1	A	682	GLU
1	A	722	VAL
1	B	59	ARG
1	B	93	CYS
1	B	158	ASP
1	B	172	LEU
1	B	187	ARG
1	B	189	LEU
1	B	193	LYS
1	B	264	LEU
1	B	342	LEU
1	B	393	LYS
1	B	399	SER
1	B	438	ILE
1	B	462	THR
1	B	463	GLU
1	B	464	PHE
1	B	474	GLU
1	B	477	ILE
1	B	493	LEU
1	B	502	LYS
1	B	511	VAL
1	B	517	GLN
1	B	523	LEU
1	B	530	LYS
1	B	533	ASP
1	B	539	SER
1	B	543	GLN
1	B	544	VAL
1	B	582	ILE
1	B	589	LYS
1	B	598	LEU
1	B	606	GLN
1	B	607	GLU
1	B	611	ASP

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Mol	Chain	Res	Type
1	B	636	ILE
1	B	670	ILE
1	C	36	MET
1	C	42	LYS
1	C	59	ARG
1	C	125	LYS
1	C	162	ARG
1	C	187	ARG
1	C	192	ILE
1	C	206	VAL
1	C	264	LEU
1	C	269	LYS
1	C	357	GLU
1	C	381	LEU
1	C	462	THR
1	C	477	ILE
1	C	493	LEU
1	C	495	LYS
1	C	512	GLU
1	C	513	ASP
1	C	514	LEU
1	C	516	ILE
1	C	517	GLN
1	C	523	LEU
1	C	527	GLU
1	C	532	LEU
1	C	548	LEU
1	C	564	LEU
1	C	569	LEU
1	C	581	ASN
1	C	602	TYR
1	C	666	LEU
1	C	674	ARG
1	C	687	SER
1	C	702	ILE
1	C	720	LEU
1	C	726	VAL
1	D	36	MET
1	D	84	ARG
1	D	118	GLN
1	D	155	ARG
1	D	172	LEU

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Mol	Chain	Res	Type
1	D	264	LEU
1	D	284	LYS
1	D	394	SER
1	D	441	LYS
1	D	449	ASN
1	D	462	THR
1	D	464	PHE
1	D	493	LEU
1	D	523	LEU
1	D	539	SER
1	D	544	VAL
1	D	564	LEU
1	D	565	LYS
1	D	569	LEU
1	D	580	LEU
1	D	602	TYR
1	D	606	GLN
1	D	652	THR
1	D	666	LEU
1	D	668	LYS
1	D	681	LEU
1	D	713	ARG
1	D	722	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	118	GLN
1	A	146	GLN
1	A	150	ASN
1	A	230	GLN
1	A	257	HIS
1	A	428	GLN
1	A	431	HIS
1	A	485	ASN
1	A	517	GLN
1	A	524	HIS
1	A	549	GLN
1	A	597	HIS
1	B	146	GLN
1	B	461	GLN

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Mol	Chain	Res	Type
1	B	485	ASN
1	B	505	HIS
1	B	526	ASN
1	B	676	ASN
1	C	95	GLN
1	C	146	GLN
1	C	147	ASN
1	C	175	HIS
1	C	257	HIS
1	C	337	ASN
1	C	348	GLN
1	C	428	GLN
1	C	431	HIS
1	C	517	GLN
1	C	526	ASN
1	C	571	HIS
1	D	87	ASN
1	D	95	GLN
1	D	146	GLN
1	D	230	GLN
1	D	257	HIS
1	D	337	ASN
1	D	431	HIS
1	D	461	GLN
1	D	517	GLN
1	D	567	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

8 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
3	SO4	B	802	-	4,4,4	0.25	0	6,6,6	0.24	0
2	ATP	D	801	-	32,33,33	1.74	9 (28%)	48,52,52	2.02	12 (25%)
2	ATP	C	801	-	32,33,33	1.76	7 (21%)	48,52,52	2.12	16 (33%)
2	ATP	A	801	-	32,33,33	1.79	7 (21%)	48,52,52	1.92	10 (20%)
2	ATP	B	801	-	32,33,33	1.70	8 (25%)	48,52,52	1.90	11 (22%)
3	SO4	D	802	-	4,4,4	0.28	0	6,6,6	0.30	0
3	SO4	A	802	-	4,4,4	0.31	0	6,6,6	0.51	0
3	SO4	C	802	-	4,4,4	0.31	0	6,6,6	0.38	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	A	801	-	-	3/22/38/38	0/3/3/3
2	ATP	D	801	-	-	6/22/38/38	0/3/3/3
2	ATP	C	801	-	-	7/22/38/38	0/3/3/3
2	ATP	B	801	-	-	5/22/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ATP	C6-N6	4.86	1.46	1.34
2	A	801	ATP	C6-N6	4.83	1.46	1.34
2	A	801	ATP	PB-O3A	4.79	1.64	1.59
2	D	801	ATP	C6-N6	4.65	1.46	1.34
2	B	801	ATP	C6-N6	4.57	1.45	1.34
2	B	801	ATP	PB-O3A	3.48	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ATP	PB-O3A	3.39	1.63	1.59
2	D	801	ATP	PB-O3A	3.14	1.62	1.59
2	C	801	ATP	C5'-C4'	-3.07	1.42	1.51
2	D	801	ATP	C5'-C4'	-3.03	1.42	1.51
2	B	801	ATP	C5'-C4'	-2.72	1.43	1.51
2	A	801	ATP	PG-O3G	-2.67	1.44	1.54
2	D	801	ATP	C2'-C3'	-2.65	1.46	1.53
2	D	801	ATP	PG-O3G	-2.64	1.45	1.54
2	C	801	ATP	PG-O3G	-2.63	1.45	1.54
2	A	801	ATP	C5'-C4'	-2.62	1.43	1.51
2	B	801	ATP	PG-O3G	-2.60	1.45	1.54
2	C	801	ATP	O5'-C5'	-2.54	1.35	1.44
2	C	801	ATP	C2'-C3'	-2.50	1.46	1.53
2	B	801	ATP	C2'-C3'	-2.50	1.46	1.53
2	A	801	ATP	C2'-C3'	-2.46	1.46	1.53
2	D	801	ATP	O5'-C5'	-2.33	1.35	1.44
2	A	801	ATP	C3'-C4'	-2.32	1.47	1.53
2	B	801	ATP	C3'-C4'	-2.27	1.47	1.53
2	A	801	ATP	PB-O3B	-2.20	1.57	1.59
2	B	801	ATP	O2'-C2'	-2.20	1.37	1.43
2	D	801	ATP	C5-N7	-2.20	1.35	1.39
2	D	801	ATP	O2'-C2'	-2.16	1.37	1.43
2	D	801	ATP	C3'-C4'	-2.11	1.47	1.53
2	B	801	ATP	PB-O3B	-2.10	1.57	1.59
2	C	801	ATP	O2'-C2'	-2.07	1.37	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ATP	C5-C4-N3	-5.36	119.34	126.72
2	D	801	ATP	C5-C4-N3	-5.24	119.50	126.72
2	B	801	ATP	C5-C4-N3	-5.00	119.83	126.72
2	C	801	ATP	C5-C4-N3	-4.85	120.04	126.72
2	C	801	ATP	N9-C8-N7	-4.76	107.19	113.94
2	D	801	ATP	N3-C2-N1	-4.69	121.48	128.58
2	C	801	ATP	N3-C2-N1	-4.60	121.62	128.58
2	A	801	ATP	N3-C2-N1	-4.59	121.63	128.58
2	A	801	ATP	N3-C4-N9	4.54	134.89	127.17
2	B	801	ATP	N3-C2-N1	-4.52	121.74	128.58
2	A	801	ATP	N9-C8-N7	-4.49	107.57	113.94
2	B	801	ATP	N3-C4-N9	4.46	134.76	127.17
2	D	801	ATP	N9-C8-N7	-4.34	107.78	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ATP	C4-N9-C8	4.28	110.23	105.74
2	B	801	ATP	N9-C8-N7	-4.19	107.99	113.94
2	D	801	ATP	N3-C4-N9	4.18	134.28	127.17
2	B	801	ATP	C4-N9-C8	4.16	110.11	105.74
2	C	801	ATP	C4-N9-C8	4.16	110.10	105.74
2	C	801	ATP	C5-N7-C8	3.86	109.52	103.45
2	D	801	ATP	C4-N9-C8	3.78	109.71	105.74
2	C	801	ATP	N3-C4-N9	3.70	133.46	127.17
2	A	801	ATP	C5-N7-C8	3.52	108.99	103.45
2	D	801	ATP	C2-N3-C4	3.52	120.42	111.83
2	D	801	ATP	C5-N7-C8	3.49	108.94	103.45
2	A	801	ATP	C2-N3-C4	3.46	120.28	111.83
2	D	801	ATP	O5'-C5'-C4'	3.42	120.64	108.99
2	C	801	ATP	C2-N3-C4	3.41	120.17	111.83
2	C	801	ATP	C4-C5-N7	-3.41	106.68	110.58
2	C	801	ATP	O4'-C4'-C5'	-3.24	98.96	109.33
2	B	801	ATP	C2-N3-C4	3.22	119.71	111.83
2	B	801	ATP	C5-N7-C8	3.11	108.33	103.45
2	C	801	ATP	O3G-PG-O3B	3.04	114.83	104.64
2	C	801	ATP	O5'-C5'-C4'	2.93	118.96	108.99
2	B	801	ATP	O3G-PG-O3B	2.84	114.17	104.64
2	D	801	ATP	C4-C5-N7	-2.82	107.35	110.58
2	D	801	ATP	O2A-PA-O3A	2.81	114.86	107.27
2	A	801	ATP	C4-C5-N7	-2.75	107.44	110.58
2	C	801	ATP	O3A-PB-O1B	-2.68	102.64	110.70
2	A	801	ATP	O3G-PG-O3B	2.66	113.57	104.64
2	C	801	ATP	O2A-PA-O3A	2.59	114.29	107.27
2	D	801	ATP	O3G-PG-O3B	2.59	113.31	104.64
2	B	801	ATP	O2B-PB-O3B	2.48	113.98	107.27
2	A	801	ATP	O5'-C5'-C4'	2.34	116.96	108.99
2	C	801	ATP	C4-N9-C1'	-2.29	121.27	126.63
2	D	801	ATP	O4'-C4'-C5'	-2.24	102.16	109.33
2	B	801	ATP	C4-C5-N7	-2.12	108.16	110.58
2	B	801	ATP	O5'-C5'-C4'	2.11	116.17	108.99
2	C	801	ATP	O3A-PA-O1A	-2.05	104.55	110.70
2	C	801	ATP	O4'-C1'-N9	2.01	111.94	108.09

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	ATP	PB-O3B-PG-O3G

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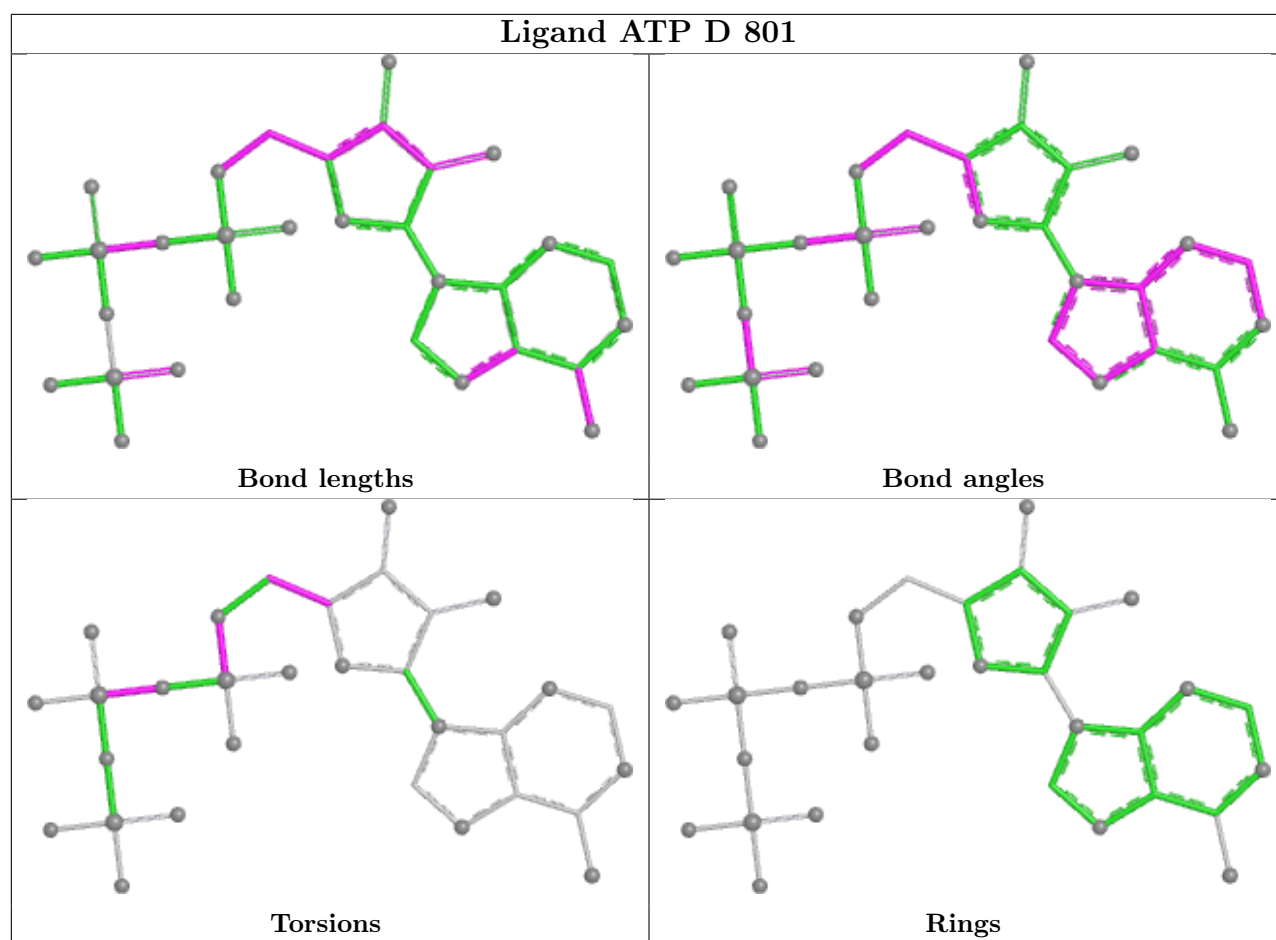
Mol	Chain	Res	Type	Atoms
2	C	801	ATP	C5'-O5'-PA-O1A
2	C	801	ATP	C5'-O5'-PA-O2A
2	C	801	ATP	C5'-O5'-PA-O3A
2	D	801	ATP	C5'-O5'-PA-O2A
2	D	801	ATP	C5'-O5'-PA-O3A
2	D	801	ATP	PA-O3A-PB-O3B
2	A	801	ATP	PB-O3A-PA-O2A
2	C	801	ATP	PA-O3A-PB-O3B
2	B	801	ATP	PB-O3A-PA-O2A
2	B	801	ATP	PB-O3B-PG-O2G
2	A	801	ATP	O4'-C4'-C5'-O5'
2	C	801	ATP	O4'-C4'-C5'-O5'
2	A	801	ATP	PB-O3A-PA-O1A
2	B	801	ATP	PB-O3A-PA-O1A
2	C	801	ATP	PA-O3A-PB-O1B
2	B	801	ATP	PB-O3B-PG-O1G
2	D	801	ATP	C3'-C4'-C5'-O5'
2	C	801	ATP	PA-O3A-PB-O2B
2	D	801	ATP	PA-O3A-PB-O2B
2	D	801	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

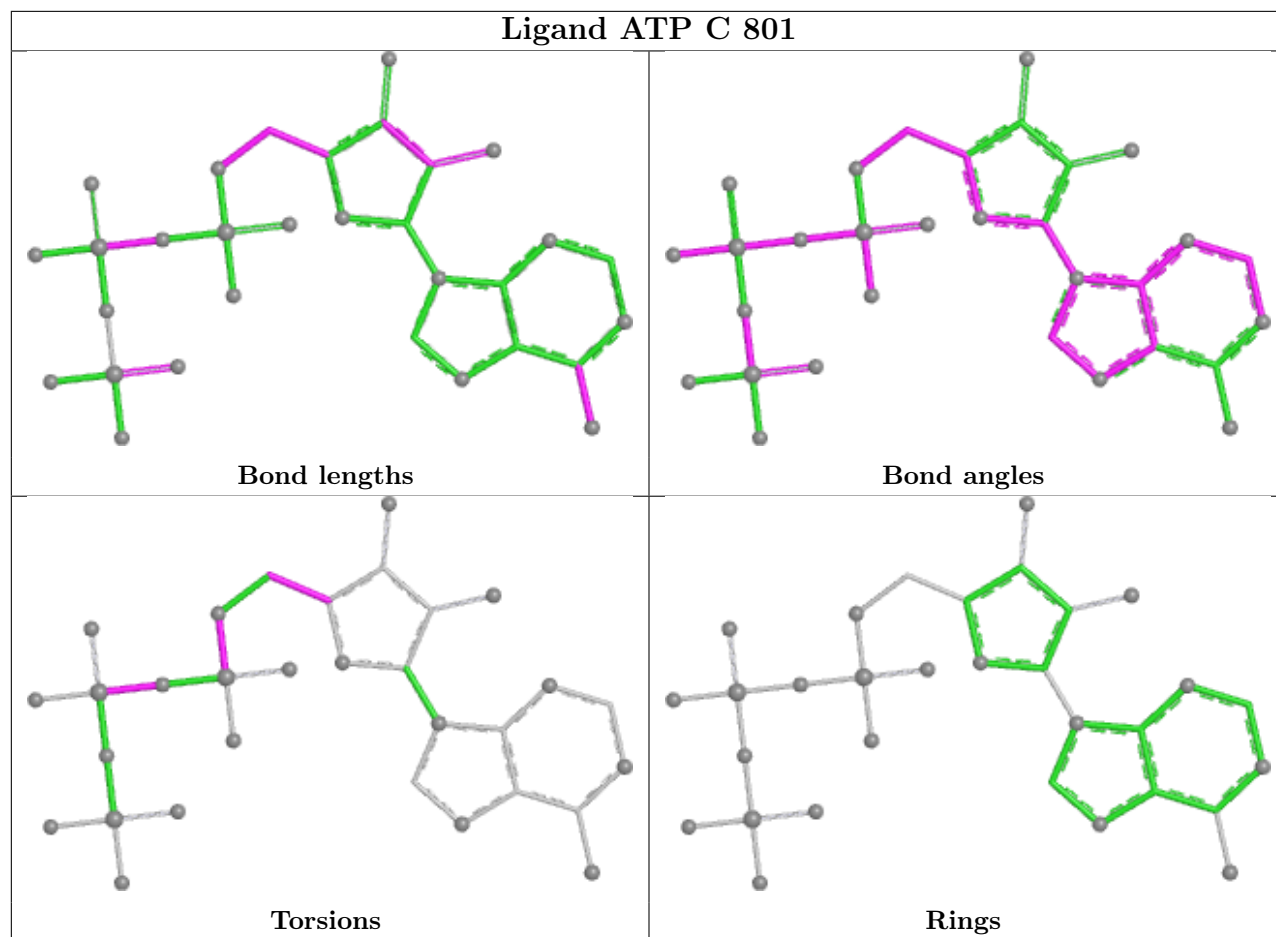
2 monomers are involved in 9 short contacts:

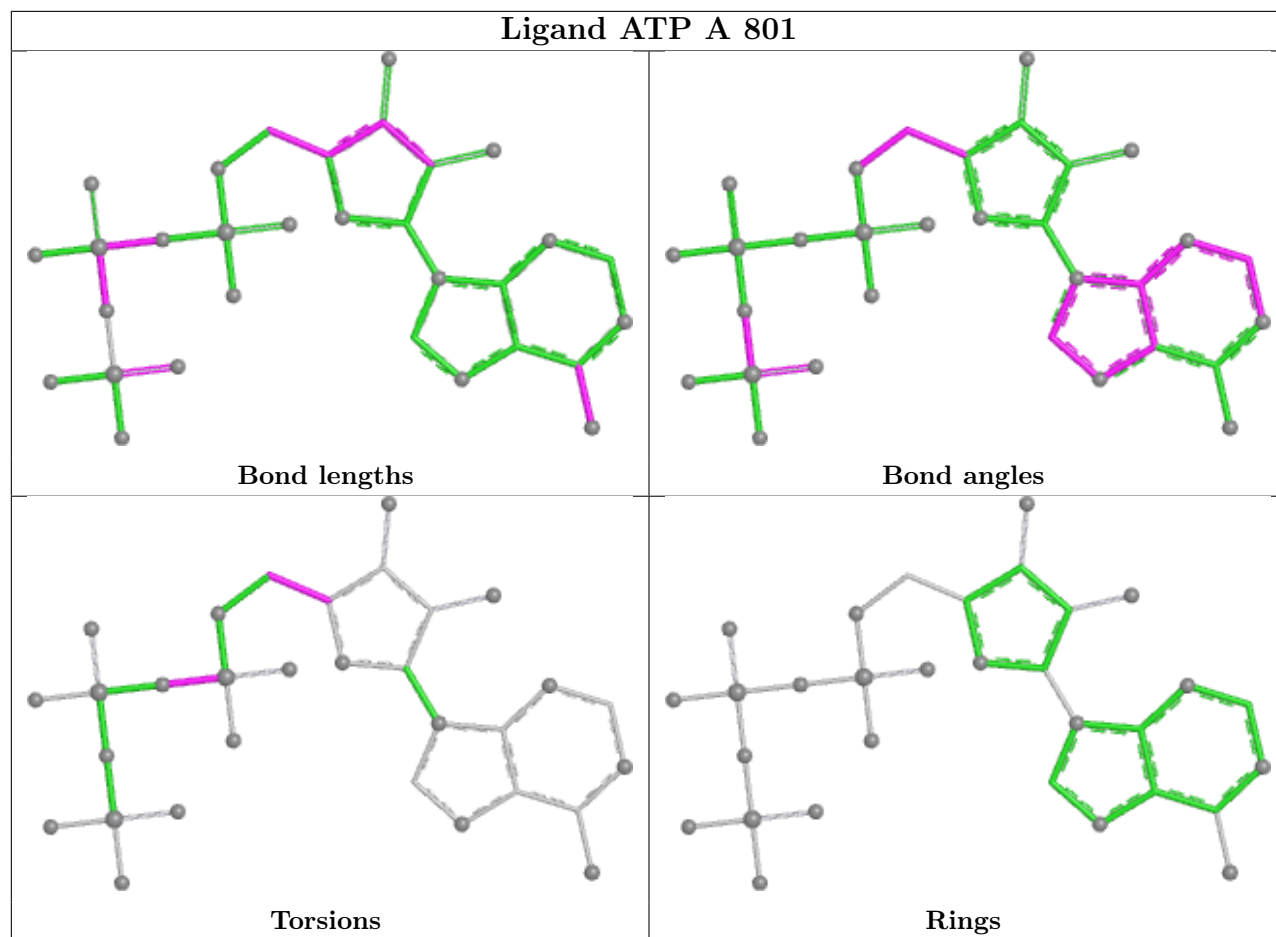
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	ATP	6	0
2	C	801	ATP	3	0

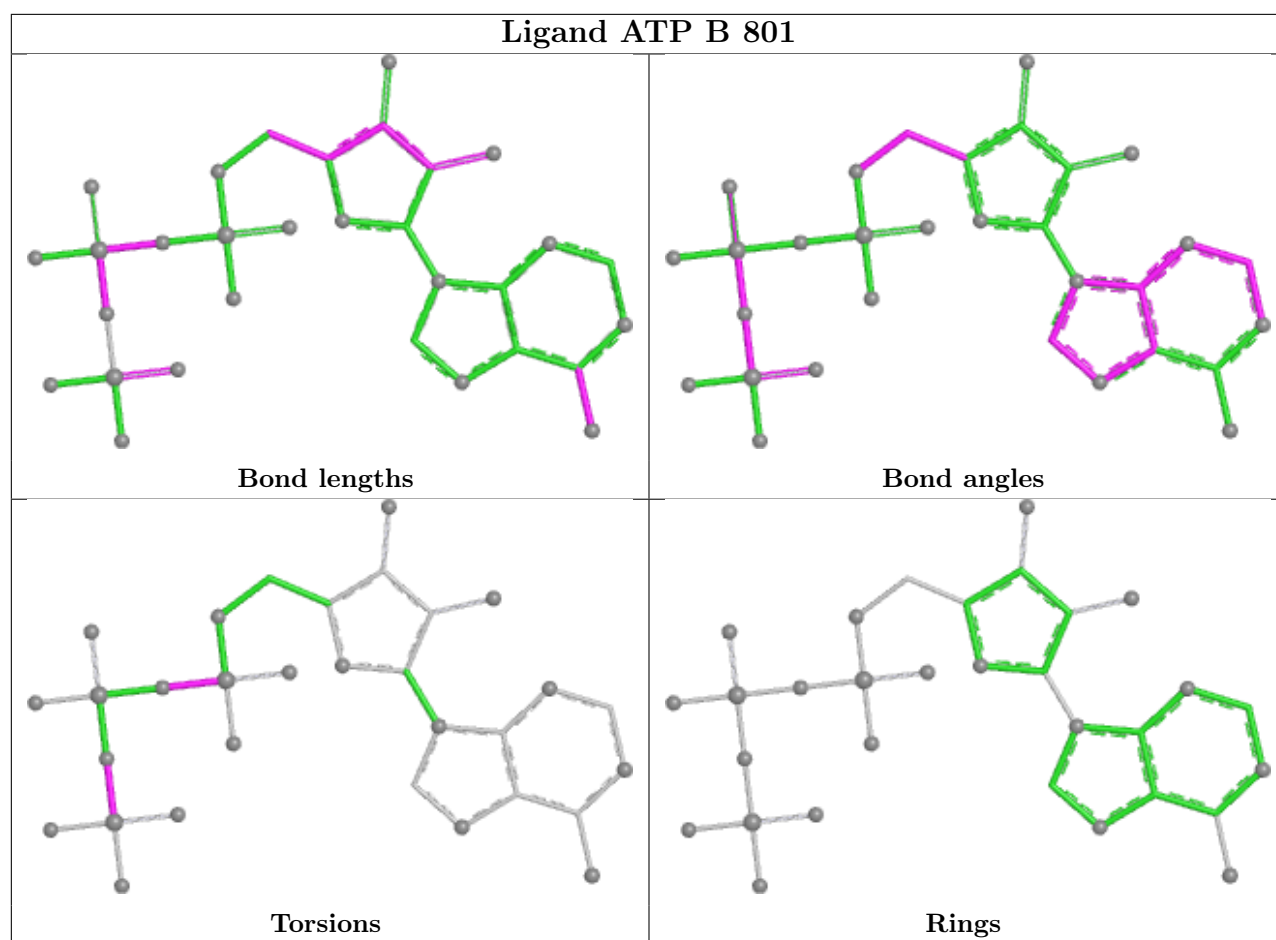
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ATP C 801







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	693/748 (92%)	-0.05	19 (2%) 56 57	20, 41, 75, 95	0
1	B	693/748 (92%)	0.00	22 (3%) 50 50	22, 42, 74, 85	0
1	C	693/748 (92%)	-0.30	15 (2%) 62 64	18, 35, 56, 101	0
1	D	692/748 (92%)	-0.08	32 (4%) 37 35	20, 37, 86, 96	0
All	All	2771/2992 (92%)	-0.11	88 (3%) 50 50	18, 38, 76, 101	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	ALA	5.5
1	A	288	VAL	4.4
1	C	516	ILE	4.3
1	C	504	ASN	4.1
1	C	288	VAL	4.0
1	A	35	ALA	3.9
1	D	569	LEU	3.9
1	A	570	ALA	3.9
1	C	514	LEU	3.8
1	A	286	ALA	3.7
1	A	563	VAL	3.7
1	D	558	ILE	3.7
1	C	513	ASP	3.6
1	D	566	ALA	3.6
1	C	36	MET	3.4
1	D	568	GLY	3.4
1	B	601	PRO	3.3
1	D	602	TYR	3.3
1	A	727	LYS	3.2
1	C	602	TYR	3.2
1	B	288	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	287	ALA	3.1
1	C	519	GLY	3.1
1	A	564	LEU	3.1
1	A	287	ALA	3.1
1	C	503	ASN	3.1
1	C	511	VAL	3.1
1	C	518	LYS	3.1
1	D	580	LEU	3.1
1	B	36	MET	3.0
1	D	556	GLU	3.0
1	D	548	LEU	2.9
1	D	564	LEU	2.9
1	D	285	SER	2.8
1	A	602	TYR	2.8
1	C	286	ALA	2.8
1	B	286	ALA	2.8
1	D	286	ALA	2.8
1	D	288	VAL	2.7
1	B	558	ILE	2.7
1	D	137	GLY	2.7
1	D	563	VAL	2.6
1	B	610	THR	2.6
1	B	505	HIS	2.6
1	B	189	LEU	2.6
1	D	612	GLY	2.6
1	A	516	ILE	2.6
1	B	579	ALA	2.6
1	B	398	PHE	2.6
1	A	524	HIS	2.5
1	D	287	ALA	2.5
1	C	35	ALA	2.5
1	D	504	ASN	2.4
1	D	598	LEU	2.4
1	B	562	VAL	2.4
1	D	36	MET	2.4
1	D	190	ARG	2.4
1	A	515	SER	2.4
1	D	604	LEU	2.4
1	B	541	ARG	2.4
1	B	546	THR	2.3
1	B	582	ILE	2.3
1	B	559	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	577	GLY	2.3
1	D	570	ALA	2.3
1	B	602	TYR	2.3
1	A	285	SER	2.2
1	B	513	ASP	2.2
1	C	505	HIS	2.2
1	B	580	LEU	2.2
1	A	36	MET	2.2
1	B	554	TYR	2.2
1	B	552	VAL	2.2
1	D	544	VAL	2.2
1	D	701	GLU	2.2
1	D	555	ALA	2.2
1	A	548	LEU	2.1
1	D	552	VAL	2.1
1	A	596	GLU	2.1
1	A	611	ASP	2.1
1	D	562	VAL	2.1
1	D	515	SER	2.1
1	D	284	LYS	2.1
1	A	595	MET	2.1
1	A	538	VAL	2.1
1	D	516	ILE	2.0
1	D	601	PRO	2.0
1	B	598	LEU	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 ⓘ

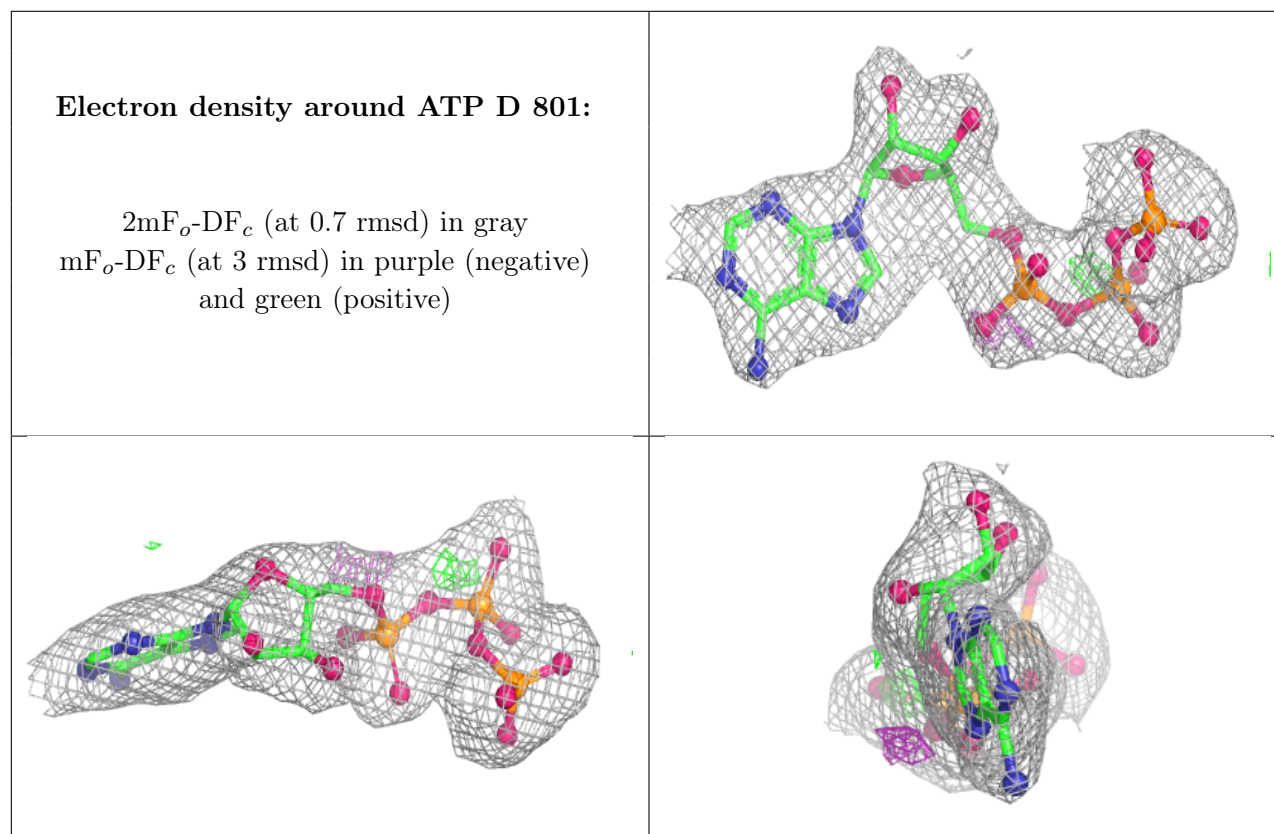
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

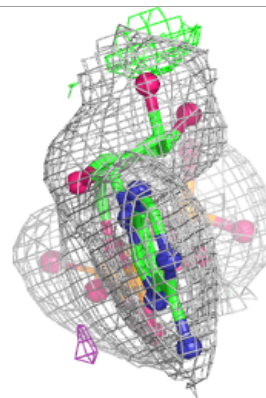
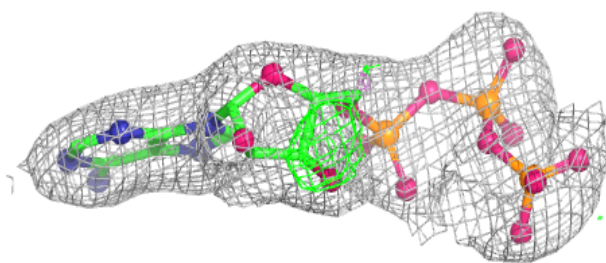
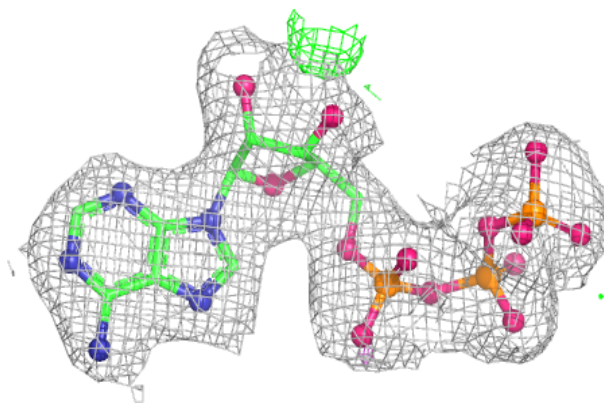
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	802	5/5	0.88	0.14	52,53,55,64	0
3	SO4	A	802	5/5	0.94	0.10	48,48,54,63	0
2	ATP	D	801	31/31	0.95	0.09	47,54,63,64	0
2	ATP	A	801	31/31	0.95	0.07	43,50,58,60	0
2	ATP	B	801	31/31	0.95	0.08	43,54,59,61	0
3	SO4	B	802	5/5	0.96	0.08	40,42,49,50	0
2	ATP	C	801	31/31	0.97	0.06	31,37,42,43	0
3	SO4	D	802	5/5	0.98	0.05	27,31,34,34	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.

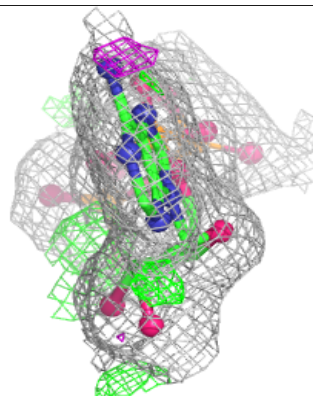
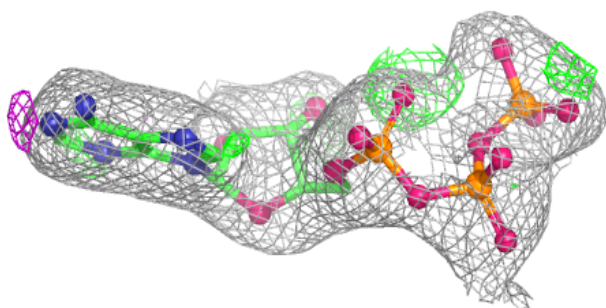
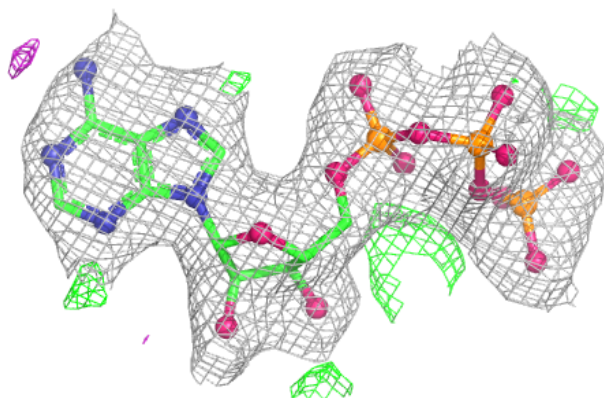


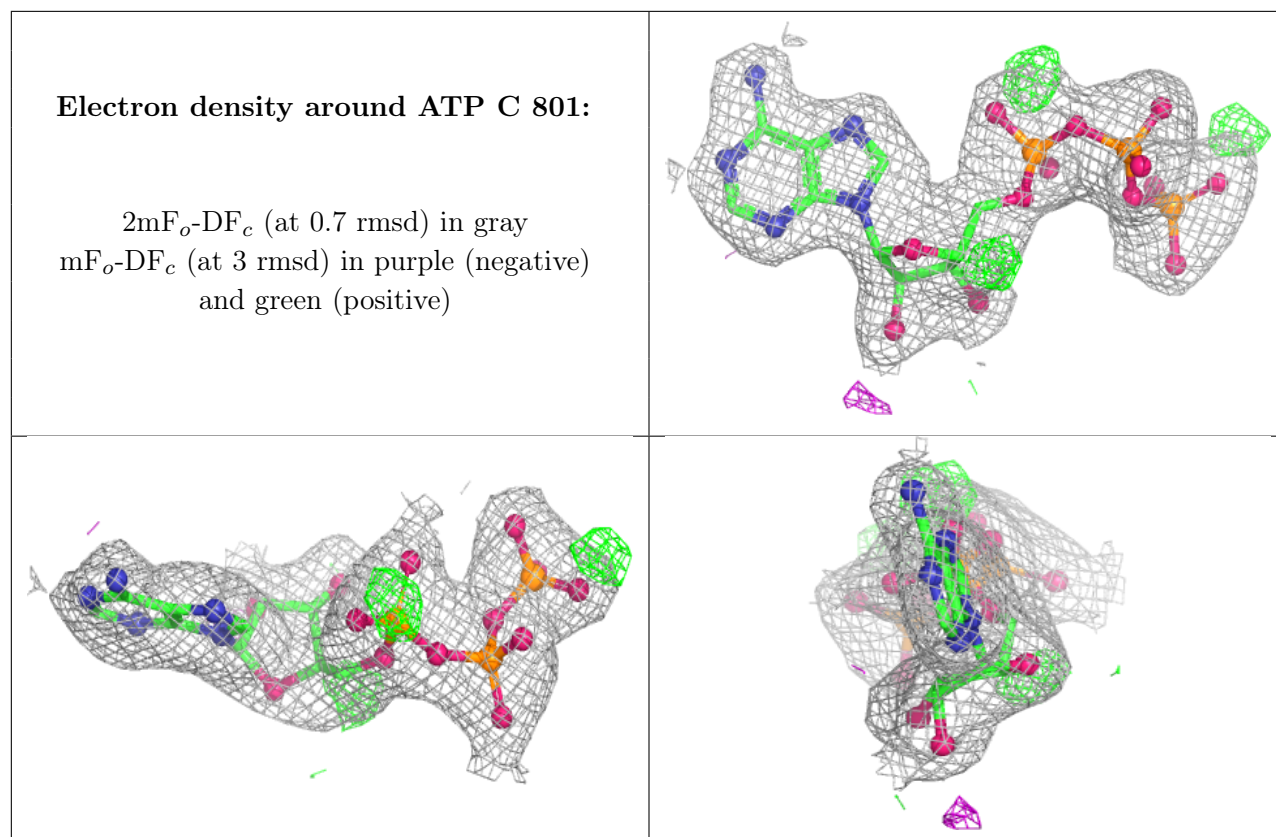
Electron density around ATP A 801:

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

**Electron density around ATP B 801:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.