



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:57 PM UTC

PDB ID : 3HNE / pdb_00003hne
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effectors TTP and ATP
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.
Deposited on : 2009-05-31
Resolution : 3.11 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

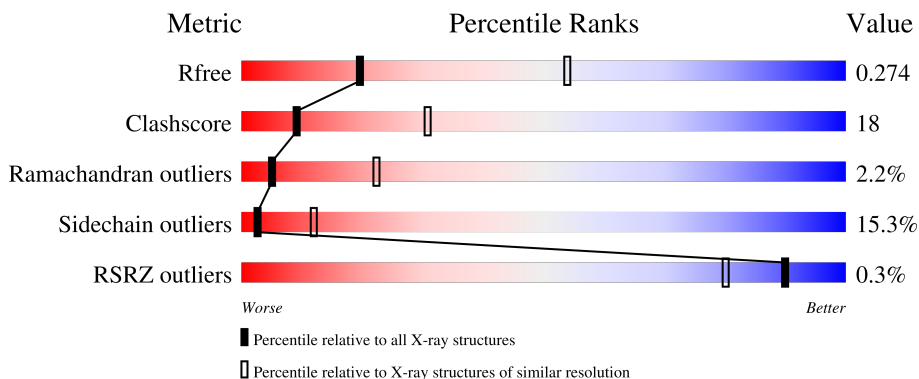
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	792	
1	B	792	

2 Entry composition [i](#)

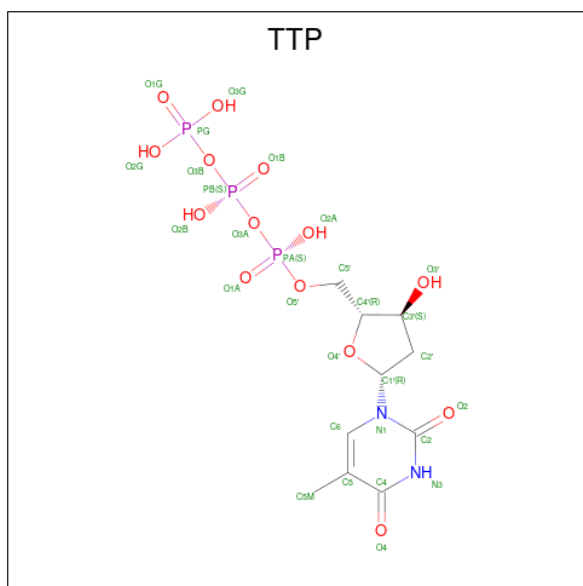
There are 6 unique types of molecules in this entry. The entry contains 11380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	6	1	0
			5568	3557	927	1051	33			
1	B	724	Total	C	N	O	S	0	0	0
			5644	3593	955	1062	34			

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	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	3	Total	Mg	0	0
			3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

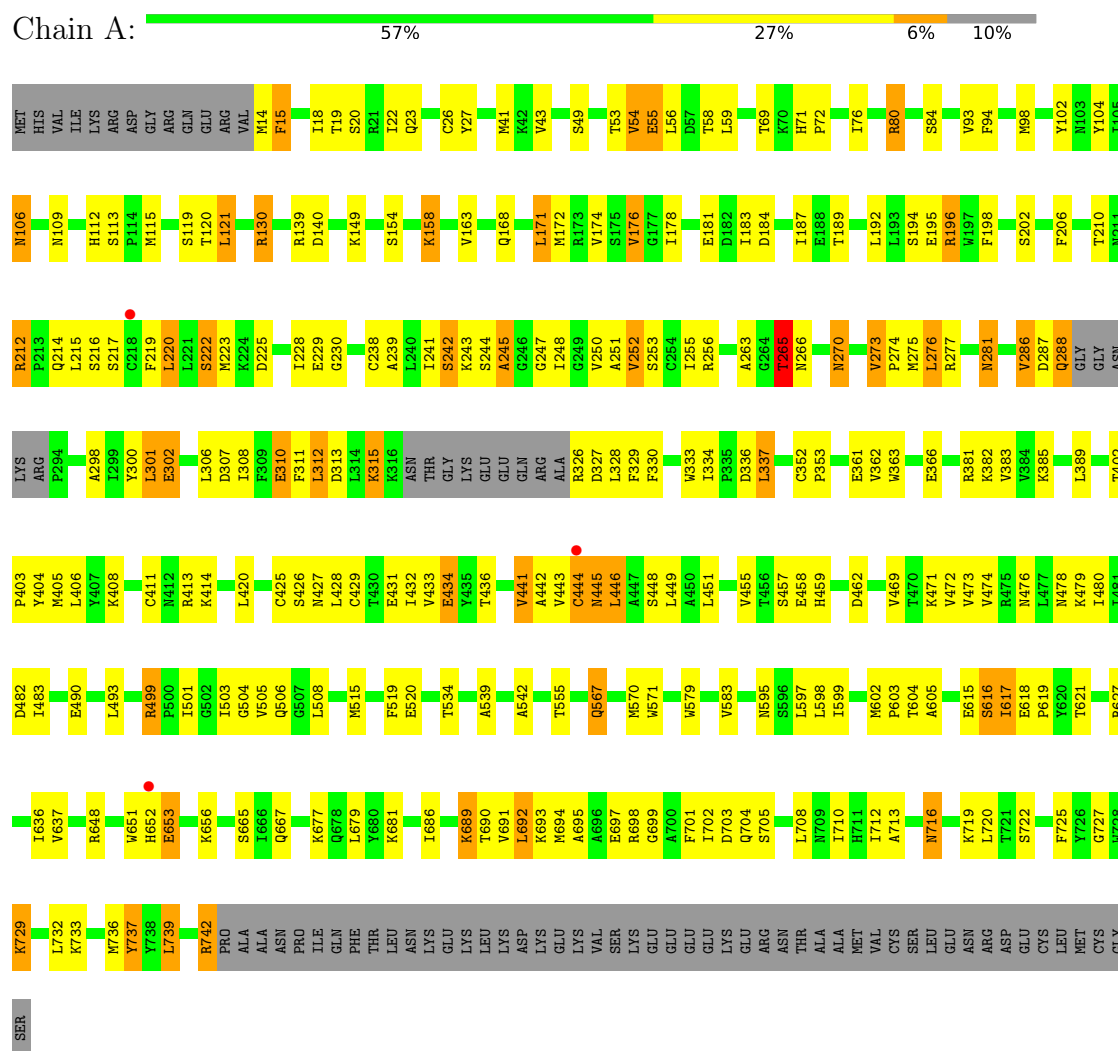
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	B	18	Total	O	0	0
			18	18		

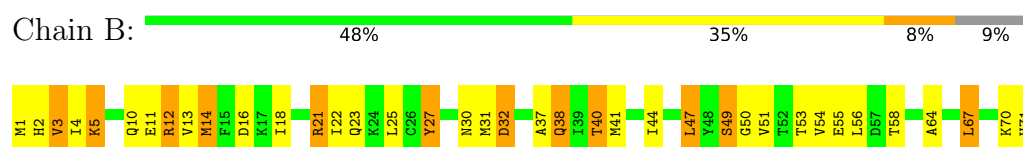
3 Residue-property plots

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

• Molecule 1: Ribonucleoside-diphosphate reductase large subunit



• Molecule 1: Ribonucleoside-diphosphate reductase large subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.15Å 114.37Å 222.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.07 – 3.11 44.07 – 3.11	Depositor EDS
% Data completeness (in resolution range)	88.5 (44.07-3.11) 88.4 (44.07-3.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.275 0.188 , 0.274	Depositor DCC
R_{free} test set	1440 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11380	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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, TTP, SO4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.89	1/5696 (0.0%)	1.10	9/7749 (0.1%)
1	B	0.88	1/5767 (0.0%)	1.15	19/7840 (0.2%)
All	All	0.89	2/11463 (0.0%)	1.12	28/15589 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	CYS	CA-C	-6.36	1.44	1.52
1	A	273	VAL	CA-CB	5.84	1.57	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ILE	N-CA-C	9.11	116.46	108.63
1	B	334	ILE	N-CA-C	8.83	116.68	107.76
1	B	302	GLU	CA-C-N	7.81	129.60	119.84
1	B	302	GLU	C-N-CA	7.81	129.60	119.84
1	B	556	TYR	N-CA-C	7.10	118.67	111.07
1	A	302	GLU	CA-C-N	7.06	126.74	119.82
1	A	302	GLU	C-N-CA	7.06	126.74	119.82
1	B	486	TYR	CA-C-N	7.01	126.62	119.19
1	B	486	TYR	C-N-CA	7.01	126.62	119.19
1	B	495	ASN	N-CA-C	6.82	118.79	111.36
1	B	499	ARG	CA-C-N	-6.24	113.86	120.66
1	B	499	ARG	C-N-CA	-6.24	113.86	120.66
1	A	385	LYS	N-CA-C	-5.96	101.21	110.10
1	B	395	GLU	N-CA-C	-5.96	104.78	111.28
1	A	56	LEU	N-CA-C	-5.85	104.60	110.97
1	B	481	ILE	CB-CA-C	-5.79	104.46	112.04
1	A	679	LEU	N-CA-C	5.66	118.18	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	MET	N-CA-C	-5.56	106.40	114.12
1	B	180	LYS	CB-CA-C	-5.45	109.82	117.23
1	B	636	ILE	N-CA-C	5.39	116.67	108.80
1	A	651	TRP	N-CA-C	5.29	117.34	109.25
1	B	551	GLY	CA-C-N	-5.25	115.17	120.21
1	B	551	GLY	C-N-CA	-5.25	115.17	120.21
1	A	618	GLU	N-CA-C	5.25	117.21	110.39
1	B	473	VAL	N-CA-C	-5.25	105.73	110.82
1	B	457	SER	N-CA-C	-5.24	105.63	112.23
1	B	285	TYR	N-CA-C	5.14	116.57	111.07
1	B	111	LYS	N-CA-C	5.02	117.50	109.96

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	5568	0	5368	179	0
1	B	5644	0	5448	227	0
2	A	29	0	13	1	0
2	B	29	0	13	4	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	15	0	0	2	0
4	B	15	0	0	1	0
5	B	31	0	12	3	0
6	A	27	0	0	3	0
6	B	18	0	0	3	0
All	All	11380	0	10854	406	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 18.

All (406) 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:445:ASN:C	1:A:446:LEU:HD23	1.34	1.49
1:A:445:ASN:O	1:A:446:LEU:HD23	1.50	1.11
1:A:445:ASN:C	1:A:446:LEU:CD2	2.30	1.03
1:A:130:ARG:HG2	1:A:130:ARG:HH11	1.18	1.01
1:A:443:VAL:HG12	1:A:444:CYS:H	1.23	0.99
1:A:567:GLN:HA	1:A:567:GLN:HE21	1.27	0.95
1:B:256:ARG:HD3	2:B:805:TTP:H4'	1.49	0.95
1:B:506:GLN:HA	1:B:616:SER:HA	1.46	0.94
1:A:446:LEU:HD23	1:A:446:LEU:N	1.67	0.94
1:B:256:ARG:CD	2:B:805:TTP:H4'	1.97	0.94
1:A:443:VAL:HG12	1:A:444:CYS:N	1.80	0.93
1:A:14:MET:HE3	1:A:15:PHE:HB3	1.56	0.88
1:B:568:TYR:HB2	1:B:573:VAL:HG12	1.54	0.87
1:A:534:THR:HG23	1:A:579:TRP:CZ2	2.13	0.84
5:B:807:ATP:H5'2	5:B:807:ATP:O1B	1.80	0.82
1:A:130:ARG:HG2	1:A:130:ARG:NH1	1.93	0.82
1:A:273:VAL:HG23	1:A:274:PRO:HD3	1.63	0.81
1:B:619:PRO:HG2	1:B:683:VAL:HG23	1.63	0.80
1:A:742:ARG:HA	1:A:742:ARG:NE	1.95	0.80
1:A:277:ARG:NH2	1:B:277:ARG:HH22	1.79	0.80
1:A:742:ARG:HA	1:A:742:ARG:HE	1.47	0.80
1:B:82:ALA:HA	1:B:85:ASN:OD1	1.81	0.80
1:B:337:LEU:HG	1:B:368:GLU:HG2	1.63	0.79
1:A:445:ASN:O	1:A:446:LEU:CD2	2.30	0.79
1:B:30:ASN:OD1	1:B:32:ASP:HB2	1.83	0.78
1:B:94:PHE:CE1	1:B:98:MET:HE3	2.18	0.78
1:A:443:VAL:CG1	1:A:444:CYS:H	1.96	0.78
1:B:695:ALA:HB1	1:B:708:LEU:HD11	1.64	0.78
1:A:534:THR:HG23	1:A:579:TRP:HZ2	1.48	0.78
1:A:310:GLU:H	1:A:310:GLU:CD	1.90	0.77
1:B:270:ASN:HB3	1:B:274:PRO:HG2	1.65	0.77
1:A:567:GLN:HA	1:A:567:GLN:NE2	2.00	0.77
1:A:736:MET:SD	1:A:739:LEU:HB2	2.25	0.77
1:B:482:ASP:CG	1:B:499:ARG:HH22	1.93	0.77
1:B:482:ASP:OD2	1:B:499:ARG:NH2	2.17	0.76
1:A:414:LYS:HG2	1:A:570:MET:HB3	1.66	0.76
1:B:416:ASN:OD1	1:B:561:VAL:HG12	1.85	0.75
1:A:273:VAL:CG2	1:A:274:PRO:HD3	2.18	0.74
1:B:172:MET:O	1:B:176:VAL:HG23	1.89	0.73
1:A:597:LEU:HA	1:A:703:ASP:OD2	1.89	0.72
1:A:140:ASP:OD2	1:A:168:GLN:HG2	1.90	0.72
1:A:616:SER:OG	1:A:617:ILE:N	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:GLY:O	1:B:150:THR:HB	1.90	0.71
1:B:533:GLU:OE2	1:B:576:THR:HG23	1.90	0.71
1:A:245:ALA:HB2	1:A:288:GLN:O	1.90	0.71
1:A:306:LEU:HD13	1:A:381:ARG:HB3	1.73	0.70
1:B:71:HIS:CG	1:B:72:PRO:HD2	2.27	0.70
1:B:71:HIS:CD2	1:B:72:PRO:HD2	2.27	0.70
1:B:420:LEU:HD22	1:B:498:HIS:HE1	1.55	0.69
1:A:474:VAL:HG22	1:A:503:ILE:HD11	1.74	0.69
1:B:261:TYR:CE1	1:B:263:ALA:HA	2.28	0.69
1:A:26:CYS:O	1:A:27:TYR:C	2.35	0.69
1:A:275:MET:HE2	1:A:276:LEU:CD1	2.23	0.68
1:A:302:GLU:HG2	1:A:333:TRP:HB3	1.74	0.68
1:A:652[B]:HIS:CD2	1:A:653:GLU:H	2.11	0.68
1:B:260:SER:OG	1:B:352:CYS:SG	2.50	0.68
1:A:599:ILE:HG22	1:A:702:ILE:HG23	1.75	0.68
1:B:248:ILE:CD1	1:B:297:PHE:HE2	2.07	0.68
1:A:478:ASN:ND2	1:A:595:ASN:OD1	2.27	0.68
1:B:362:VAL:CG2	1:B:366:GLU:HB3	2.24	0.67
1:B:397:GLN:HG3	1:B:403:PRO:HD2	1.76	0.67
1:A:265:THR:O	1:A:266:ASN:HB2	1.95	0.67
1:A:270:ASN:HB2	1:A:274:PRO:HG2	1.75	0.67
1:B:284:ARG:NH2	1:B:324:ARG:HB3	2.09	0.67
1:B:415:SER:O	1:B:418:GLN:HB2	1.95	0.67
1:B:170:MET:O	1:B:174:VAL:HG23	1.95	0.67
1:B:386:ALA:HB3	6:B:933:HOH:O	1.94	0.66
1:B:23:GLN:NE2	1:B:31:MET:HE2	2.10	0.66
1:B:475:ARG:HG2	1:B:546:LEU:HD11	1.78	0.66
1:B:374:TYR:HE2	1:B:379:ARG:NH2	1.93	0.66
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.77	0.65
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.62	0.65
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.79	0.65
1:A:275:MET:HE2	1:A:276:LEU:HD13	1.79	0.64
1:A:446:LEU:HB3	1:A:602:MET:HE2	1.80	0.64
1:A:298:ALA:HB2	1:A:428:LEU:HA	1.80	0.63
1:B:533:GLU:HG2	1:B:701:PHE:CZ	2.34	0.63
1:A:742:ARG:HE	1:A:742:ARG:CA	2.12	0.63
1:B:568:TYR:HB2	1:B:573:VAL:CG1	2.29	0.62
1:A:652[B]:HIS:CG	1:A:653:GLU:H	2.17	0.62
1:A:71:HIS:CE1	1:A:72:PRO:HD2	2.34	0.62
1:A:241:ILE:CG2	1:A:248:ILE:HD11	2.30	0.62
1:A:420:LEU:HD21	1:A:555:THR:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD22	1:B:125:LEU:HD12	1.82	0.62
1:B:93:VAL:HG13	1:B:96:ASP:HB2	1.81	0.61
1:B:315:LYS:HD2	1:B:326:ARG:HG2	1.82	0.61
1:B:689:LYS:HB2	4:B:810:SO4:O3	2.01	0.61
1:B:12:ARG:HH21	1:B:14:MET:HE3	1.65	0.60
1:A:429:CYS:HB2	1:A:431:GLU:OE2	2.01	0.60
1:B:302:GLU:HG2	1:B:333:TRP:HB3	1.84	0.60
1:A:71:HIS:ND1	1:A:72:PRO:HD2	2.17	0.60
1:B:23:GLN:HE22	1:B:31:MET:HE2	1.67	0.60
1:B:493:LEU:HD11	1:B:497:ARG:NH1	2.17	0.60
1:B:308:ILE:O	1:B:311:PHE:HB3	2.02	0.60
1:B:1:MET:HE1	1:B:47:LEU:HD12	1.83	0.60
1:B:94:PHE:CE1	1:B:172:MET:HB3	2.37	0.59
1:B:206:PHE:HB3	1:B:207:ASN:HD22	1.67	0.59
1:B:394:ILE:HD12	1:B:395:GLU:N	2.17	0.59
1:B:625:TYR:HD1	1:B:625:TYR:C	2.11	0.59
1:B:651:TRP:CD1	1:B:651:TRP:C	2.80	0.59
1:B:287:ASP:C	1:B:289:GLY:H	2.10	0.59
1:A:474:VAL:HG21	1:A:539:ALA:HA	1.84	0.59
1:B:37:ALA:O	1:B:41:MET:HG2	2.03	0.59
1:A:251:ALA:HB2	1:A:425:CYS:HB3	1.85	0.59
1:A:228:ILE:O	1:A:229:GLU:C	2.45	0.58
1:B:89:GLU:O	1:B:90:THR:HB	2.02	0.58
1:B:248:ILE:HD13	1:B:297:PHE:CE2	2.39	0.58
1:A:225:ASP:HB3	1:A:230:GLY:HA3	1.85	0.58
1:A:219:PHE:N	1:A:247:GLY:O	2.35	0.58
1:A:270:ASN:H	1:A:270:ASN:ND2	2.00	0.58
1:B:223:MET:HE2	1:B:231:ILE:HA	1.85	0.58
1:A:352:CYS:HB3	1:A:381:ARG:NH2	2.18	0.58
1:A:501:ILE:HG13	1:A:598:LEU:HA	1.84	0.57
1:A:214:GLN:HG3	1:A:244:SER:CB	2.34	0.57
1:A:94:PHE:CE1	1:A:98:MET:HE3	2.38	0.57
1:B:206:PHE:CB	1:B:207:ASN:HD22	2.17	0.57
1:B:408:LYS:HD3	6:B:924:HOH:O	2.04	0.57
5:B:807:ATP:O1B	5:B:807:ATP:C5'	2.52	0.57
1:A:698:ARG:O	1:A:702:ILE:HG13	2.04	0.57
1:B:117:ALA:H	1:B:210:THR:HA	1.69	0.57
1:B:195:GLU:C	1:B:196:ARG:HG3	2.29	0.57
1:A:315:LYS:HZ1	1:A:326:ARG:HA	1.70	0.57
1:B:248:ILE:HD13	1:B:297:PHE:HE2	1.70	0.57
1:B:553:TYR:HB3	1:B:594:ARG:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:CYS:O	1:B:443:VAL:HA	2.05	0.57
1:A:426:SER:OG	1:A:427:ASN:N	2.38	0.56
1:B:346:GLN:HG3	1:B:347:ASP:H	1.69	0.56
1:A:433:VAL:H	1:A:704:GLN:HB3	1.71	0.56
1:B:394:ILE:HD12	1:B:394:ILE:C	2.30	0.56
1:A:18:ILE:O	1:A:22:ILE:HG12	2.06	0.56
1:A:76:ILE:O	1:A:80:ARG:HG3	2.06	0.56
1:A:222:SER:OG	1:A:436:THR:OG1	2.22	0.56
1:A:441:VAL:HG13	1:A:490:GLU:HB3	1.86	0.56
1:A:14:MET:CE	1:A:15:PHE:HB3	2.33	0.56
1:B:83:VAL:HG11	1:B:140:ASP:HB3	1.86	0.55
1:B:18:ILE:HB	1:B:40:THR:HG23	1.87	0.55
1:B:673:PRO:HB2	1:B:675:ASP:OD1	2.06	0.55
1:A:219:PHE:CE2	1:A:443:VAL:HG22	2.42	0.55
1:B:443:VAL:CG2	1:B:491:ALA:HB1	2.37	0.55
1:B:166:ARG:HD2	1:B:169:HIS:CE1	2.42	0.55
1:B:675:ASP:OD1	1:B:675:ASP:N	2.39	0.55
1:A:432:ILE:HG22	1:A:434:GLU:HG3	1.89	0.54
1:B:248:ILE:CD1	1:B:297:PHE:CE2	2.90	0.54
1:A:471:LYS:HA	1:A:542:ALA:HB2	1.89	0.54
1:B:625:TYR:C	1:B:625:TYR:CD1	2.84	0.54
1:A:308:ILE:O	1:A:312:LEU:HD22	2.07	0.54
1:B:129:ASP:OD2	1:B:129:ASP:N	2.37	0.54
1:A:627:ARG:HG2	1:A:636:ILE:HD12	1.89	0.54
1:A:652[B]:HIS:CD2	1:A:653:GLU:N	2.76	0.54
1:B:541:GLU:O	1:B:542:ALA:C	2.49	0.54
1:A:310:GLU:CD	1:A:310:GLU:N	2.61	0.54
1:B:87:HIS:NE2	1:B:140:ASP:OD1	2.30	0.54
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.43	0.54
1:B:443:VAL:HG12	1:B:444:CYS:N	2.22	0.54
1:B:448:SER:HA	1:B:504:GLY:O	2.07	0.54
1:B:567:GLN:CD	1:B:703:ASP:HA	2.32	0.54
1:A:172:MET:O	1:A:176:VAL:HG22	2.07	0.53
1:B:256:ARG:HG3	1:B:354:ASN:HB2	1.90	0.53
1:A:695:ALA:HA	1:A:698:ARG:NH1	2.23	0.53
1:B:248:ILE:HD12	1:B:297:PHE:HE2	1.73	0.53
1:B:287:ASP:O	1:B:289:GLY:N	2.38	0.53
1:B:416:ASN:HA	1:B:560:PRO:HG2	1.91	0.53
1:B:79:ALA:HB2	1:B:145:TYR:N	2.23	0.53
1:B:94:PHE:HE1	1:B:98:MET:HE3	1.73	0.53
1:A:174:VAL:HG12	1:A:178:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LYS:NZ	1:A:326:ARG:HA	2.23	0.53
1:B:284:ARG:CZ	1:B:324:ARG:HB3	2.38	0.53
1:B:102:TYR:CG	1:B:121:LEU:HD12	2.44	0.53
1:A:315:LYS:NZ	1:A:328:LEU:O	2.42	0.52
1:B:624:ILE:HG22	1:B:664:GLY:HA2	1.91	0.52
1:B:727:GLY:O	1:B:730:GLN:HB2	2.08	0.52
1:A:479:LYS:HA	6:A:910:HOH:O	2.10	0.52
1:A:457:SER:C	1:A:459:HIS:H	2.17	0.52
1:B:602:MET:HE2	1:B:604:THR:HG22	1.90	0.52
1:A:212:ARG:O	1:A:214:GLN:N	2.37	0.52
1:B:326:ARG:O	1:B:327:ASP:HB2	2.08	0.52
1:B:687:SER:HB3	1:B:690:THR:OG1	2.09	0.52
1:B:696:ALA:O	1:B:699:GLY:N	2.42	0.52
1:B:64:ALA:HB3	1:B:78:ALA:HB2	1.90	0.52
1:B:275:MET:HE2	1:B:276:LEU:HD13	1.91	0.52
1:A:183:ILE:O	1:A:184:ASP:C	2.52	0.52
1:B:362:VAL:HG23	1:B:366:GLU:OE2	2.10	0.52
1:B:420:LEU:HD22	1:B:498:HIS:CE1	2.40	0.52
1:B:5:LYS:HE2	1:B:11:GLU:CD	2.34	0.52
1:A:27:TYR:O	1:A:80:ARG:NH2	2.42	0.51
1:B:346:GLN:CG	1:B:347:ASP:H	2.23	0.51
1:A:275:MET:HE2	1:A:276:LEU:HD12	1.92	0.51
1:B:394:ILE:HD11	1:B:717:TYR:CE1	2.45	0.51
1:A:198:PHE:CE2	1:A:473:VAL:HG22	2.45	0.51
1:A:382:LYS:HG2	1:A:383:VAL:N	2.26	0.51
1:A:189:THR:CG2	1:A:476:ASN:HD21	2.23	0.51
1:B:3:VAL:HG23	1:B:11:GLU:O	2.10	0.51
1:B:601:PRO:HG2	1:B:702:ILE:HD13	1.91	0.51
1:A:139:ARG:HD3	1:A:194:SER:HB2	1.91	0.51
1:A:310:GLU:HA	1:A:313:ASP:HB2	1.93	0.51
1:B:12:ARG:NH2	1:B:14:MET:HE3	2.26	0.51
1:B:602:MET:HB2	1:B:603:PRO:HD2	1.93	0.51
1:A:652[B]:HIS:CG	1:A:653:GLU:N	2.77	0.50
1:B:101:LEU:O	1:B:115:MET:HB2	2.11	0.50
1:B:212:ARG:HG2	1:B:485:TYR:CZ	2.46	0.50
1:A:195:GLU:O	1:A:196:ARG:HB2	2.11	0.50
1:A:402:THR:HB	1:A:403:PRO:HA	1.92	0.50
1:A:520:GLU:HB2	1:A:690:THR:HG21	1.92	0.50
1:B:454:TYR:HB2	1:B:461:TYR:CZ	2.46	0.50
1:B:464:LYS:O	1:B:468:GLU:HG2	2.11	0.50
1:B:443:VAL:HG23	1:B:491:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:VAL:CG2	1:A:366:GLU:HB2	2.42	0.50
1:B:22:ILE:HG23	1:B:77:LEU:HD21	1.94	0.50
1:B:474:VAL:HG21	1:B:539:ALA:HA	1.93	0.50
1:B:532:PHE:CE2	1:B:698:ARG:HD3	2.47	0.49
1:B:734:THR:HG22	1:B:736:MET:H	1.76	0.49
1:A:26:CYS:C	1:A:27:TYR:O	2.48	0.49
1:B:735:GLY:O	1:B:736:MET:HB2	2.11	0.49
1:B:206:PHE:HB3	1:B:207:ASN:ND2	2.27	0.49
1:B:261:TYR:CE2	1:B:266:ASN:O	2.66	0.49
1:B:420:LEU:CD2	1:B:498:HIS:HE1	2.23	0.49
1:B:202:SER:O	1:B:203:PRO:C	2.56	0.49
1:B:446:LEU:HD13	1:B:602:MET:HG3	1.94	0.49
1:A:26:CYS:O	1:A:27:TYR:O	2.30	0.49
1:A:242:SER:HB3	1:A:286:VAL:HG22	1.95	0.49
1:B:374:TYR:CE2	1:B:379:ARG:NH2	2.77	0.49
1:B:498:HIS:CE1	1:B:555:THR:HG21	2.48	0.49
1:A:333:TRP:CD1	1:A:408:LYS:HD2	2.48	0.49
1:A:716:ASN:O	1:A:719:LYS:N	2.46	0.49
1:A:71:HIS:CG	1:A:72:PRO:CD	2.97	0.48
1:B:441:VAL:O	1:B:491:ALA:HA	2.14	0.48
1:B:695:ALA:CB	1:B:708:LEU:HD11	2.39	0.48
1:A:482:ASP:OD1	1:A:499:ARG:NH2	2.47	0.48
1:A:102:TYR:CG	1:A:121:LEU:HD12	2.48	0.48
1:B:220:LEU:N	1:B:220:LEU:HD23	2.29	0.48
1:B:94:PHE:HB2	1:B:135:ILE:CD1	2.44	0.48
1:A:219:PHE:HB2	1:A:247:GLY:O	2.14	0.48
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.62	0.48
1:B:277:ARG:O	1:B:281:ASN:HB2	2.14	0.48
1:B:443:VAL:CG1	1:B:444:CYS:N	2.77	0.48
1:A:220:LEU:HG	1:A:442:ALA:HB3	1.95	0.48
1:B:4:ILE:O	1:B:53:THR:HG23	2.14	0.48
1:A:275:MET:CE	1:A:276:LEU:CD1	2.90	0.47
1:A:431:GLU:HG2	1:A:432:ILE:CD1	2.44	0.47
1:A:692:LEU:CD1	1:A:710:ILE:HD11	2.44	0.47
1:B:300:TYR:CE2	1:B:406:LEU:HD13	2.46	0.47
1:A:202:SER:OG	4:A:812:SO4:O4	2.29	0.47
1:A:307:ASP:C	1:A:310:GLU:OE1	2.57	0.47
1:A:432:ILE:CG2	1:A:434:GLU:HG3	2.44	0.47
1:B:652:HIS:CG	1:B:653:GLU:H	2.32	0.47
1:A:330:PHE:N	1:A:330:PHE:CD2	2.83	0.47
1:A:459:HIS:O	1:A:515:MET:HE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:SER:HB2	1:B:506:GLN:HG2	1.97	0.47
1:B:544:CYS:SG	1:B:587:LYS:HG2	2.54	0.47
1:B:237:GLN:O	1:B:241:ILE:HG13	2.14	0.47
1:A:690:THR:O	1:A:691:VAL:C	2.57	0.47
1:B:518:PRO:HB3	1:B:678:GLN:O	2.15	0.47
1:A:411:CYS:HA	1:A:733:LYS:HG2	1.95	0.47
1:B:27:TYR:HE1	1:B:80:ARG:NH1	2.13	0.47
1:B:273:VAL:HG21	1:B:310:GLU:HB3	1.97	0.47
1:A:427:ASN:HB2	6:A:903:HOH:O	2.14	0.47
1:A:443:VAL:CG1	1:A:444:CYS:N	2.52	0.47
1:B:130:ARG:NH1	1:B:187:ILE:HD13	2.29	0.47
1:B:257:ALA:HB1	1:B:306:LEU:HD23	1.97	0.46
1:B:137:TYR:HE2	1:B:169:HIS:NE2	2.13	0.46
1:A:14:MET:HE3	1:A:15:PHE:CB	2.35	0.46
1:B:610:ILE:HG22	1:B:611:LEU:HD23	1.96	0.46
1:A:202:SER:HB3	1:A:206:PHE:CE1	2.51	0.46
1:A:198:PHE:CD2	1:A:473:VAL:HG22	2.51	0.46
1:B:528:ASN:O	1:B:529:LYS:C	2.59	0.46
1:B:566:LEU:O	1:B:567:GLN:C	2.58	0.46
1:B:542:ALA:O	1:B:546:LEU:HD12	2.16	0.46
1:B:695:ALA:O	1:B:706:GLN:NE2	2.49	0.46
1:A:192:LEU:HD23	1:A:469:VAL:HG13	1.96	0.45
1:B:49:SER:O	1:B:51:VAL:N	2.49	0.45
1:B:94:PHE:HB2	1:B:135:ILE:HD13	1.98	0.45
1:B:261:TYR:HE2	1:B:266:ASN:O	1.98	0.45
1:B:79:ALA:O	1:B:83:VAL:HG23	2.16	0.45
1:B:199:THR:HG21	1:B:607:THR:HB	1.97	0.45
1:B:420:LEU:CD2	1:B:498:HIS:CE1	3.00	0.45
1:B:508:LEU:HD13	1:B:512:PHE:CE2	2.51	0.45
1:A:667:GLN:O	1:A:677:LYS:HE2	2.17	0.45
1:B:21:ARG:HD2	1:B:21:ARG:O	2.16	0.45
1:B:220:LEU:HD22	1:B:427:ASN:HB3	1.97	0.45
1:B:315:LYS:NZ	1:B:326:ARG:HB3	2.32	0.45
1:B:408:LYS:HE3	6:B:926:HOH:O	2.15	0.45
1:B:218:CYS:SG	1:B:432:ILE:HG13	2.56	0.45
1:A:158:LYS:HD3	1:A:163:VAL:HG23	1.98	0.45
1:A:681:LYS:HB2	1:A:686:ILE:HD11	1.99	0.45
1:B:223:MET:HE3	1:B:234:THR:HB	1.97	0.45
1:A:71:HIS:ND1	1:A:72:PRO:CD	2.80	0.45
1:B:622:SER:OG	1:B:664:GLY:HA3	2.15	0.45
1:A:603:PRO:O	1:A:604:THR:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:VAL:N	1:B:298:ALA:O	2.47	0.45
1:A:281:ASN:HD22	1:A:281:ASN:HA	1.52	0.44
1:A:665:SER:OG	1:A:667:GLN:HG2	2.17	0.44
1:B:22:ILE:CG2	1:B:77:LEU:HD21	2.48	0.44
1:B:652:HIS:CD2	1:B:653:GLU:H	2.36	0.44
1:B:493:LEU:CD1	1:B:497:ARG:NH1	2.80	0.44
1:A:215:LEU:HD11	1:A:483:ILE:HD11	1.99	0.44
1:A:519:PHE:CE2	1:A:619:PRO:HG3	2.53	0.44
1:B:287:ASP:C	1:B:289:GLY:N	2.75	0.44
1:A:602:MET:SD	1:A:602:MET:N	2.89	0.44
1:B:207:ASN:O	1:B:210:THR:OG1	2.28	0.44
1:A:275:MET:CE	1:A:276:LEU:HD12	2.48	0.44
1:A:363:TRP:CH2	1:A:413:ARG:HA	2.53	0.44
1:B:2:HIS:ND1	1:B:10:GLN:HG2	2.33	0.44
1:B:451:LEU:CD1	1:B:508:LEU:HD23	2.48	0.44
1:A:742:ARG:HE	1:A:742:ARG:C	2.26	0.44
1:B:214:GLN:HG3	1:B:244:SER:HB3	2.00	0.44
1:B:312:LEU:HD21	1:B:393:ILE:HG12	1.99	0.44
1:B:501:ILE:HG13	1:B:598:LEU:HA	1.99	0.44
1:A:742:ARG:NE	1:A:742:ARG:CA	2.71	0.43
1:B:451:LEU:HD13	1:B:508:LEU:HD23	2.00	0.43
1:A:336:ASP:O	1:A:337:LEU:C	2.60	0.43
1:B:120:THR:O	1:B:124:VAL:HG23	2.18	0.43
1:A:404:TYR:CZ	1:A:737:TYR:HE1	2.37	0.43
1:A:308:ILE:O	1:A:311:PHE:HB3	2.18	0.43
1:B:136:ILE:HB	1:B:139:ARG:HG3	2.00	0.43
1:B:708:LEU:O	1:B:737:TYR:HB3	2.18	0.43
1:A:120:THR:O	1:A:121:LEU:C	2.60	0.43
1:A:216:SER:HB3	1:A:443:VAL:CG1	2.48	0.43
1:B:226:ASP:OD1	1:B:256:ARG:HD2	2.18	0.43
1:A:337:LEU:HD22	1:A:337:LEU:HA	1.74	0.43
1:B:346:GLN:HG3	1:B:347:ASP:N	2.33	0.43
1:B:653:GLU:O	1:B:655:MET:N	2.51	0.43
1:A:252:VAL:HG12	1:A:300:TYR:O	2.18	0.43
1:B:283:ALA:HB2	1:B:297:PHE:CD1	2.54	0.43
1:B:362:VAL:HG23	1:B:366:GLU:HB3	1.98	0.43
1:B:523:GLU:OE2	1:B:523:GLU:N	2.31	0.42
1:A:216:SER:CB	1:A:443:VAL:CG1	2.96	0.42
1:A:265:THR:CG2	1:B:288:GLN:HG2	2.50	0.42
1:A:256:ARG:HA	1:A:353:PRO:HD2	2.01	0.42
1:A:263:ALA:HB3	2:A:806:TTP:O1G	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ASP:OD2	1:A:462:ASP:C	2.63	0.42
1:B:256:ARG:HH21	1:B:262:ILE:HA	1.85	0.42
1:B:523:GLU:H	1:B:523:GLU:CD	2.21	0.42
1:B:3:VAL:HG22	1:B:13:VAL:HG22	2.01	0.42
1:B:551:GLY:O	1:B:594:ARG:NH1	2.50	0.42
1:A:20:SER:O	1:A:23:GLN:HB3	2.19	0.42
1:A:54:VAL:HG13	1:A:55:GLU:HG3	2.00	0.42
1:A:106:ASN:HD21	1:A:109:ASN:H	1.67	0.42
1:A:265:THR:HG21	1:B:288:GLN:HG2	2.01	0.42
1:A:414:LYS:HD2	1:A:571:TRP:NE1	2.35	0.42
1:B:256:ARG:HD2	2:B:805:TTP:H4'	1.91	0.42
1:B:483:ILE:HD12	1:B:483:ILE:HA	1.92	0.42
1:B:611:LEU:HB2	1:B:613:ASN:HD22	1.85	0.42
1:A:627:ARG:CG	1:A:636:ILE:HD12	2.49	0.42
1:B:112:HIS:CE1	1:B:114:PRO:HG3	2.55	0.42
1:B:515:MET:O	1:B:516:ARG:HB2	2.18	0.42
1:B:83:VAL:CG1	1:B:140:ASP:HB3	2.48	0.42
1:A:241:ILE:HG22	1:A:248:ILE:HD11	2.01	0.42
1:B:414:LYS:HG2	1:B:570:MET:HB2	2.01	0.42
1:B:441:VAL:HG12	1:B:490:GLU:HB2	2.02	0.42
1:A:71:HIS:CG	1:A:72:PRO:HD2	2.55	0.41
1:B:516:ARG:HH21	1:B:679:LEU:CD1	2.33	0.41
1:B:645:LEU:HD23	1:B:645:LEU:HA	1.87	0.41
1:A:106:ASN:ND2	1:A:109:ASN:H	2.18	0.41
1:B:219:PHE:CE2	1:B:443:VAL:HG22	2.55	0.41
1:B:222:SER:HA	1:B:251:ALA:HB3	2.02	0.41
1:B:308:ILE:HG13	1:B:312:LEU:HD13	2.02	0.41
1:B:368:GLU:O	1:B:369:LYS:C	2.63	0.41
1:B:416:ASN:CG	1:B:561:VAL:HG12	2.45	0.41
1:B:445:ASN:ND2	1:B:445:ASN:N	2.68	0.41
1:B:626:THR:HG22	1:B:635:GLN:HA	2.01	0.41
1:A:446:LEU:CD2	1:A:446:LEU:N	2.43	0.41
1:B:67:LEU:O	1:B:70:LYS:N	2.52	0.41
1:A:238:CYS:O	1:A:239:ALA:C	2.62	0.41
1:A:330:PHE:N	1:A:330:PHE:HD2	2.19	0.41
1:B:38:GLN:NE2	1:B:38:GLN:HA	2.35	0.41
1:B:300:TYR:HE2	1:B:406:LEU:CD1	2.30	0.41
1:B:336:ASP:O	1:B:337:LEU:C	2.62	0.41
5:B:807:ATP:H5'2	5:B:807:ATP:PB	2.60	0.41
1:A:451:LEU:HG	1:A:505:VAL:HB	2.02	0.41
1:A:689:LYS:HB2	4:A:809:SO4:O1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:PHE:N	1:B:330:PHE:CD2	2.88	0.41
1:A:171:LEU:HD23	1:A:194:SER:HA	2.03	0.41
1:A:694:MET:HE2	1:A:694:MET:HB3	1.77	0.41
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.83	0.41
1:A:270:ASN:ND2	1:A:270:ASN:N	2.67	0.41
1:A:520:GLU:HG2	6:A:914:HOH:O	2.21	0.41
1:A:692:LEU:HD13	1:A:710:ILE:HD11	2.03	0.41
1:B:253:SER:OG	1:B:301:LEU:HD23	2.21	0.41
1:B:570:MET:HE2	1:B:570:MET:HB3	1.93	0.41
1:B:705:SER:OG	1:B:706:GLN:N	2.54	0.41
1:A:405:MET:C	1:A:406:LEU:HD12	2.46	0.41
1:B:128:LYS:O	1:B:132:ASN:ND2	2.49	0.41
1:B:471:LYS:HA	1:B:542:ALA:HB2	2.02	0.41
1:A:104:TYR:HD2	1:A:113:SER:HB2	1.86	0.40
1:A:192:LEU:HD22	1:A:472:VAL:HG11	2.03	0.40
1:A:448:SER:HB2	1:A:506:GLN:HG2	2.03	0.40
1:A:725:PHE:O	1:A:729:LYS:HB2	2.21	0.40
1:B:365:GLU:H	1:B:365:GLU:HG2	1.43	0.40
1:A:301:LEU:HD12	1:A:311:PHE:CG	2.56	0.40
1:A:329:PHE:C	1:A:330:PHE:HD2	2.29	0.40
1:B:151:LEU:HD23	1:B:155:TYR:HB2	2.03	0.40
1:B:337:LEU:HD23	1:B:337:LEU:HA	1.95	0.40
1:A:215:LEU:CD1	1:A:483:ILE:HD11	2.51	0.40
1:A:695:ALA:CB	1:A:708:LEU:HD11	2.51	0.40
1:A:727:GLY:CA	1:A:732:LEU:HD12	2.51	0.40
1:B:1:MET:HB3	1:B:1:MET:HE2	1.69	0.40
1:B:233:ASP:O	1:B:234:THR:C	2.64	0.40
1:B:533:GLU:HG2	1:B:701:PHE:CE1	2.55	0.40
1:A:243:LYS:NZ	2:B:805:TTP:O1B	2.52	0.40
1:A:699:GLY:C	1:A:701:PHE:H	2.28	0.40
1:B:93:VAL:HG23	1:B:132:ASN:OD1	2.22	0.40
1:A:448:SER:HA	1:A:504:GLY:O	2.22	0.40
1:B:41:MET:HA	1:B:41:MET:HE2	2.04	0.40
1:B:325:ALA:C	1:B:326:ARG:HG3	2.46	0.40
1:B:389:LEU:O	1:B:390:TRP:C	2.64	0.40
1:B:477:LEU:HD23	1:B:477: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	710/792 (90%)	636 (90%)	61 (9%)	13 (2%)	6	26
1	B	716/792 (90%)	616 (86%)	82 (12%)	18 (2%)	4	20
All	All	1426/1584 (90%)	1252 (88%)	143 (10%)	31 (2%)	5	22

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
1	B	130	ARG
1	B	288	GLN
1	B	316	LYS
1	B	327	ASP
1	B	653	GLU
1	B	654	GLU
1	A	245	ALA
1	A	444	CYS
1	A	458	GLU
1	A	605	ALA
1	A	616	SER
1	A	713	ALA
1	A	737	TYR
1	B	50	GLY
1	B	484	ASN
1	B	736	MET
1	B	128	LYS
1	B	258	THR
1	B	313	ASP
1	B	576	THR
1	B	661	ALA
1	B	737	TYR
1	A	112	HIS
1	A	196	ARG

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Mol	Chain	Res	Type
1	B	537	TYR
1	A	49	SER
1	A	265	THR
1	B	303	PRO
1	B	245	ALA
1	A	212	ARG

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	586/693 (85%)	509 (87%)	77 (13%)	4	17
1	B	593/693 (86%)	490 (83%)	103 (17%)	2	9
All	All	1179/1386 (85%)	999 (85%)	180 (15%)	3	12

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	19	THR
1	A	41	MET
1	A	43	VAL
1	A	53	THR
1	A	54	VAL
1	A	55	GLU
1	A	58	THR
1	A	59	LEU
1	A	69	THR
1	A	80	ARG
1	A	84	SER
1	A	93	VAL
1	A	106	ASN
1	A	119	SER
1	A	121	LEU
1	A	130	ARG

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Mol	Chain	Res	Type
1	A	149	LYS
1	A	154	SER
1	A	158	LYS
1	A	171	LEU
1	A	176	VAL
1	A	181	GLU
1	A	187	ILE
1	A	210	THR
1	A	217	SER
1	A	220	LEU
1	A	222	SER
1	A	242	SER
1	A	250	VAL
1	A	252	VAL
1	A	253	SER
1	A	265	THR
1	A	270	ASN
1	A	276	LEU
1	A	281	ASN
1	A	286	VAL
1	A	287	ASP
1	A	288	GLN
1	A	301	LEU
1	A	310	GLU
1	A	312	LEU
1	A	315	LYS
1	A	337	LEU
1	A	361	GLU
1	A	389	LEU
1	A	434	GLU
1	A	441	VAL
1	A	445	ASN
1	A	446	LEU
1	A	449	LEU
1	A	455	VAL
1	A	480	ILE
1	A	493	LEU
1	A	499	ARG
1	A	508	LEU
1	A	567	GLN
1	A	583	VAL
1	A	615	GLU

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Mol	Chain	Res	Type
1	A	617	ILE
1	A	621	THR
1	A	637	VAL
1	A	648	ARG
1	A	653	GLU
1	A	656	LYS
1	A	689	LYS
1	A	692	LEU
1	A	693	LYS
1	A	697	GLU
1	A	705	SER
1	A	712	ILE
1	A	716	ASN
1	A	720	LEU
1	A	722	SER
1	A	729	LYS
1	A	739	LEU
1	A	742	ARG
1	B	3	VAL
1	B	5	LYS
1	B	12	ARG
1	B	14	MET
1	B	16	ASP
1	B	21	ARG
1	B	25	LEU
1	B	27	TYR
1	B	32	ASP
1	B	38	GLN
1	B	40	THR
1	B	44	ILE
1	B	47	LEU
1	B	49	SER
1	B	54	VAL
1	B	55	GLU
1	B	56	LEU
1	B	58	THR
1	B	67	LEU
1	B	85	ASN
1	B	88	LYS
1	B	92	LYS
1	B	93	VAL
1	B	109	ASN

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Mol	Chain	Res	Type
1	B	121	LEU
1	B	123	ILE
1	B	125	LEU
1	B	127	ASN
1	B	129	ASP
1	B	149	LYS
1	B	153	ARG
1	B	154	SER
1	B	159	ILE
1	B	162	LYS
1	B	171	LEU
1	B	175	SER
1	B	188	GLU
1	B	196	ARG
1	B	216	SER
1	B	218	CYS
1	B	220	LEU
1	B	229	GLU
1	B	234	THR
1	B	241	ILE
1	B	252	VAL
1	B	256	ARG
1	B	265	THR
1	B	272	LEU
1	B	276	LEU
1	B	277	ARG
1	B	286	VAL
1	B	288	GLN
1	B	301	LEU
1	B	313	ASP
1	B	314	LEU
1	B	324	ARG
1	B	326	ARG
1	B	337	LEU
1	B	359	LEU
1	B	361	GLU
1	B	365	GLU
1	B	366	GLU
1	B	383	VAL
1	B	389	LEU
1	B	410	SER
1	B	420	LEU

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Mol	Chain	Res	Type
1	B	426	SER
1	B	439	ASP
1	B	441	VAL
1	B	445	ASN
1	B	457	SER
1	B	503	ILE
1	B	506	GLN
1	B	508	LEU
1	B	525	GLN
1	B	541	GLU
1	B	546	LEU
1	B	561	VAL
1	B	570	MET
1	B	573	VAL
1	B	588	ILE
1	B	597	LEU
1	B	615	GLU
1	B	617	ILE
1	B	618	GLU
1	B	625	TYR
1	B	626	THR
1	B	655	MET
1	B	657	ASN
1	B	671	GLU
1	B	675	ASP
1	B	678	GLN
1	B	683	VAL
1	B	685	GLU
1	B	690	THR
1	B	692	LEU
1	B	697	GLU
1	B	707	SER
1	B	708	LEU
1	B	719	LYS
1	B	723	MET
1	B	739	LEU
1	B	740	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN

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Mol	Chain	Res	Type
1	A	85	ASN
1	A	106	ASN
1	A	200	HIS
1	A	211	ASN
1	A	270	ASN
1	A	281	ASN
1	A	354	ASN
1	A	387	GLN
1	A	388	GLN
1	A	418	GLN
1	A	476	ASN
1	A	478	ASN
1	A	567	GLN
1	A	595	ASN
1	A	716	ASN
1	B	23	GLN
1	B	38	GLN
1	B	207	ASN
1	B	281	ASN
1	B	445	ASN
1	B	459	HIS
1	B	525	GLN
1	B	530	GLN
1	B	614	ASN
1	B	623	ASN
1	B	652	HIS
1	B	711	HIS

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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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
4	SO4	B	813	-	4,4,4	0.27	0	6,6,6	0.56	0
4	SO4	B	810	-	4,4,4	0.31	0	6,6,6	0.30	0
4	SO4	A	808	-	4,4,4	0.29	0	6,6,6	0.41	0
4	SO4	A	812	-	4,4,4	0.25	0	6,6,6	0.39	0
4	SO4	A	809	-	4,4,4	0.24	0	6,6,6	0.30	0
2	TTP	A	806	3	29,30,30	1.32	6 (20%)	43,47,47	1.93	9 (20%)
5	ATP	B	807	3	32,33,33	1.96	8 (25%)	48,52,52	2.06	16 (33%)
4	SO4	B	811	-	4,4,4	0.28	0	6,6,6	0.53	0
2	TTP	B	805	3	29,30,30	1.41	6 (20%)	43,47,47	1.68	7 (16%)

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	TTP	A	806	3	-	11/22/34/34	0/2/2/2
5	ATP	B	807	3	-	5/22/38/38	0/3/3/3
2	TTP	B	805	3	-	1/22/34/34	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	807	ATP	PB-O3B	5.59	1.65	1.59
5	B	807	ATP	C5-C4	4.89	1.47	1.39
5	B	807	ATP	PA-O3A	3.77	1.63	1.59
5	B	807	ATP	PB-O3A	3.52	1.63	1.59
5	B	807	ATP	C5-C6	3.05	1.49	1.41
2	A	806	TTP	C4-C5	2.96	1.49	1.44
2	A	806	TTP	C4-N3	-2.88	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	805	TTP	C6-C5	2.85	1.39	1.34
2	B	805	TTP	C4-C5	2.81	1.49	1.44
2	A	806	TTP	C2-N1	2.54	1.42	1.38
2	B	805	TTP	C6-N1	-2.53	1.33	1.38
2	B	805	TTP	C4-N3	-2.48	1.34	1.38
2	B	805	TTP	PB-O3B	2.48	1.62	1.59
5	B	807	ATP	O4'-C1'	2.36	1.47	1.42
2	A	806	TTP	C6-N1	-2.36	1.34	1.38
2	A	806	TTP	C2-N3	-2.28	1.34	1.38
5	B	807	ATP	C8-N7	2.26	1.36	1.31
2	B	805	TTP	C2-N3	-2.17	1.34	1.38
5	B	807	ATP	C5-N7	-2.10	1.35	1.39
2	A	806	TTP	C6-C5	2.01	1.37	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	807	ATP	C5-C4-N3	-5.73	118.83	126.72
2	A	806	TTP	C4-N3-C2	-5.35	120.32	127.34
2	A	806	TTP	C5-C6-N1	-5.11	117.76	123.31
2	A	806	TTP	N3-C2-N1	4.74	121.06	114.89
2	B	805	TTP	C4-N3-C2	-4.66	121.22	127.34
5	B	807	ATP	C4-C5-N7	-4.32	105.64	110.58
2	B	805	TTP	C5-C6-N1	-4.19	118.76	123.31
2	B	805	TTP	N3-C2-N1	4.16	120.30	114.89
2	A	806	TTP	C5-C4-N3	4.15	118.94	115.32
2	B	805	TTP	C5-C4-N3	4.09	118.88	115.32
5	B	807	ATP	N3-C4-N9	4.08	134.11	127.17
2	A	806	TTP	O2B-PB-O3B	3.91	117.83	107.27
5	B	807	ATP	C2-N3-C4	3.42	120.18	111.83
5	B	807	ATP	O4'-C1'-N9	3.31	114.45	108.09
5	B	807	ATP	O4'-C4'-C5'	3.11	119.31	109.33
5	B	807	ATP	C5-N7-C8	3.09	108.31	103.45
5	B	807	ATP	O2B-PB-O3B	-3.08	98.94	107.27
2	B	805	TTP	O4-C4-C5	-2.83	121.67	124.92
2	A	806	TTP	O2B-PB-O3A	2.75	114.71	107.27
2	A	806	TTP	O4-C4-C5	-2.63	121.90	124.92
2	A	806	TTP	C5M-C5-C6	-2.59	119.35	122.85
5	B	807	ATP	C6-C5-N7	2.58	137.06	132.09
5	B	807	ATP	O3G-PG-O2G	2.58	117.47	107.80
5	B	807	ATP	O3G-PG-O1G	2.47	120.45	110.83
5	B	807	ATP	N3-C2-N1	-2.46	124.86	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	805	TTP	C5M-C5-C4	2.42	121.37	118.78
5	B	807	ATP	C4-N9-C8	2.39	108.25	105.74
5	B	807	ATP	N9-C8-N7	-2.25	110.74	113.94
2	A	806	TTP	C6-C5-C4	2.17	119.81	118.02
5	B	807	ATP	C2'-C1'-N9	-2.14	107.98	113.30
2	B	805	TTP	O2B-PB-O3B	2.11	112.98	107.27
5	B	807	ATP	O4'-C4'-C3'	-2.03	101.13	105.15

There are no chirality outliers.

All (17) torsion outliers are listed below:

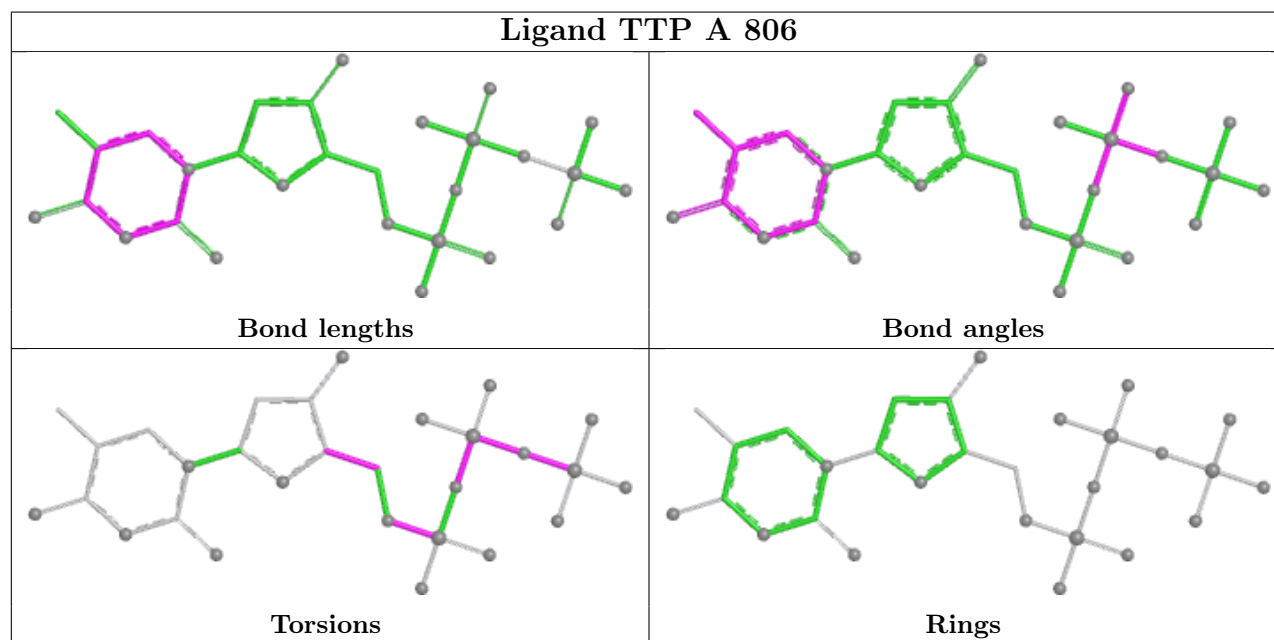
Mol	Chain	Res	Type	Atoms
2	A	806	TTP	C5'-O5'-PA-O1A
2	A	806	TTP	C5'-O5'-PA-O2A
2	A	806	TTP	C5'-O5'-PA-O3A
5	B	807	ATP	C5'-O5'-PA-O1A
5	B	807	ATP	C5'-O5'-PA-O2A
5	B	807	ATP	C5'-O5'-PA-O3A
2	A	806	TTP	O4'-C4'-C5'-O5'
2	A	806	TTP	C3'-C4'-C5'-O5'
2	A	806	TTP	PB-O3B-PG-O3G
2	B	805	TTP	PA-O3A-PB-O2B
2	A	806	TTP	PA-O3A-PB-O2B
5	B	807	ATP	C4'-C5'-O5'-PA
2	A	806	TTP	PA-O3A-PB-O1B
2	A	806	TTP	PG-O3B-PB-O1B
2	A	806	TTP	PB-O3B-PG-O2G
2	A	806	TTP	PG-O3B-PB-O2B
5	B	807	ATP	PG-O3B-PB-O2B

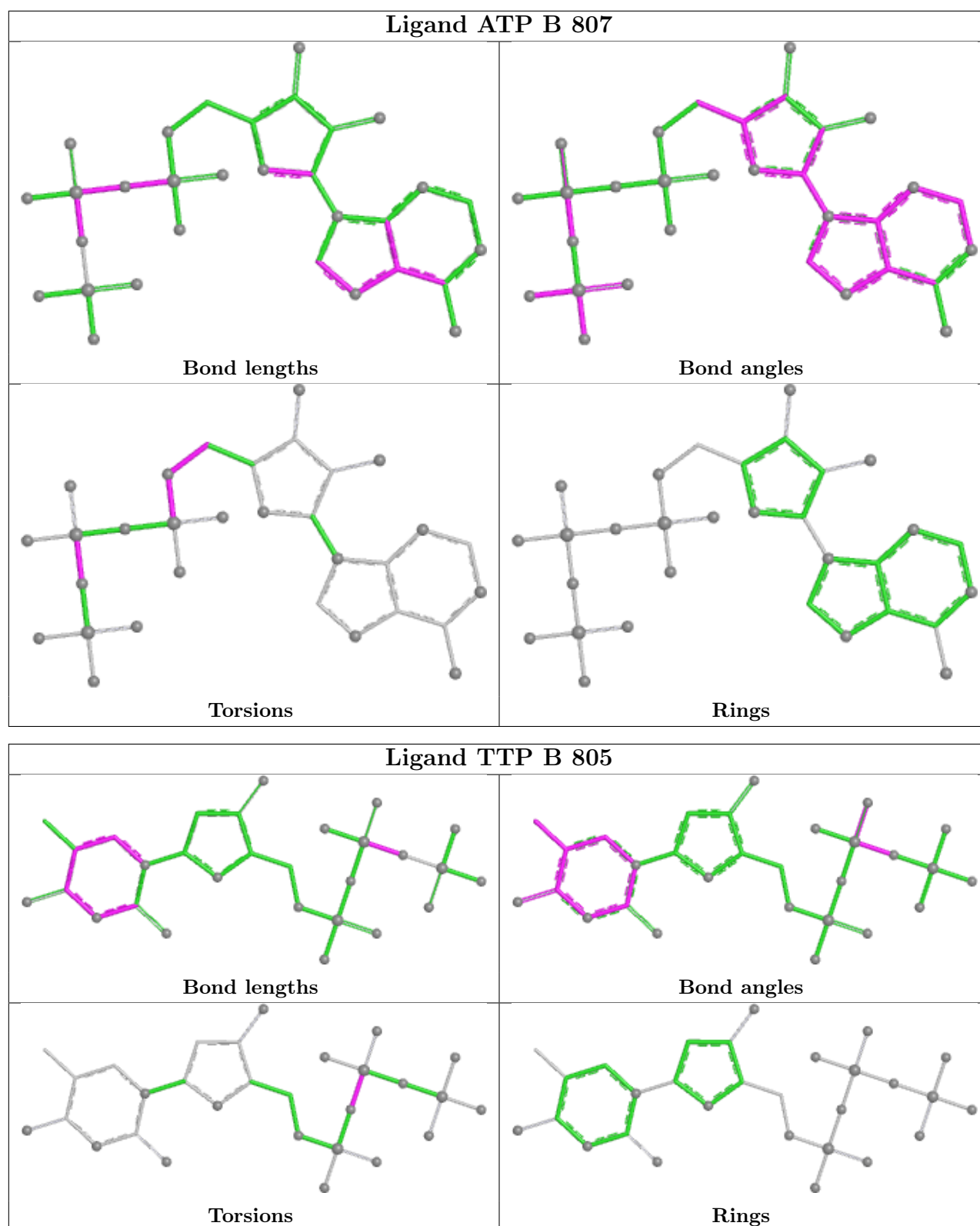
There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	810	SO4	1	0
4	A	812	SO4	1	0
4	A	809	SO4	1	0
2	A	806	TTP	1	0
5	B	807	ATP	3	0
2	B	805	TTP	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	715/792 (90%)	-0.54	3 (0%)	88 76	13, 61, 81, 110	3 (0%)
1	B	724/792 (91%)	-0.52	1 (0%)	92 86	46, 65, 94, 126	0
All	All	1439/1584 (90%)	-0.53	4 (0%)	90 80	13, 63, 90, 126	3 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	8.5
1	A	218	CYS	6.5
1	B	634	PHE	2.6
1	A	652[A]	HIS	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	MG	B	804	1/1	0.85	0.15	47,47,47,47	0

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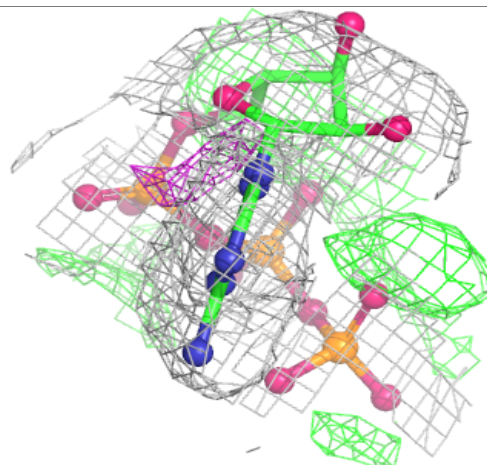
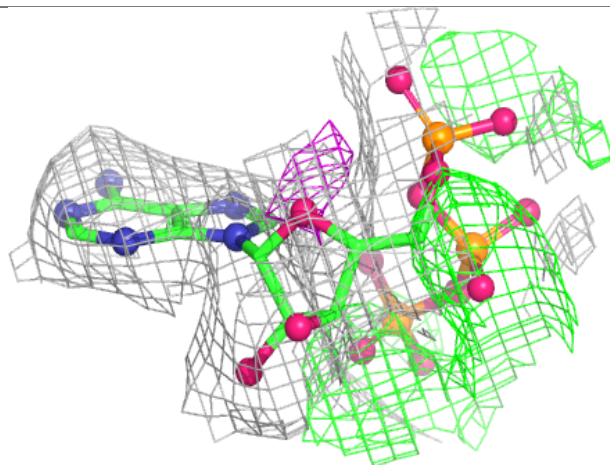
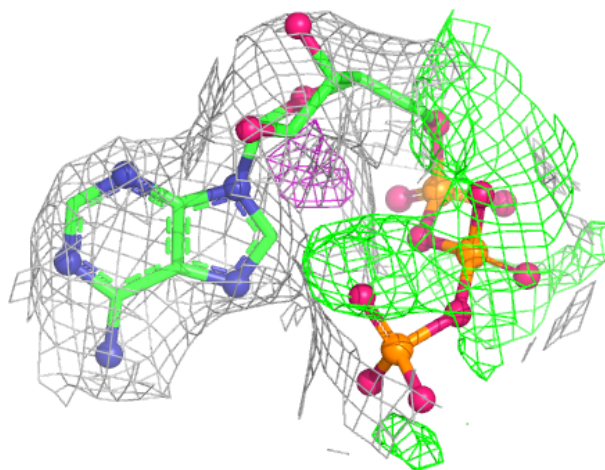
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	803	1/1	0.86	0.19	42,42,42,42	0
4	SO4	A	809	5/5	0.86	0.08	127,127,127,127	0
5	ATP	B	807	31/31	0.87	0.10	65,69,76,76	0
3	MG	A	801	1/1	0.88	0.13	56,56,56,56	0
4	SO4	B	813	5/5	0.90	0.07	70,70,72,72	0
4	SO4	B	811	5/5	0.90	0.08	99,100,100,100	0
3	MG	B	802	1/1	0.91	0.08	62,62,62,62	0
4	SO4	A	812	5/5	0.92	0.09	83,83,85,86	0
4	SO4	B	810	5/5	0.93	0.06	79,79,80,81	0
4	SO4	A	808	5/5	0.93	0.08	86,87,87,87	0
2	TTP	B	805	29/29	0.96	0.07	72,75,83,85	0
2	TTP	A	806	29/29	0.96	0.07	59,63,74,75	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.

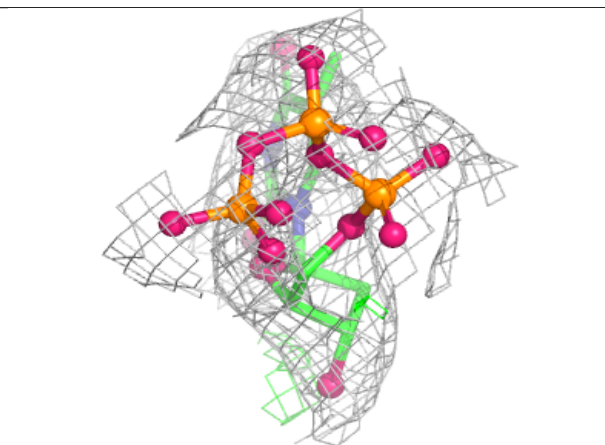
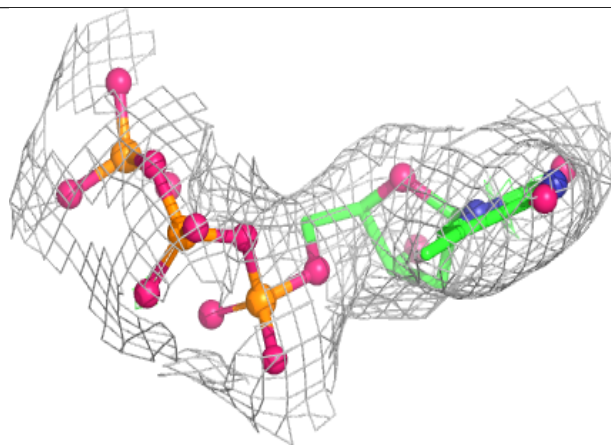
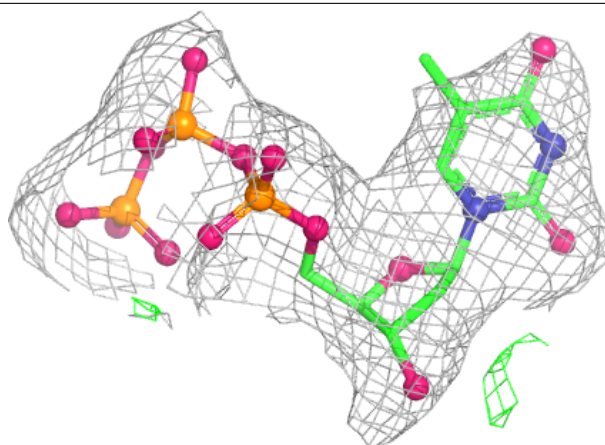
Electron density around ATP B 807:

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

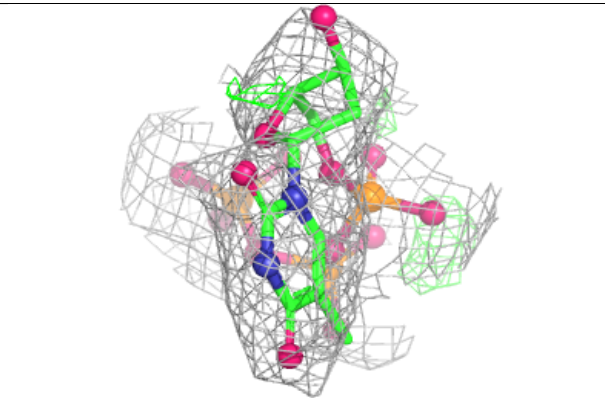
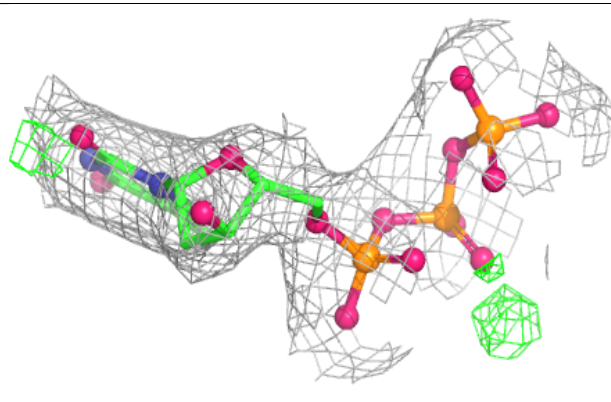
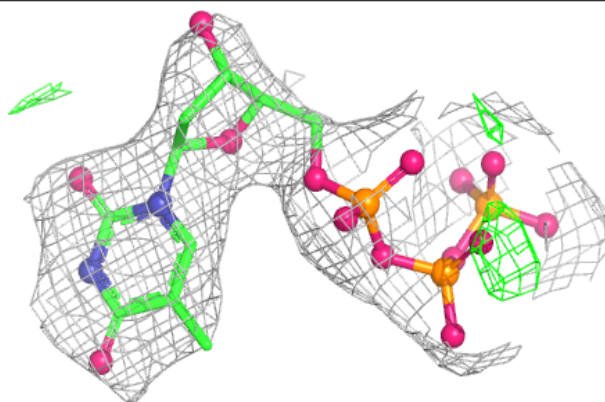


Electron density around TTP B 805:

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

**Electron density around TTP A 806:**

$2mF_o-DF_c$ (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.