



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:49 AM UTC

PDB ID : 3HNF / pdb_00003hnf
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effectors TTP and dATP
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.
Deposited on : 2009-05-31
Resolution : 3.16 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

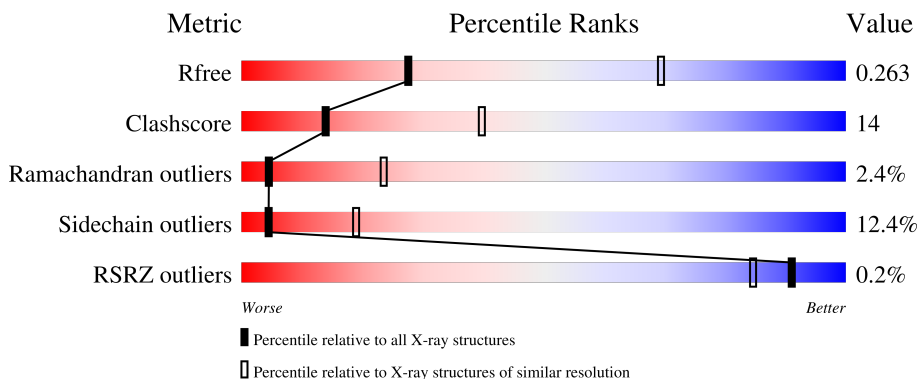
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 11549 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.

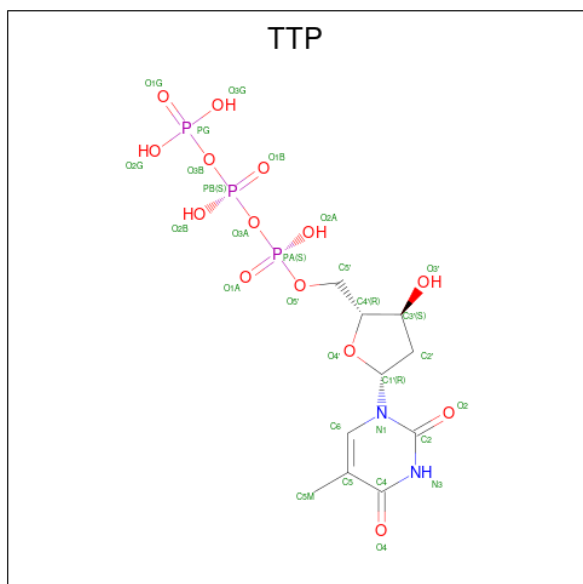
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	6	0	0
			5596	3579	925	1059	33			
1	B	737	Total	C	N	O	S	0	0	0
			5795	3698	980	1083	34			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

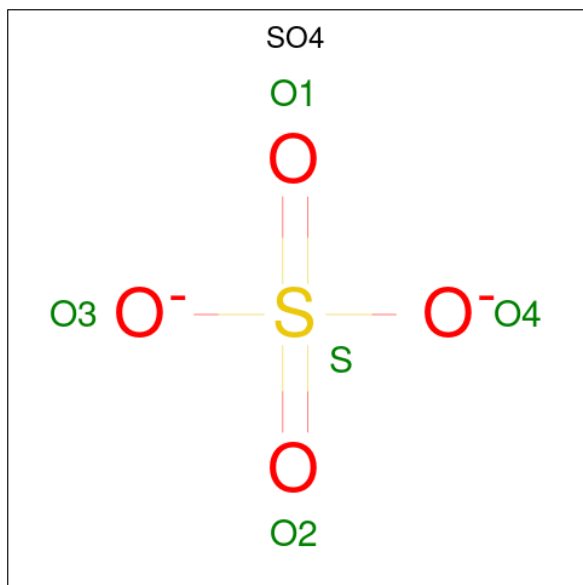
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



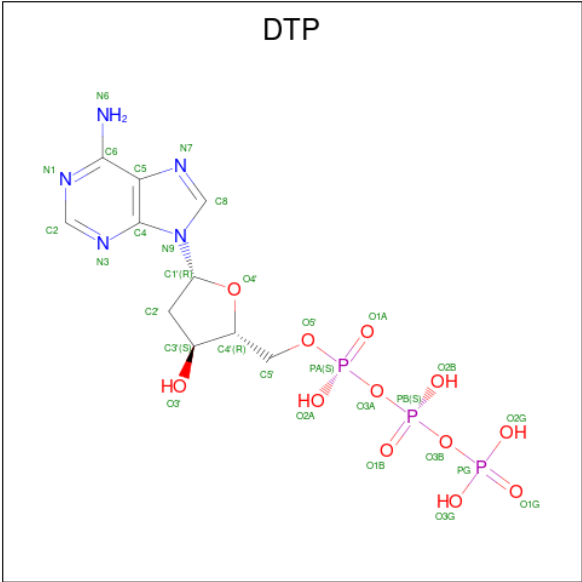
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
3	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- 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	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	22	Total O	0	0
			22 22		
6	B	26	Total O	0	0
			26 26		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.86Å 114.39Å 220.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.86 – 3.16 40.86 – 3.16	Depositor EDS
% Data completeness (in resolution range)	89.4 (40.86-3.16) 89.3 (40.86-3.16)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.260 0.185 , 0.263	Depositor DCC
R_{free} test set	1335 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11549	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: TTP, MG, SO4, DTP

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	0.73	1/5721 (0.0%)	1.03	15/7782 (0.2%)
1	B	0.71	0/5920	1.01	8/8035 (0.1%)
All	All	0.72	1/11641 (0.0%)	1.02	23/15817 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	VAL	CA-CB	5.26	1.60	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	GLN	N-CA-C	8.61	119.61	108.34
1	A	443	VAL	CB-CA-C	-6.30	102.56	111.19
1	A	53	THR	N-CA-C	6.27	124.15	110.80
1	B	425	CYS	N-CA-C	6.16	116.69	108.38
1	A	669	ILE	CA-C-N	5.91	125.61	119.05
1	A	669	ILE	C-N-CA	5.91	125.61	119.05
1	B	533	GLU	N-CA-C	-5.69	104.77	110.97
1	A	533	GLU	N-CA-C	-5.68	105.09	111.28
1	A	554	GLU	N-CA-C	5.65	119.43	112.54
1	B	623	ASN	N-CA-C	-5.60	106.45	113.28
1	A	486	TYR	CA-C-N	5.50	125.02	119.19
1	A	486	TYR	C-N-CA	5.50	125.02	119.19
1	B	76	ILE	N-CA-C	-5.42	105.09	111.00
1	A	549	GLU	N-CA-C	5.33	117.17	111.36
1	B	625	TYR	N-CA-C	5.31	116.07	108.74
1	A	327	ASP	N-CA-C	-5.29	99.53	110.80
1	A	602	MET	CA-C-N	5.26	125.32	119.32
1	A	602	MET	C-N-CA	5.26	125.32	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	ALA	N-CA-C	-5.20	105.69	111.36
1	A	207	ASN	N-CA-C	5.17	120.44	113.72
1	B	440	GLU	N-CA-C	5.08	116.59	107.80
1	B	250	VAL	N-CA-C	5.01	115.93	108.46
1	B	334	ILE	N-CA-C	5.01	113.44	107.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5596	0	5436	165	0
1	B	5795	0	5687	167	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	13	4	0
3	B	29	0	13	6	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
5	B	30	0	12	1	0
6	A	22	0	0	0	0
6	B	26	0	0	1	0
All	All	11549	0	11161	326	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 14.

All (326) 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:219:PHE:C	1:A:220:LEU:HD23	1.40	1.46
1:A:443:VAL:HG12	1:A:444:CYS:N	1.67	1.10
1:A:220:LEU:HD23	1:A:220:LEU:N	1.48	1.09
1:A:219:PHE:C	1:A:220:LEU:CD2	2.30	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ASN:OD1	1:B:561:VAL:CG2	2.09	1.00
1:B:130:ARG:HG2	1:B:130:ARG:HH11	1.30	0.97
1:B:90:THR:HG21	1:B:166:ARG:HG3	1.47	0.95
1:A:443:VAL:CG1	1:A:444:CYS:N	2.29	0.94
1:A:220:LEU:N	1:A:220:LEU:CD2	2.30	0.92
1:B:689:LYS:HG2	4:B:809:SO4:O1	1.71	0.90
1:A:742:ARG:HH11	1:A:742:ARG:HB2	1.39	0.87
1:B:223:MET:CE	1:B:231:ILE:HA	2.04	0.87
1:B:416:ASN:OD1	1:B:561:VAL:HG22	1.74	0.86
1:B:223:MET:HE2	1:B:231:ILE:HA	1.57	0.85
1:A:92:LYS:HD2	1:A:166:ARG:HH12	1.42	0.84
1:B:416:ASN:OD1	1:B:561:VAL:HG23	1.77	0.82
1:B:130:ARG:HG2	1:B:130:ARG:NH1	1.91	0.82
1:A:219:PHE:O	1:A:220:LEU:HD23	1.78	0.81
1:A:243:LYS:HG3	3:B:803:TTP:HM52	1.59	0.81
1:B:273:VAL:HB	1:B:274:PRO:HD3	1.61	0.81
1:B:212:ARG:HH11	1:B:485:TYR:HE1	1.28	0.81
1:A:219:PHE:O	1:A:220:LEU:CD2	2.30	0.78
1:A:311:PHE:CZ	1:A:330:PHE:HB3	2.19	0.77
1:B:107:PRO:HG2	1:B:160:ASN:ND2	1.99	0.77
1:B:26:CYS:HA	1:B:29:LEU:HD12	1.67	0.76
1:A:471:LYS:HG2	1:A:542:ALA:HB2	1.68	0.76
1:A:106:ASN:OD1	1:A:108:HIS:HB3	1.84	0.76
1:A:53:THR:HA	1:A:56:LEU:HG	1.67	0.73
1:A:219:PHE:CD2	1:A:443:VAL:HG22	2.24	0.73
1:B:416:ASN:CG	1:B:561:VAL:CG2	2.61	0.72
1:A:256:ARG:NH1	3:A:804:TTP:O3G	2.22	0.72
1:B:490:GLU:OE1	1:B:490:GLU:N	2.18	0.72
1:B:212:ARG:NH1	1:B:485:TYR:HE1	1.87	0.71
1:B:273:VAL:HB	1:B:274:PRO:CD	2.20	0.71
1:A:302:GLU:HG2	1:A:333:TRP:HB3	1.72	0.69
1:B:107:PRO:HG2	1:B:160:ASN:HD21	1.57	0.69
1:B:149:LYS:HE2	1:B:152:GLU:OE2	1.91	0.69
1:A:443:VAL:CG1	1:A:444:CYS:H	2.04	0.69
1:A:515:MET:O	1:A:516:ARG:HB2	1.93	0.69
1:B:30:ASN:HD21	1:B:33:PHE:HD1	1.40	0.69
1:B:314:LEU:HD23	1:B:323:GLN:O	1.94	0.68
1:A:92:LYS:HD2	1:A:166:ARG:NH1	2.06	0.68
1:B:561:VAL:C	1:B:563:LYS:H	2.02	0.67
1:B:212:ARG:NH1	1:B:485:TYR:CE1	2.60	0.66
1:A:219:PHE:CE2	1:A:443:VAL:HG22	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD22	1:B:125:LEU:HG	1.76	0.66
1:B:1:MET:HE1	1:B:47:LEU:HD13	1.78	0.65
1:B:52:THR:HB	1:B:54:VAL:HG13	1.79	0.65
1:B:362:VAL:HG22	1:B:366:GLU:OE1	1.97	0.64
1:B:481:ILE:HG23	1:B:495:ASN:HD22	1.61	0.64
1:A:584:LEU:O	1:A:588:ILE:HG13	1.97	0.64
1:B:222:SER:HA	1:B:251:ALA:HB3	1.80	0.64
3:A:804:TTP:HM52	1:B:243:LYS:HB2	1.78	0.64
1:A:243:LYS:NZ	3:B:803:TTP:O3A	2.31	0.63
1:B:6:ARG:HG3	1:B:53:THR:HG21	1.79	0.63
1:B:441:VAL:HG13	1:B:490:GLU:HB2	1.81	0.63
1:A:43:VAL:HG22	1:A:59:LEU:HD22	1.81	0.63
1:B:90:THR:HB	1:B:166:ARG:HE	1.62	0.63
1:B:471:LYS:HG3	1:B:542:ALA:HB2	1.81	0.62
1:B:302:GLU:HG2	1:B:333:TRP:HB3	1.80	0.62
1:B:478:ASN:HD21	1:B:594:ARG:HG2	1.64	0.62
1:A:93:VAL:HG13	1:A:96:ASP:HB2	1.81	0.62
1:B:260:SER:OG	1:B:352:CYS:SG	2.46	0.61
1:B:644:ASP:N	1:B:644:ASP:OD1	2.33	0.61
1:A:704:GLN:O	1:A:733:LYS:HD2	2.00	0.61
1:B:395:GLU:O	1:B:399:GLU:HG2	2.00	0.61
1:B:644:ASP:O	1:B:648:ARG:HG3	2.01	0.60
1:A:231:ILE:HD13	1:A:275:MET:HG3	1.83	0.60
1:B:226:ASP:OD1	1:B:256:ARG:HD2	2.01	0.60
1:A:103:ASN:O	1:A:104:TYR:C	2.44	0.60
1:B:167:PRO:O	1:B:171:LEU:HD22	2.01	0.60
1:B:130:ARG:HH11	1:B:130:ARG:CG	2.08	0.59
1:B:256:ARG:HD3	3:B:803:TTP:H4'	1.85	0.59
1:A:243:LYS:HG3	3:B:803:TTP:C5M	2.31	0.59
1:B:224:LYS:O	1:B:225:ASP:HB3	2.02	0.58
1:B:525:GLN:HB3	6:B:813:HOH:O	2.03	0.58
1:B:373:SER:O	1:B:377:GLN:HG3	2.04	0.58
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.84	0.58
1:B:552:PRO:HA	1:B:593:ILE:O	2.04	0.58
1:B:43:VAL:HG13	1:B:59:LEU:HD12	1.85	0.58
1:A:94:PHE:HB3	1:A:132:ASN:OD1	2.05	0.57
1:A:533:GLU:OE1	1:A:576:THR:HG22	2.05	0.57
1:B:602:MET:HE2	1:B:604:THR:HG22	1.87	0.57
1:A:120:THR:O	1:A:124:VAL:HG23	2.05	0.57
1:A:170:MET:SD	1:A:170:MET:C	2.88	0.57
1:B:174:VAL:HG22	1:B:208:ALA:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:SER:O	1:B:418:GLN:HB2	2.04	0.56
1:B:695:ALA:O	1:B:699:GLY:N	2.38	0.56
1:B:280:ASN:O	1:B:284:ARG:HG3	2.05	0.56
1:A:710:ILE:HG12	1:A:736:MET:HG3	1.88	0.56
1:A:439:ASP:O	1:A:490:GLU:HB3	2.06	0.55
1:A:462:ASP:OD2	1:A:462:ASP:C	2.49	0.55
1:B:561:VAL:O	1:B:563:LYS:N	2.39	0.55
1:A:229:GLU:HG3	1:B:240:LEU:HD11	1.87	0.55
1:B:561:VAL:C	1:B:563:LYS:N	2.61	0.55
1:A:284:ARG:NH2	1:B:277:ARG:NH2	2.55	0.55
1:B:478:ASN:OD1	1:B:595:ASN:ND2	2.37	0.55
1:A:683:VAL:HA	1:A:686:ILE:HD12	1.89	0.55
1:A:362:VAL:CG1	1:A:366:GLU:HB2	2.37	0.55
1:A:380:VAL:HG12	1:A:382:LYS:H	1.72	0.54
1:A:378:GLY:O	1:A:380:VAL:N	2.40	0.54
1:B:516:ARG:NH2	1:B:644:ASP:OD2	2.40	0.54
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.73	0.54
1:A:273:VAL:HG13	1:A:314:LEU:HD11	1.90	0.54
1:A:406:LEU:HD11	1:A:430:THR:HB	1.89	0.54
1:B:531:ILE:O	1:B:534:THR:HB	2.08	0.54
1:A:607:THR:HA	1:A:610:ILE:HD12	1.88	0.54
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.88	0.53
1:A:30:ASN:OD1	1:A:32:ASP:HB2	2.08	0.53
1:A:278:VAL:HA	1:B:281:ASN:ND2	2.23	0.53
1:A:159:ILE:O	1:A:160:ASN:C	2.52	0.53
1:A:281:ASN:HD22	1:B:281:ASN:HB2	1.74	0.53
1:A:529:LYS:HE2	1:A:697:GLU:HG2	1.91	0.53
1:A:382:LYS:HE3	1:A:384:VAL:HG13	1.91	0.53
1:A:281:ASN:HD22	1:B:281:ASN:CB	2.22	0.53
1:A:513:ILE:HG23	1:A:679:LEU:HD11	1.91	0.53
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.09	0.53
1:B:310:GLU:CD	1:B:310:GLU:N	2.67	0.53
1:A:295:GLY:O	1:A:296:ALA:HB2	2.09	0.53
1:A:146:PHE:HE1	1:A:634:PHE:HB2	1.74	0.52
1:A:102:TYR:O	1:A:114:PRO:HA	2.10	0.52
1:B:431:GLU:OE2	1:B:431:GLU:N	2.39	0.52
1:A:478:ASN:OD1	1:A:499:ARG:NH1	2.43	0.52
1:B:1:MET:HG2	1:B:49:SER:HB2	1.92	0.52
3:A:804:TTP:HM52	1:B:243:LYS:HE2	1.92	0.52
1:A:170:MET:O	1:A:174:VAL:HG23	2.10	0.51
1:A:445:ASN:ND2	1:A:445:ASN:N	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:PRO:HG2	1:A:490:GLU:OE1	2.11	0.51
1:B:87:HIS:CD2	1:B:166:ARG:HD3	2.46	0.51
1:B:224:LYS:O	1:B:225:ASP:CB	2.58	0.51
1:B:135:ILE:HD11	1:B:172:MET:HG2	1.92	0.51
1:B:298:ALA:HA	1:B:329:PHE:O	2.11	0.51
1:A:336:ASP:O	1:A:337:LEU:C	2.53	0.51
1:A:136:ILE:HG23	4:A:808:SO4:O1	2.11	0.50
1:B:83:VAL:HG11	1:B:140:ASP:HB3	1.93	0.50
1:A:621:THR:HA	1:A:683:VAL:HG12	1.94	0.50
1:A:373:SER:O	1:A:377:GLN:HG3	2.11	0.50
1:B:1:MET:HE1	1:B:47:LEU:CD1	2.41	0.50
1:B:313:ASP:HA	1:B:316:LYS:HD3	1.93	0.50
1:B:416:ASN:ND2	1:B:561:VAL:CG2	2.75	0.50
1:A:720:LEU:O	1:A:723:MET:HB2	2.11	0.50
1:B:551:GLY:O	1:B:594:ARG:NH1	2.45	0.50
1:A:615:GLU:CD	1:A:615:GLU:H	2.20	0.50
1:A:105:ILE:O	1:A:107:PRO:HD3	2.12	0.49
1:B:256:ARG:CD	3:B:803:TTP:H4'	2.41	0.49
1:A:159:ILE:O	1:A:160:ASN:O	2.30	0.49
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.94	0.49
1:B:364:GLY:O	1:B:368:GLU:HG3	2.13	0.49
1:A:222:SER:OG	1:A:424:LYS:HD2	2.12	0.49
1:B:170:MET:HG2	1:B:173:ARG:NH2	2.27	0.49
1:A:281:ASN:ND2	1:B:281:ASN:HB2	2.27	0.49
1:A:515:MET:O	1:A:516:ARG:CB	2.59	0.49
1:A:306:LEU:HD13	1:A:381:ARG:HB3	1.94	0.49
1:B:256:ARG:HH21	1:B:262:ILE:HA	1.76	0.49
1:B:226:ASP:CG	1:B:256:ARG:HD2	2.38	0.49
1:A:742:ARG:HB2	1:A:742:ARG:NH1	2.19	0.48
1:B:109:ASN:O	1:B:111:LYS:N	2.46	0.48
1:B:330:PHE:N	1:B:330:PHE:CD2	2.81	0.48
1:B:98:MET:HG3	1:B:124:VAL:HG11	1.96	0.48
1:B:256:ARG:NH1	3:B:803:TTP:H5'1	2.28	0.48
1:A:93:VAL:HG22	1:A:96:ASP:H	1.78	0.48
1:B:115:MET:HE2	1:B:157:LEU:HD22	1.95	0.48
1:A:405:MET:HG3	1:A:724:HIS:CE1	2.49	0.48
1:B:485:TYR:C	1:B:485:TYR:CD2	2.92	0.48
1:A:600:ALA:HB2	1:A:704:GLN:HB2	1.96	0.48
1:B:678:GLN:O	1:B:681:LYS:HG3	2.13	0.48
1:B:277:ARG:HD2	1:B:322:GLU:O	2.13	0.48
1:B:540:LEU:HB2	1:B:584:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:VAL:HG13	1:A:444:CYS:H	1.78	0.48
1:A:600:ALA:O	1:A:602:MET:HE3	2.14	0.48
1:A:429:CYS:C	1:A:430:THR:HG23	2.39	0.47
1:B:601:PRO:HG2	1:B:702:ILE:HD13	1.95	0.47
1:B:553:TYR:O	1:B:554:GLU:C	2.56	0.47
1:B:715:PRO:HG3	1:B:741:THR:HG21	1.95	0.47
1:A:219:PHE:O	1:A:220:LEU:HD22	2.12	0.47
1:A:244:SER:O	1:A:245:ALA:HB3	2.14	0.47
1:A:446:LEU:HB3	1:A:602:MET:HE2	1.97	0.47
1:A:217:SER:O	1:A:217:SER:OG	2.30	0.47
1:B:637:VAL:O	1:B:638:ASN:C	2.57	0.47
1:A:48:TYR:CE2	1:A:51:VAL:HG12	2.50	0.47
1:A:53:THR:HA	1:A:56:LEU:CG	2.41	0.47
1:A:156:LEU:HD21	1:A:167:PRO:HA	1.96	0.47
1:B:566:LEU:O	1:B:569:ASP:HB2	2.15	0.47
1:A:43:VAL:HG13	1:A:59:LEU:HD13	1.97	0.47
1:A:144:ASN:OD1	1:A:144:ASN:C	2.58	0.47
1:B:140:ASP:OD2	1:B:168:GLN:HG2	2.14	0.47
1:A:149:LYS:HG2	1:A:629:VAL:HG13	1.97	0.47
1:B:429:CYS:C	1:B:430:THR:HG23	2.40	0.47
1:B:619:PRO:HG2	1:B:683:VAL:HG23	1.96	0.47
1:A:603:PRO:O	1:A:604:THR:C	2.58	0.47
1:A:170:MET:HG2	1:A:173:ARG:NH2	2.29	0.46
1:B:215:LEU:HD13	1:B:480:ILE:HG12	1.97	0.46
1:B:490:GLU:H	1:B:490:GLU:CD	2.16	0.46
1:B:659:ILE:HG22	1:B:664:GLY:HA2	1.97	0.46
1:A:76:ILE:O	1:A:80:ARG:HG3	2.15	0.46
1:A:478:ASN:ND2	1:A:595:ASN:HD21	2.13	0.46
1:A:603:PRO:HD3	1:A:707:SER:OG	2.15	0.46
1:B:5:LYS:HE3	1:B:11:GLU:HG3	1.97	0.46
1:A:334:ILE:O	1:A:408:LYS:HB3	2.16	0.46
1:A:567:GLN:HG3	1:A:700:ALA:O	2.16	0.46
1:B:273:VAL:CB	1:B:274:PRO:CD	2.91	0.46
1:A:667:GLN:O	1:A:677:LYS:HE2	2.15	0.46
1:A:148:PHE:HA	1:A:151:LEU:HD12	1.98	0.46
1:B:265:THR:C	1:B:267:GLY:H	2.23	0.46
1:B:152:GLU:HA	1:B:156:LEU:HD12	1.97	0.45
1:A:349:SER:HB3	1:A:380:VAL:HG11	1.98	0.45
1:B:53:THR:HG21	5:B:805:DTP:O2B	2.16	0.45
1:B:406:LEU:HD22	1:B:426:SER:HB2	1.99	0.45
1:B:667:GLN:O	1:B:677:LYS:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLY:O	1:A:362:VAL:HG23	2.17	0.45
1:A:679:LEU:HD12	1:A:680:TYR:CZ	2.52	0.45
1:B:519:PHE:CD2	1:B:619:PRO:HB3	2.52	0.45
1:B:39:ILE:O	1:B:40:THR:C	2.57	0.45
1:A:484:ASN:HB3	1:A:486:TYR:CE2	2.51	0.45
1:B:14:MET:HE3	1:B:14:MET:HB2	1.83	0.45
1:B:445:ASN:ND2	1:B:445:ASN:H	2.15	0.45
1:A:446:LEU:HA	1:A:502:GLY:O	2.17	0.45
1:B:6:ARG:CG	1:B:53:THR:HG21	2.45	0.45
1:A:227:SER:HB2	3:A:804:TTP:O2A	2.16	0.45
1:A:452:ASN:ND2	1:A:453:MET:HG2	2.32	0.44
1:A:526:LEU:O	1:A:530:GLN:HG3	2.17	0.44
1:B:308:ILE:HD11	1:B:332:LEU:HD21	1.99	0.44
1:A:216:SER:OG	1:A:443:VAL:HG11	2.16	0.44
1:A:434:GLU:OE1	1:A:442:ALA:HB1	2.17	0.44
1:B:199:THR:HG21	1:B:607:THR:HB	1.99	0.44
1:B:202:SER:N	1:B:203:PRO:HD2	2.32	0.44
1:B:16:ASP:HA	1:B:19:THR:HG23	1.99	0.44
1:B:140:ASP:OD2	1:B:167:PRO:HB2	2.17	0.44
1:B:255:ILE:HB	1:B:272:LEU:HD21	1.98	0.44
1:A:441:VAL:O	1:A:491:ALA:HA	2.18	0.44
1:B:79:ALA:O	1:B:83:VAL:HG23	2.16	0.44
1:A:135:ILE:HG23	1:A:168:GLN:HB3	1.99	0.44
1:A:456:THR:C	1:A:458:GLU:H	2.26	0.44
1:A:106:ASN:C	1:A:108:HIS:H	2.26	0.44
1:B:566:LEU:O	1:B:567:GLN:C	2.61	0.44
1:A:485:TYR:C	1:A:485:TYR:CD2	2.95	0.43
1:B:563:LYS:HB2	1:B:565:ILE:HD12	2.00	0.43
1:A:287:ASP:HB2	1:A:294:PRO:HD2	2.00	0.43
1:B:68:THR:C	1:B:70:LYS:H	2.26	0.43
1:B:223:MET:HE1	1:B:279:TYR:OH	2.17	0.43
1:B:320:LYS:O	1:B:324:ARG:HG2	2.18	0.43
1:B:27:TYR:O	1:B:80:ARG:NH2	2.51	0.43
1:B:674:ASP:OD1	1:B:674:ASP:N	2.49	0.43
1:B:280:ASN:ND2	1:B:284:ARG:HD2	2.33	0.43
1:B:123:ILE:O	1:B:124:VAL:C	2.60	0.43
1:B:147:GLY:HA2	1:B:610:ILE:HA	2.00	0.43
1:B:648:ARG:HG2	1:B:648:ARG:HH11	1.83	0.43
1:B:107:PRO:CG	1:B:160:ASN:HD21	2.28	0.43
1:B:481:ILE:HG23	1:B:495:ASN:ND2	2.31	0.43
1:B:546:LEU:O	1:B:547:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:ND1	1:A:72:PRO:HD2	2.34	0.43
1:A:223:MET:HE2	1:A:223:MET:HB2	1.83	0.43
1:A:722:SER:O	1:A:726:TYR:N	2.43	0.43
1:A:202:SER:HB3	1:A:206:PHE:CE1	2.54	0.43
1:A:223:MET:HB2	1:A:251:ALA:O	2.19	0.43
1:A:474:VAL:O	1:A:478:ASN:HB2	2.18	0.43
1:B:225:ASP:O	1:B:227:SER:N	2.49	0.43
1:B:618:GLU:OE1	1:B:711:HIS:HE1	2.00	0.43
1:A:448:SER:HA	1:A:504:GLY:O	2.19	0.43
1:A:551:GLY:O	1:A:594:ARG:NH1	2.52	0.43
1:A:83:VAL:O	1:A:84:SER:C	2.62	0.42
1:B:205:LEU:HD23	1:B:205:LEU:HA	1.93	0.42
1:B:303:PRO:HD3	1:B:333:TRP:O	2.18	0.42
1:B:443:VAL:HG12	1:B:444:CYS:N	2.34	0.42
1:A:298:ALA:HA	1:A:329:PHE:O	2.20	0.42
1:A:396:SER:HB3	1:A:403:PRO:HD2	2.01	0.42
1:A:622:SER:OG	1:A:664:GLY:HA3	2.18	0.42
1:A:218:CYS:C	1:A:219:PHE:CD1	2.97	0.42
1:B:170:MET:SD	1:B:170:MET:C	3.02	0.42
1:A:23:GLN:O	1:A:26:CYS:HB2	2.19	0.42
1:A:628:ARG:HA	1:A:632:GLY:O	2.19	0.42
1:A:637:VAL:HG22	1:A:642:LEU:HB2	2.01	0.42
1:B:136:ILE:HG13	1:B:139:ARG:CZ	2.50	0.42
1:A:306:LEU:HA	1:A:350:LEU:HB3	2.02	0.42
1:A:306:LEU:HD22	1:A:381:ARG:HG2	2.02	0.42
1:A:480:ILE:O	1:A:484:ASN:HB2	2.19	0.42
1:A:650:LEU:HD22	1:A:671:GLU:HG3	2.01	0.42
1:B:588:ILE:HG23	1:B:593:ILE:HG23	2.02	0.42
1:A:43:VAL:C	1:A:45:GLN:H	2.28	0.42
1:A:273:VAL:HB	1:A:274:PRO:HD3	2.02	0.42
1:A:21:ARG:HA	1:A:24:LYS:HG2	2.02	0.41
1:A:287:ASP:OD1	1:A:288:GLN:N	2.54	0.41
1:A:297:PHE:N	1:A:297:PHE:CD2	2.87	0.41
1:B:47:LEU:HD23	1:B:56:LEU:HD21	2.02	0.41
1:B:416:ASN:CG	1:B:561:VAL:HG22	2.40	0.41
1:A:584:LEU:HG	1:A:588:ILE:HD11	2.03	0.41
1:B:333:TRP:CD1	1:B:408:LYS:HD2	2.55	0.41
1:A:489:PRO:O	1:A:492:CYS:HB3	2.20	0.41
1:A:94:PHE:HB2	1:A:135:ILE:HD12	2.01	0.41
1:A:146:PHE:CE1	1:A:634:PHE:HB2	2.53	0.41
1:A:183:ILE:O	1:A:186:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ILE:O	1:A:398:THR:HG23	2.21	0.41
1:A:414:LYS:HA	1:A:570:MET:SD	2.61	0.41
1:B:344:THR:O	1:B:346:GLN:HG3	2.21	0.41
1:B:710:ILE:HG12	1:B:736:MET:HG3	2.02	0.41
1:A:387:GLN:O	1:A:390:TRP:HB3	2.20	0.41
1:A:477:LEU:HD23	1:A:477:LEU:HA	1.83	0.41
1:A:528:ASN:O	1:A:532:PHE:HD2	2.03	0.41
1:A:618:GLU:HA	1:A:619:PRO:HD3	1.93	0.41
1:B:416:ASN:ND2	1:B:561:VAL:HG21	2.36	0.41
1:B:536:TYR:CZ	1:B:540:LEU:HD11	2.56	0.41
1:A:215:LEU:C	1:A:216:SER:O	2.61	0.41
1:A:441:VAL:HG22	1:A:491:ALA:HA	2.02	0.41
1:B:97:VAL:HG21	1:B:169:HIS:CE1	2.56	0.41
1:A:156:LEU:HD22	1:A:165:GLU:O	2.21	0.41
1:A:315:LYS:CB	1:A:330:PHE:HE2	2.34	0.41
1:A:638:ASN:HA	1:A:639:PRO:HD2	1.89	0.41
1:A:402:THR:HB	1:A:403:PRO:HA	2.03	0.41
1:A:498:HIS:O	1:A:499:ARG:C	2.63	0.41
1:B:248:ILE:HG22	1:B:249:GLY:N	2.35	0.41
1:B:647:GLU:C	1:B:649:GLY:H	2.28	0.41
1:B:338:PHE:O	1:B:342:VAL:HG23	2.21	0.40
1:B:547:ALA:O	1:B:551:GLY:N	2.39	0.40
1:B:18:ILE:O	1:B:22:ILE:HG12	2.21	0.40
1:B:304:TRP:C	1:B:304:TRP:CE3	2.99	0.40
1:A:19:THR:C	1:A:21:ARG:H	2.30	0.40
1:B:324:ARG:HG3	1:B:326:ARG:NH2	2.35	0.40
1:B:359:LEU:HD12	1:B:359:LEU:HA	1.96	0.40
1:B:452:ASN:OD1	1:B:452:ASN:N	2.50	0.40
1:B:553:TYR:CZ	1:B:596:SER:HB3	2.55	0.40
1:A:71:HIS:CG	1:A:72:PRO:HD2	2.57	0.40
1:B:90:THR:HG22	1:B:91:LYS:O	2.21	0.40
1:A:135:ILE:CG2	1:A:168:GLN:HB3	2.52	0.40
1:A:179:HIS:O	1:A:180:LYS:C	2.64	0.40
1:A:191:ASN:O	1:A:192:LEU:C	2.65	0.40
1:B:648:ARG:HE	1:B:676:LEU:HD11	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	709/792 (90%)	633 (89%)	54 (8%)	22 (3%)	3	18
1	B	731/792 (92%)	639 (87%)	79 (11%)	13 (2%)	6	29
All	All	1440/1584 (91%)	1272 (88%)	133 (9%)	35 (2%)	4	23

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	296	ALA
1	A	327	ASP
1	A	379	ARG
1	B	110	GLY
1	B	225	ASP
1	B	713	ALA
1	A	104	TYR
1	A	162	LYS
1	A	218	CYS
1	A	245	ALA
1	A	246	GLY
1	A	345	ASN
1	A	516	ARG
1	B	327	ASP
1	A	180	LYS
1	A	457	SER
1	A	653	GLU
1	A	663	ASN
1	A	713	ALA
1	B	6	ARG
1	B	226	ASP
1	B	345	ASN
1	B	516	ARG
1	B	562	SER

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Mol	Chain	Res	Type
1	A	53	THR
1	A	737	TYR
1	B	7	ASP
1	B	601	PRO
1	A	285	TYR
1	A	312	LEU
1	B	267	GLY
1	B	493	LEU
1	A	106	ASN
1	A	44	ILE

5.3.2 Protein sidechains [i](#)

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	597/693 (86%)	531 (89%)	66 (11%)	6	22
1	B	617/693 (89%)	533 (86%)	84 (14%)	3	16
All	All	1214/1386 (88%)	1064 (88%)	150 (12%)	4	19

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	45	GLN
1	A	53	THR
1	A	59	LEU
1	A	66	THR
1	A	67	LEU
1	A	93	VAL
1	A	95	SER
1	A	108	HIS
1	A	120	THR
1	A	121	LEU
1	A	130	ARG
1	A	149	LYS

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Mol	Chain	Res	Type
1	A	158	LYS
1	A	171	LEU
1	A	176	VAL
1	A	192	LEU
1	A	210	THR
1	A	214	GLN
1	A	220	LEU
1	A	221	LEU
1	A	222	SER
1	A	225	ASP
1	A	242	SER
1	A	250	VAL
1	A	272	LEU
1	A	275	MET
1	A	276	LEU
1	A	282	THR
1	A	286	VAL
1	A	301	LEU
1	A	312	LEU
1	A	337	LEU
1	A	382	LYS
1	A	387	GLN
1	A	389	LEU
1	A	396	SER
1	A	429	CYS
1	A	441	VAL
1	A	445	ASN
1	A	455	VAL
1	A	457	SER
1	A	460	THR
1	A	490	GLU
1	A	505	VAL
1	A	508	LEU
1	A	550	GLN
1	A	562	SER
1	A	573	VAL
1	A	574	THR
1	A	591	TYR
1	A	615	GLU
1	A	631	SER
1	A	635	GLN
1	A	637	VAL

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Mol	Chain	Res	Type
1	A	648	ARG
1	A	656	LYS
1	A	669	ILE
1	A	674	ASP
1	A	679	LEU
1	A	692	LEU
1	A	693	LYS
1	A	697	GLU
1	A	739	LEU
1	A	741	THR
1	A	742	ARG
1	B	5	LYS
1	B	11	GLU
1	B	16	ASP
1	B	19	THR
1	B	30	ASN
1	B	41	MET
1	B	47	LEU
1	B	53	THR
1	B	54	VAL
1	B	58	THR
1	B	59	LEU
1	B	66	THR
1	B	69	THR
1	B	76	ILE
1	B	80	ARG
1	B	84	SER
1	B	93	VAL
1	B	106	ASN
1	B	113	SER
1	B	121	LEU
1	B	129	ASP
1	B	130	ARG
1	B	136	ILE
1	B	149	LYS
1	B	154	SER
1	B	171	LEU
1	B	187	ILE
1	B	192	LEU
1	B	217	SER
1	B	256	ARG
1	B	265	THR

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Mol	Chain	Res	Type
1	B	273	VAL
1	B	276	LEU
1	B	281	ASN
1	B	301	LEU
1	B	312	LEU
1	B	313	ASP
1	B	326	ARG
1	B	327	ASP
1	B	337	LEU
1	B	349	SER
1	B	359	LEU
1	B	362	VAL
1	B	380	VAL
1	B	389	LEU
1	B	396	SER
1	B	431	GLU
1	B	441	VAL
1	B	444	CYS
1	B	445	ASN
1	B	446	LEU
1	B	449	LEU
1	B	455	VAL
1	B	464	LYS
1	B	471	LYS
1	B	478	ASN
1	B	480	ILE
1	B	493	LEU
1	B	508	LEU
1	B	541	GLU
1	B	554	GLU
1	B	555	THR
1	B	561	VAL
1	B	570	MET
1	B	583	VAL
1	B	587	LYS
1	B	615	GLU
1	B	617	ILE
1	B	621	THR
1	B	622	SER
1	B	627	ARG
1	B	629	VAL
1	B	642	LEU

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Mol	Chain	Res	Type
1	B	644	ASP
1	B	655	MET
1	B	678	GLN
1	B	679	LEU
1	B	685	GLU
1	B	692	LEU
1	B	708	LEU
1	B	723	MET
1	B	739	LEU
1	B	740	ARG
1	B	742	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	108	HIS
1	A	127	ASN
1	A	214	GLN
1	A	281	ASN
1	A	387	GLN
1	A	478	ASN
1	A	550	GLN
1	A	623	ASN
1	A	652	HIS
1	A	657	ASN
1	B	2	HIS
1	B	10	GLN
1	B	30	ASN
1	B	45	GLN
1	B	106	ASN
1	B	237	GLN
1	B	268	ASN
1	B	445	ASN
1	B	459	HIS
1	B	495	ASN
1	B	614	ASN
1	B	652	HIS
1	B	663	ASN
1	B	709	ASN
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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
3	TTP	A	804	2	29,30,30	1.93	8 (27%)	43,47,47	2.16	10 (23%)
4	SO4	B	806	-	4,4,4	0.29	0	6,6,6	0.40	0
5	DTP	B	805	-	31,32,32	1.73	6 (19%)	46,50,50	1.85	9 (19%)
4	SO4	B	809	-	4,4,4	0.30	0	6,6,6	0.18	0
4	SO4	A	807	-	4,4,4	0.28	0	6,6,6	0.18	0
3	TTP	B	803	2	29,30,30	1.45	6 (20%)	43,47,47	2.13	10 (23%)
4	SO4	A	808	-	4,4,4	0.25	0	6,6,6	0.26	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
3	TTP	A	804	2	-	9/22/34/34	0/2/2/2
5	DTP	B	805	-	-	4/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTP	B	803	2	-	4/22/34/34	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	805	DTP	C5-C4	4.76	1.47	1.39
3	A	804	TTP	PB-O3A	4.58	1.64	1.59
5	B	805	DTP	PA-O3A	4.23	1.64	1.59
3	A	804	TTP	C2-N1	3.87	1.44	1.38
5	B	805	DTP	PB-O3A	3.71	1.63	1.59
3	B	803	TTP	C2-N1	3.59	1.44	1.38
3	A	804	TTP	C4-N3	-3.54	1.32	1.38
3	B	803	TTP	C4-C5	3.33	1.50	1.44
3	A	804	TTP	C6-C5	3.27	1.39	1.34
3	A	804	TTP	PA-O3A	3.27	1.63	1.59
3	A	804	TTP	PB-O3B	3.16	1.62	1.59
3	A	804	TTP	C4-C5	3.11	1.49	1.44
3	B	803	TTP	C4-N3	-3.00	1.33	1.38
5	B	805	DTP	C5-C6	2.90	1.49	1.41
3	B	803	TTP	C6-C5	2.70	1.39	1.34
3	B	803	TTP	C6-N1	-2.54	1.33	1.38
5	B	805	DTP	C5-N7	-2.43	1.34	1.39
5	B	805	DTP	C8-N7	2.32	1.36	1.31
3	A	804	TTP	C6-N1	-2.15	1.34	1.38
3	B	803	TTP	C2-N3	-2.05	1.34	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	TTP	N3-C2-N1	7.19	124.25	114.89
3	B	803	TTP	N3-C2-N1	6.77	123.70	114.89
3	B	803	TTP	C4-N3-C2	-6.27	119.12	127.34
5	B	805	DTP	C5-C4-N3	-6.09	118.33	126.72
3	A	804	TTP	C4-N3-C2	-5.59	120.01	127.34
5	B	805	DTP	N3-C4-N9	4.87	135.45	127.17
3	B	803	TTP	C5-C6-N1	-4.46	118.47	123.31
3	A	804	TTP	C5-C6-N1	-4.44	118.49	123.31
3	A	804	TTP	C6-C5-C4	4.24	121.51	118.02
5	B	805	DTP	C2-N3-C4	4.09	121.81	111.83
3	B	803	TTP	C5-C4-N3	3.84	118.66	115.32
5	B	805	DTP	N3-C2-N1	-3.77	122.87	128.58
3	A	804	TTP	O2-C2-N3	-3.52	114.99	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	805	DTP	C4-C5-N7	-3.40	106.70	110.58
3	B	803	TTP	O2-C2-N3	-3.31	115.39	121.49
3	B	803	TTP	C5M-C5-C6	-3.30	118.39	122.85
3	A	804	TTP	C5M-C5-C6	-3.13	118.61	122.85
3	A	804	TTP	O4'-C1'-N1	3.10	113.37	107.86
3	A	804	TTP	C6-N1-C2	-3.09	118.22	121.30
3	B	803	TTP	C6-C5-C4	2.97	120.47	118.02
5	B	805	DTP	O4'-C1'-N9	2.77	112.94	107.96
3	A	804	TTP	C5-C4-N3	2.52	117.52	115.32
5	B	805	DTP	C5-N7-C8	2.50	107.38	103.45
5	B	805	DTP	C4-N9-C8	2.40	108.25	105.74
3	B	803	TTP	O4-C4-C5	-2.39	122.18	124.92
3	B	803	TTP	C1'-N1-C2	2.38	122.32	117.66
3	B	803	TTP	C5M-C5-C4	2.21	121.14	118.78
5	B	805	DTP	C6-C5-N7	2.19	136.31	132.09
3	A	804	TTP	O2B-PB-O3A	2.14	113.06	107.27

There are no chirality outliers.

All (17) torsion outliers are listed below:

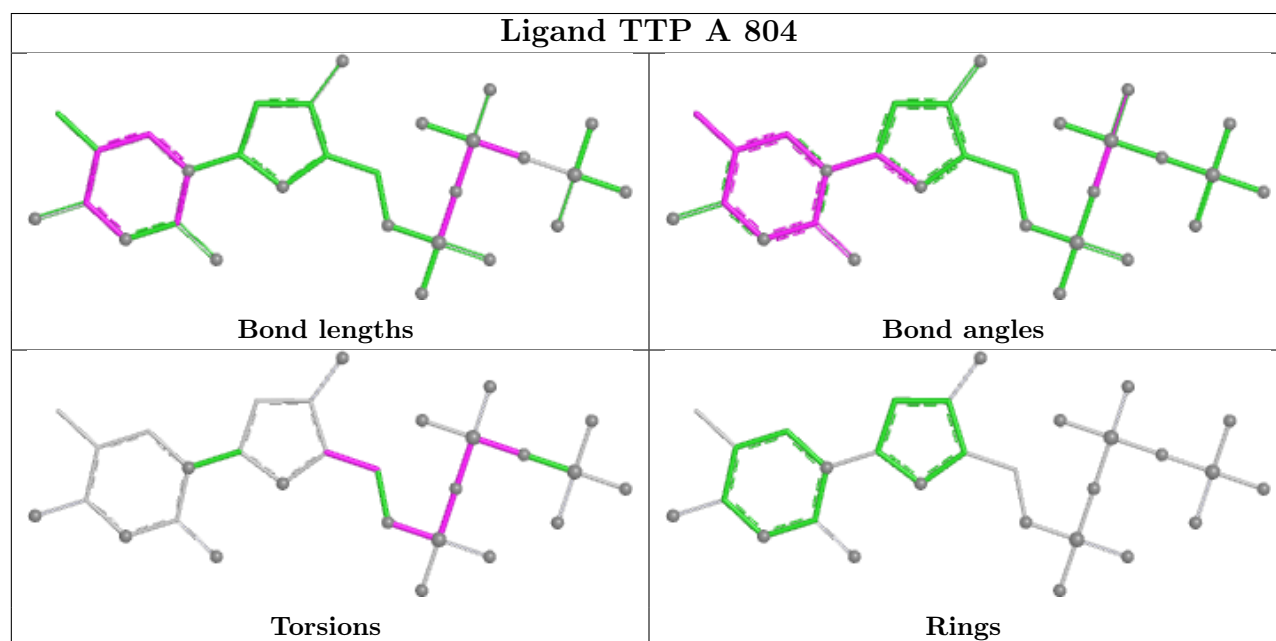
Mol	Chain	Res	Type	Atoms
3	A	804	TTP	C5'-O5'-PA-O1A
3	B	803	TTP	C5'-O5'-PA-O1A
3	B	803	TTP	O4'-C4'-C5'-O5'
3	B	803	TTP	C3'-C4'-C5'-O5'
3	A	804	TTP	O4'-C4'-C5'-O5'
3	A	804	TTP	C3'-C4'-C5'-O5'
5	B	805	DTP	PB-O3B-PG-O1G
3	A	804	TTP	PB-O3A-PA-O2A
3	A	804	TTP	PA-O3A-PB-O2B
3	A	804	TTP	PG-O3B-PB-O1B
5	B	805	DTP	PG-O3B-PB-O1B
3	A	804	TTP	C5'-O5'-PA-O3A
3	B	803	TTP	PB-O3B-PG-O3G
3	A	804	TTP	PB-O3A-PA-O1A
3	A	804	TTP	PG-O3B-PB-O2B
5	B	805	DTP	PG-O3B-PB-O2B
5	B	805	DTP	C2'-C1'-N9-C4

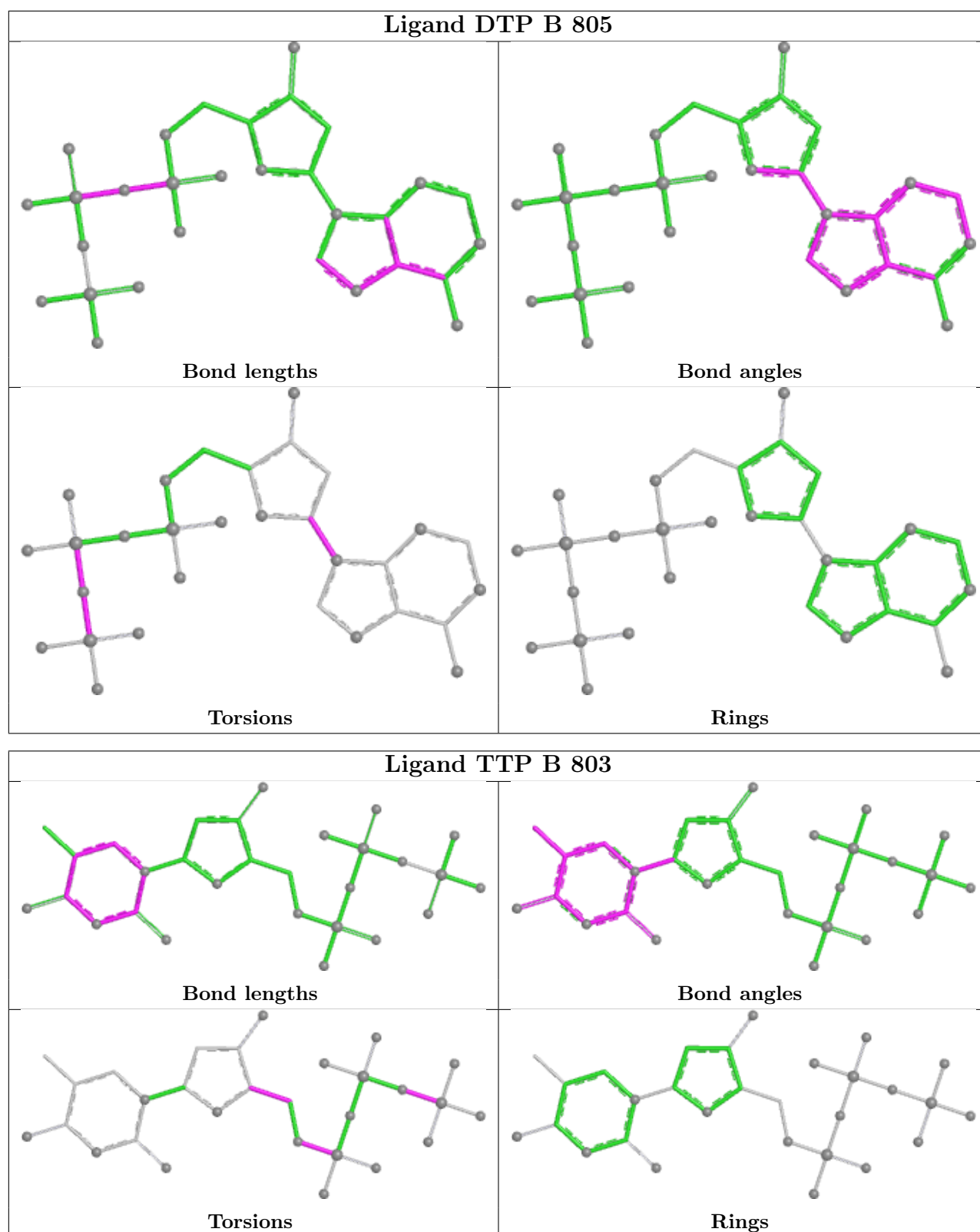
There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	TTP	4	0
5	B	805	DTP	1	0
4	B	809	SO4	1	0
3	B	803	TTP	6	0
4	A	808	SO4	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.53	3 (0%) 88 78	12, 63, 85, 123	2 (0%)
1	B	737/792 (93%)	-0.59	0 100 100	38, 58, 94, 110	0
All	All	1452/1584 (91%)	-0.56	3 (0%) 91 84	12, 61, 91, 123	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	9.2
1	A	218	CYS	5.5
1	A	51	VAL	2.3

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.

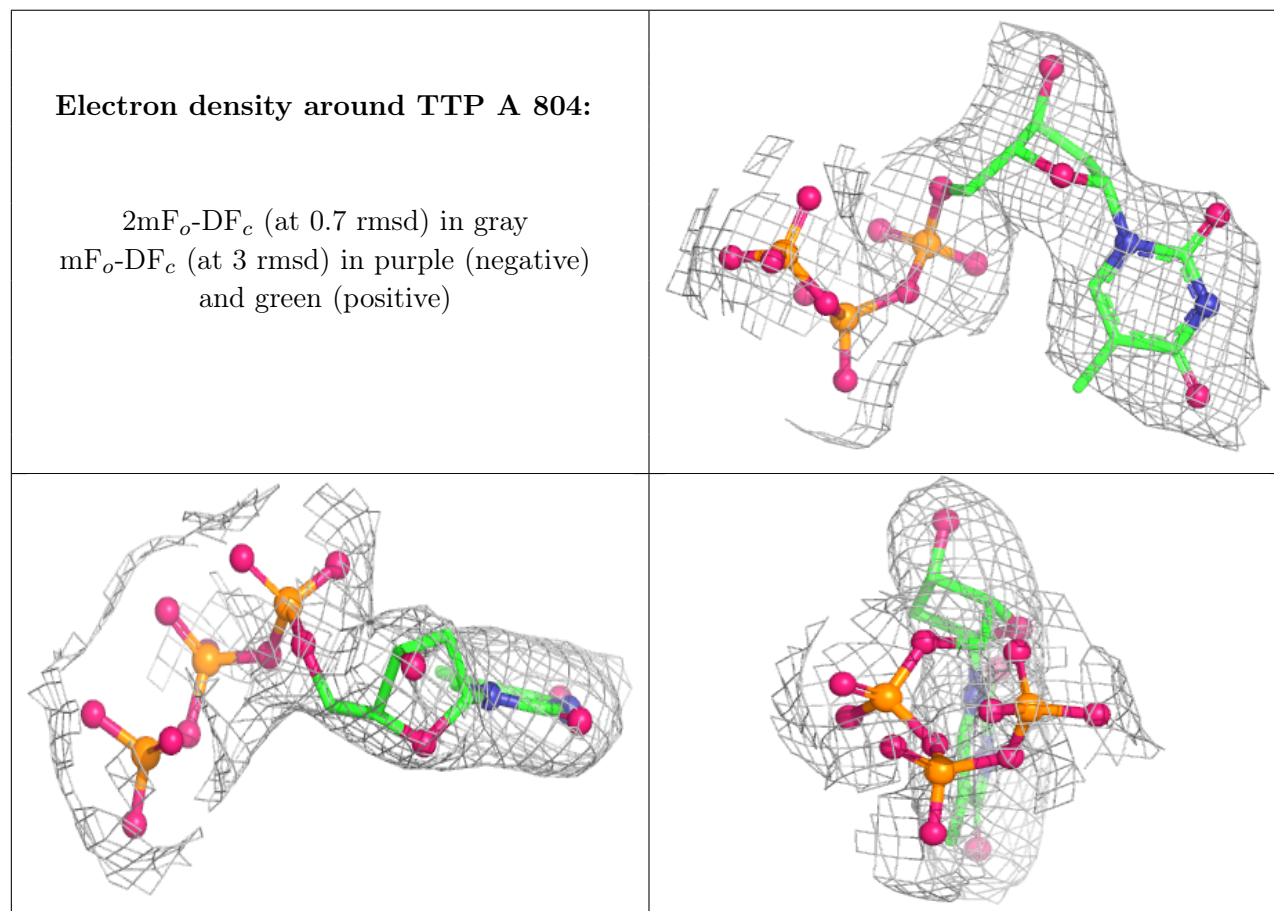
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	801	1/1	0.87	0.10	46,46,46,46	0
4	SO4	B	806	5/5	0.91	0.10	101,102,102,102	0

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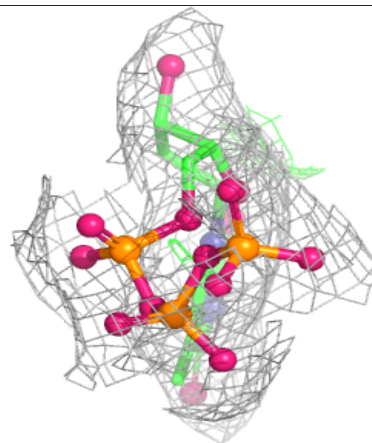
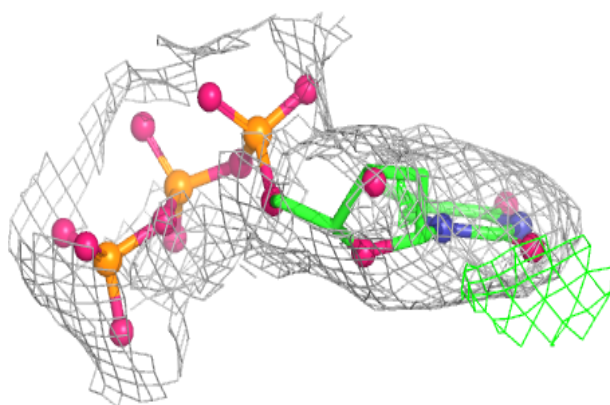
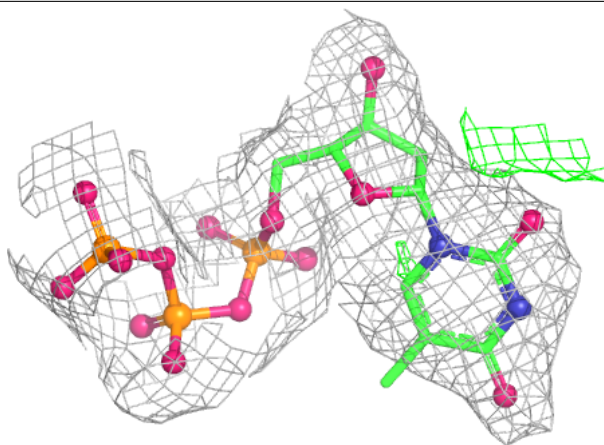
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	808	5/5	0.94	0.06	76,76,77,78	0
4	SO4	A	807	5/5	0.95	0.07	91,91,91,91	0
2	MG	B	802	1/1	0.95	0.09	48,48,48,48	0
3	TTP	A	804	29/29	0.95	0.07	58,60,66,67	0
3	TTP	B	803	29/29	0.96	0.07	54,57,66,67	0
4	SO4	B	809	5/5	0.96	0.05	74,75,75,75	0
5	DTP	B	805	30/30	0.96	0.07	83,84,88,89	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.

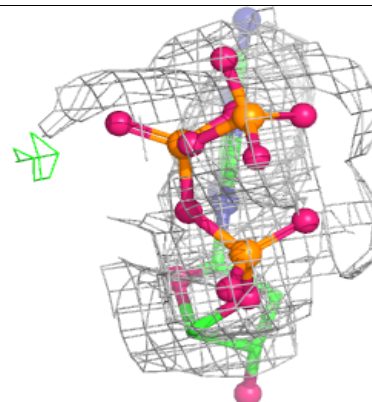
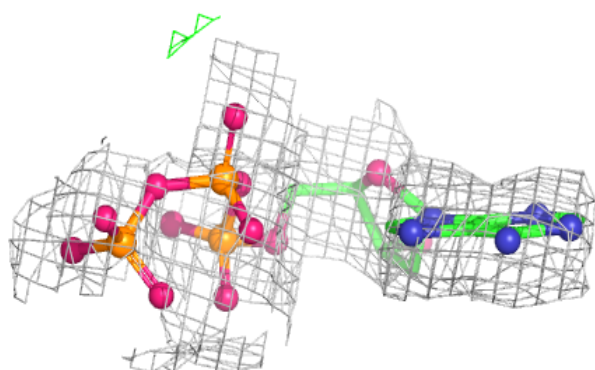
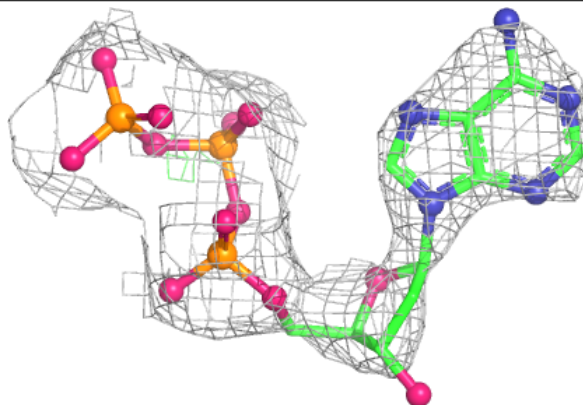


Electron density around TTP B 803:

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

**Electron density around DTP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.