



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 05:30 AM EDT

PDB ID : 3HNC
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effector TTP
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.
Deposited on : unknown
Resolution : 2.41 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

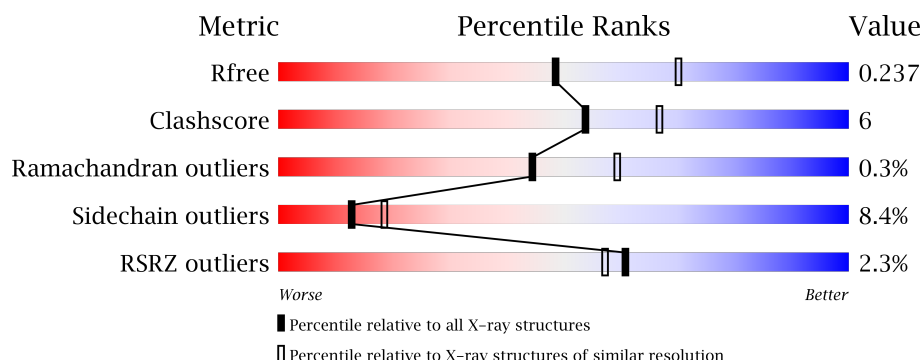
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	100719	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	792	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>•</div> <div>7%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11778 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.

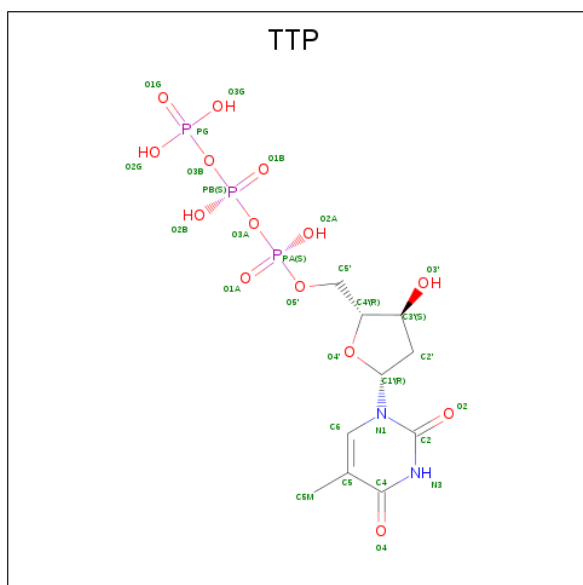
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	6	0	0
			5577	3567	926	1052	32			
1	B	738	Total	C	N	O	S	0	0	0
			5751	3669	968	1080	34			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



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 (three-letter code: 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	187	Total	O	0	0
			187	187		
5	B	173	Total	O	0	0
			173	173		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 2% 74% 14% 10%
- | Position | Amino Acid |
|----------|------------|
| 1 | MET |
| 2 | VAL |
| 3 | ILE |
| 4 | LYS |
| 5 | ARG |
| 6 | ASP |
| 7 | GLY |
| 8 | ARG |
| 9 | GLN |
| 10 | GLU |
| 11 | ARG |
| 12 | VAL |
| 13 | F15 |
| 14 | I18 |
| 15 | R21 |
| 16 | I22 |
| 17 | Y27 |
| 18 | D85 |
| 19 | Q38 |
| 20 | M41 |
| 21 | K42 |
| 22 | V43 |
| 23 | I44 |
| 24 | Q45 |
| 25 | G46 |
| 26 | L47 |
| 27 | G50 |
| 28 | V51 |
| 29 | T52 |
| 30 | T53 |
| 31 | L56 |
| 32 | L59 |
| 33 | L67 |
| 34 | I76 |
| 35 | A79 |
| 36 | R80 |
| 37 | V83 |
| 38 | V93 |
| 39 | L121 |
| 40 | L125 |
| 41 | P140 |

- Chain B:
-
- 77% 3% 15% 7%

MET	L692
CYS	S707
GLY	L708
SER	P715
	M723
	H724
	L739
	R740
	T741
	R742
	PRO
	ALA
	ALA
	ASN
	PRO
	ILE
	GLN
	PHI
	THR
	LEU
	ASN
	LYS
	LYS
	LYS
	LYS
	ASP
	LYS
	GLU
	LYS
	VAL
	SER
	LYS
	GLU
	GLU
	GLU
	LYS
	GLU
	ARG
	ASN
	THR
	ALA
	ALA
	MET
	VAL
	CYS
	SER
	LEU
	GLU
	ASN
	ARG
	ASP
	GLU
	CYS
	LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.98Å 114.10Å 219.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 2.41 37.67 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.53-2.41) 97.0 (37.67-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.236 0.187 , 0.237	Depositor DCC
R_{free} test set	3306 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.2	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	0.95	EDS
Total number of atoms	11778	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TTP, 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	0.52	0/5700	0.63	3/7754 (0.0%)
1	B	0.45	0/5877	0.60	1/7989 (0.0%)
All	All	0.49	0/11577	0.61	4/15743 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	LEU	CA-CB-CG	7.01	131.42	115.30
1	A	499	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	A	220	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	508	LEU	CA-CB-CG	5.29	127.47	115.30

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	5577	0	5418	64	0
1	B	5751	0	5586	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	29	0	13	6	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	187	0	0	3	0
5	B	173	0	0	3	0
All	All	11778	0	11030	136	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 6.

All (136) 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:B:123:ILE:CD1	1:B:180:LYS:HG2	1.86	1.06
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.69	0.75
1:B:448:SER:HB3	1:B:602:MET:CE	2.17	0.75
1:B:123:ILE:HD13	1:B:180:LYS:HG2	1.70	0.73
1:B:413:ARG:HD2	5:B:827:HOH:O	1.87	0.73
1:B:196:ARG:HG2	1:B:611:LEU:HD22	1.71	0.72
1:B:123:ILE:CD1	1:B:180:LYS:CG	2.70	0.68
1:B:402:THR:HB	1:B:403:PRO:HA	1.74	0.68
1:B:256:ARG:HD3	3:B:802:TTP:H4'	1.76	0.67
1:A:416:ASN:OD1	1:A:561:VAL:HG13	1.95	0.67
1:A:478:ASN:HD22	1:A:499:ARG:HH11	1.44	0.66
1:B:80:ARG:HD3	1:B:141:PHE:HB3	1.76	0.66
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.79	0.65
1:B:90:THR:HG21	1:B:166:ARG:HG3	1.77	0.65
1:B:123:ILE:HD13	1:B:180:LYS:CG	2.26	0.64
1:B:270:ASN:HB3	1:B:274:PRO:HG2	1.80	0.64
1:A:498:HIS:ND1	1:A:555:THR:HG21	2.13	0.63
1:B:180:LYS:HG3	5:B:935:HOH:O	2.00	0.62
1:B:220:LEU:HG	1:B:442:ALA:HB3	1.82	0.62
1:B:256:ARG:CD	3:B:802:TTP:H4'	2.28	0.62
1:B:226:ASP:OD1	1:B:256:ARG:HD2	2.00	0.62
1:B:218:CYS:HB3	1:B:444:CYS:SG	2.40	0.62
1:B:123:ILE:HD11	1:B:180:LYS:HG2	1.80	0.61
1:A:283:ALA:HB1	1:A:295:GLY:O	2.00	0.61
1:B:645:LEU:HD21	1:B:672:ILE:HD12	1.83	0.60
1:B:415:SER:O	1:B:418:GLN:HB2	2.02	0.60
1:B:221:LEU:HD13	1:B:248:ILE:HG21	1.84	0.60
1:B:448:SER:HB3	1:B:602:MET:HE1	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ALA:HB2	1:B:288:GLN:OE1	2.03	0.59
1:A:456:THR:HG23	1:A:458:GLU:H	1.68	0.59
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.66	0.58
1:A:482:ASP:OD2	1:A:499:ARG:NH2	2.32	0.58
1:B:535:ILE:HG22	1:B:599:ILE:HD12	1.86	0.58
1:A:456:THR:CG2	1:A:458:GLU:H	2.17	0.57
1:A:248:ILE:HD12	1:A:297:PHE:CE2	2.40	0.56
1:B:324:ARG:HG3	1:B:326:ARG:NH2	2.20	0.56
1:A:362:VAL:HG22	1:A:366:GLU:HB3	1.87	0.56
1:B:3:VAL:HG22	1:B:13:VAL:HG22	1.87	0.56
1:A:478:ASN:ND2	1:A:499:ARG:HH11	2.04	0.55
1:A:637:VAL:HG22	1:A:642:LEU:HB2	1.88	0.55
1:A:655:MET:HE3	1:A:672:ILE:HD11	1.89	0.55
1:A:281:ASN:ND2	1:B:281:ASN:OD1	2.31	0.55
1:A:27:TYR:O	1:A:80:ARG:NH2	2.39	0.54
1:B:448:SER:HB3	1:B:602:MET:HE3	1.87	0.54
1:B:221:LEU:HD13	1:B:248:ILE:CG2	2.38	0.54
1:A:153:ARG:NH1	1:A:153:ARG:HB2	2.23	0.54
1:A:402:THR:HB	1:A:403:PRO:HA	1.90	0.53
1:A:275:MET:CE	1:A:276:LEU:HD13	2.38	0.53
1:A:637:VAL:HG13	1:A:642:LEU:HD22	1.89	0.53
1:B:223:MET:HE2	1:B:231:ILE:HG12	1.92	0.52
1:B:362:VAL:CG1	1:B:367:PHE:HA	2.40	0.51
1:B:130:ARG:CG	1:B:130:ARG:HH11	2.22	0.51
1:B:482:ASP:OD2	1:B:499:ARG:NH2	2.44	0.51
1:A:121:LEU:HD22	1:A:125:LEU:HG	1.93	0.51
1:A:478:ASN:HD22	1:A:499:ARG:NH1	2.06	0.50
1:B:441:VAL:O	1:B:491:ALA:HA	2.11	0.50
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.10	0.50
1:A:243:LYS:HG3	3:B:802:TTP:C5M	2.41	0.50
1:A:260:SER:OG	1:A:381:ARG:NH2	2.44	0.50
1:B:444:CYS:HA	5:B:863:HOH:O	2.12	0.50
1:A:655:MET:CE	1:A:672:ILE:HD11	2.41	0.50
1:A:553:TYR:CE1	1:A:555:THR:HG22	2.47	0.50
1:A:652:HIS:O	1:A:655:MET:HB3	2.12	0.49
1:B:256:ARG:NH2	3:B:802:TTP:O2G	2.45	0.49
1:A:221:LEU:CD1	1:A:248:ILE:HG23	2.42	0.49
1:B:27:TYR:O	1:B:80:ARG:NH2	2.46	0.49
1:B:287:ASP:HB3	1:B:294:PRO:HA	1.94	0.48
1:A:535:ILE:HG22	1:A:599:ILE:HD12	1.95	0.48
1:A:18:ILE:O	1:A:22:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:CYS:HB3	1:B:374:TYR:CD1	2.49	0.48
1:A:359:LEU:HB2	5:A:800:HOH:O	2.14	0.48
1:A:35:ASP:HB3	1:A:38:GLN:HG3	1.96	0.47
1:A:364:GLY:O	1:A:368:GLU:HG3	2.14	0.47
1:B:80:ARG:CD	1:B:141:PHE:HB3	2.42	0.47
1:B:275:MET:HE2	1:B:276:LEU:HD13	1.96	0.47
1:A:416:ASN:CG	1:A:561:VAL:HG13	2.34	0.47
1:A:621:THR:HA	1:A:683:VAL:HG12	1.96	0.47
1:B:627:ARG:HB2	1:B:636:ILE:HD12	1.95	0.47
1:B:123:ILE:HD12	1:B:180:LYS:HG2	1.86	0.46
1:B:416:ASN:CG	1:B:561:VAL:HG13	2.36	0.46
1:B:341:ARG:HD2	1:B:347:ASP:O	2.16	0.46
1:A:362:VAL:HG13	1:A:367:PHE:HA	1.98	0.46
1:B:627:ARG:HB2	1:B:636:ILE:CD1	2.46	0.45
1:B:715:PRO:HG3	1:B:741:THR:HG21	1.98	0.45
1:B:223:MET:HE3	1:B:231:ILE:HA	1.98	0.45
1:B:556:TYR:HE2	1:B:561:VAL:CG2	2.29	0.45
1:A:285:TYR:O	1:B:270:ASN:ND2	2.50	0.45
1:B:406:LEU:HD22	1:B:426:SER:HB2	1.99	0.45
1:A:300:TYR:HE2	1:A:406:LEU:HD13	1.81	0.45
1:B:221:LEU:CD1	1:B:248:ILE:CG2	2.95	0.45
1:B:454:TYR:HB2	1:B:461:TYR:CZ	2.52	0.45
1:B:603:PRO:HD3	1:B:707:SER:OG	2.16	0.45
1:B:275:MET:CE	1:B:276:LEU:HD13	2.47	0.44
1:B:319:GLY:HA3	1:B:324:ARG:NH1	2.32	0.44
1:B:83:VAL:HG11	1:B:140:ASP:HB3	1.99	0.44
1:A:474:VAL:HG21	1:A:539:ALA:HA	1.99	0.44
1:B:284:ARG:HD2	1:B:327:ASP:OD2	2.16	0.44
1:A:76:ILE:O	1:A:80:ARG:HG3	2.18	0.44
1:B:482:ASP:CG	1:B:499:ARG:HH22	2.20	0.44
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.53	0.44
1:B:256:ARG:HG3	1:B:354:ASN:HB2	1.99	0.43
1:A:427:ASN:HB2	5:A:920:HOH:O	2.18	0.43
1:B:140:ASP:OD2	1:B:168:GLN:HG2	2.18	0.43
1:B:432:ILE:HG13	1:B:444:CYS:SG	2.58	0.43
1:B:251:ALA:HB2	1:B:425:CYS:HB3	1.99	0.43
1:A:362:VAL:CG1	1:A:367:PHE:HA	2.49	0.43
1:A:270:ASN:HB3	1:A:274:PRO:HG3	2.01	0.43
1:A:441:VAL:HG22	1:A:491:ALA:HB2	2.01	0.42
1:A:199:THR:HG21	1:A:607:THR:HB	2.00	0.42
1:B:90:THR:HG22	1:B:91:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:VAL:HG13	1:B:490:GLU:HB2	2.01	0.42
1:A:306:LEU:HD22	1:A:381:ARG:HG2	2.02	0.42
1:A:192:LEU:HD23	1:A:472:VAL:HG11	2.02	0.42
1:A:220:LEU:HG	1:A:442:ALA:HB3	2.02	0.42
1:A:593:ILE:HD12	1:A:595:ASN:O	2.20	0.42
1:A:379:ARG:HG2	1:A:379:ARG:H	1.64	0.41
1:A:423:ILE:HA	5:A:926:HOH:O	2.18	0.41
1:A:405:MET:HG3	1:A:724:HIS:CE1	2.55	0.41
1:B:35:ASP:O	1:B:38:GLN:HB2	2.21	0.41
1:A:362:VAL:HG13	1:A:367:PHE:CA	2.50	0.41
1:A:553:TYR:HE1	1:A:555:THR:HG22	1.85	0.41
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.84	0.41
1:B:221:LEU:CD1	1:B:248:ILE:HG23	2.51	0.41
1:A:243:LYS:HG3	3:B:802:TTP:HM53	2.03	0.41
1:A:373:SER:O	1:A:377:GLN:HG3	2.21	0.41
1:A:669:ILE:HA	1:A:670:PRO:HD3	1.96	0.41
1:A:529:LYS:O	1:A:533:GLU:HG3	2.21	0.41
1:A:275:MET:HE3	1:A:276:LEU:HD13	2.02	0.40
1:A:79:ALA:O	1:A:83:VAL:HG23	2.21	0.40
1:A:710:ILE:HG12	1:A:736:MET:HG3	2.04	0.40
1:B:130:ARG:NH1	1:B:130:ARG:CG	2.82	0.40
1:B:264:GLY:HA3	3:B:802:TTP:O1B	2.20	0.40
1:A:216:SER:OG	1:A:484:ASN:ND2	2.54	0.40
1:A:556:TYR:HE2	1:A:561:VAL:HG22	1.87	0.40
1:B:196:ARG:HG2	1:B:611:LEU:CD2	2.46	0.40
1:B:1:MET:HE3	1:B:47:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	708/792 (89%)	685 (97%)	21 (3%)	2 (0%)	44	59
1	B	732/792 (92%)	702 (96%)	28 (4%)	2 (0%)	44	59
All	All	1440/1584 (91%)	1387 (96%)	49 (3%)	4 (0%)	44	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	B	224	LYS
1	A	737	TYR
1	B	601	PRO

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	592/693 (85%)	545 (92%)	47 (8%)	14	21
1	B	607/693 (88%)	553 (91%)	54 (9%)	11	16
All	All	1199/1386 (86%)	1098 (92%)	101 (8%)	13	18

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	44	ILE
1	A	59	LEU
1	A	67	LEU
1	A	93	VAL
1	A	121	LEU
1	A	149	LYS
1	A	153	ARG
1	A	171	LEU
1	A	192	LEU
1	A	214	GLN
1	A	220	LEU

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Mol	Chain	Res	Type
1	A	252	VAL
1	A	276	LEU
1	A	286	VAL
1	A	287	ASP
1	A	301	LEU
1	A	312	LEU
1	A	327	ASP
1	A	337	LEU
1	A	359	LEU
1	A	362	VAL
1	A	379	ARG
1	A	383	VAL
1	A	389	LEU
1	A	441	VAL
1	A	443	VAL
1	A	444	CYS
1	A	449	LEU
1	A	455	VAL
1	A	456	THR
1	A	458	GLU
1	A	493	LEU
1	A	555	THR
1	A	606	SER
1	A	637	VAL
1	A	653	GLU
1	A	679	LEU
1	A	692	LEU
1	A	693	LYS
1	A	703	ASP
1	A	708	LEU
1	A	716	ASN
1	A	720	LEU
1	A	739	LEU
1	A	741	THR
1	A	742	ARG
1	B	3	VAL
1	B	12	ARG
1	B	47	LEU
1	B	56	LEU
1	B	59	LEU
1	B	67	LEU
1	B	80	ARG

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Mol	Chain	Res	Type
1	B	93	VAL
1	B	108	HIS
1	B	121	LEU
1	B	130	ARG
1	B	149	LYS
1	B	171	LEU
1	B	180	LYS
1	B	192	LEU
1	B	217	SER
1	B	218	CYS
1	B	220	LEU
1	B	225	ASP
1	B	252	VAL
1	B	256	ARG
1	B	276	LEU
1	B	286	VAL
1	B	301	LEU
1	B	312	LEU
1	B	316	LYS
1	B	318	THR
1	B	337	LEU
1	B	359	LEU
1	B	361	GLU
1	B	362	VAL
1	B	365	GLU
1	B	380	VAL
1	B	381	ARG
1	B	389	LEU
1	B	441	VAL
1	B	449	LEU
1	B	455	VAL
1	B	493	LEU
1	B	508	LEU
1	B	516	ARG
1	B	543	SER
1	B	561	VAL
1	B	602	MET
1	B	615	GLU
1	B	627	ARG
1	B	648	ARG
1	B	671	GLU
1	B	678	GLN

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Mol	Chain	Res	Type
1	B	679	LEU
1	B	692	LEU
1	B	708	LEU
1	B	723	MET
1	B	739	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	281	ASN
1	B	281	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	802	2	22,30,30	0.69	0	25,47,47	1.81	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	804	-	4,4,4	0.19	0	6,6,6	0.20	0
4	SO4	A	805	-	4,4,4	0.90	0	6,6,6	0.25	0
4	SO4	A	809	-	4,4,4	0.86	0	6,6,6	0.18	0
3	TTP	B	802	2	22,30,30	0.63	0	25,47,47	1.65	3 (12%)
4	SO4	B	803	-	4,4,4	0.21	0	6,6,6	0.18	0
4	SO4	B	806	-	4,4,4	0.86	0	6,6,6	0.10	0
4	SO4	B	807	-	4,4,4	0.92	0	6,6,6	0.19	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	802	2	-	0/18/34/34	0/2/2/2
4	SO4	A	804	-	-	0/0/0/0	0/0/0/0
4	SO4	A	805	-	-	0/0/0/0	0/0/0/0
4	SO4	A	809	-	-	0/0/0/0	0/0/0/0
3	TTP	B	802	2	-	0/18/34/34	0/2/2/2
4	SO4	B	803	-	-	0/0/0/0	0/0/0/0
4	SO4	B	806	-	-	0/0/0/0	0/0/0/0
4	SO4	B	807	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	TTP	C5-C4-N3	-5.11	119.61	125.24
3	B	802	TTP	C5-C4-N3	-4.97	119.76	125.24
3	B	802	TTP	C5-C6-N1	-2.61	119.33	122.15
3	A	802	TTP	C5-C6-N1	-2.46	119.49	122.15
3	B	802	TTP	C4-N3-C2	5.18	119.69	115.16
3	A	802	TTP	C4-N3-C2	6.36	120.72	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	TTP	6	0

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	714/792 (90%)	-0.19	13 (1%)	69 66	31, 44, 63, 87	2 (0%)
1	B	738/792 (93%)	-0.11	21 (2%)	53 50	31, 46, 74, 88	0
All	All	1452/1584 (91%)	-0.15	34 (2%)	61 57	31, 44, 71, 88	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	13.9
1	A	218	CYS	11.8
1	B	107	PRO	4.8
1	B	108	HIS	4.7
1	A	53	THR	3.7
1	A	43	VAL	3.5
1	B	48	TYR	3.4
1	A	314	LEU	3.3
1	B	318	THR	3.2
1	B	633	GLU	3.0
1	A	47	LEU	2.9
1	B	290	GLY	2.8
1	B	180	LYS	2.6
1	B	264	GLY	2.6
1	B	655	MET	2.6
1	A	50	GLY	2.6
1	B	675	ASP	2.5
1	B	105	ILE	2.5
1	B	27	TYR	2.4
1	B	113	SER	2.4
1	B	663	ASN	2.4
1	B	291	ASN	2.3
1	A	631	SER	2.3
1	B	635	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	659	ILE	2.2
1	A	56	LEU	2.2
1	B	660	ILE	2.2
1	A	41	MET	2.1
1	A	52	THR	2.1
1	B	632	GLY	2.1
1	B	317	ASN	2.1
1	B	662	CYS	2.0
1	A	46	GLY	2.0
1	A	15	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	A	809	5/5	0.93	0.18	1.35	83,83,84,85	0
4	SO4	B	807	5/5	0.93	0.20	0.49	75,75,76,77	0
3	TTP	A	802	29/29	0.97	0.10	-1.11	37,40,49,49	0
3	TTP	B	802	29/29	0.97	0.10	-1.23	39,41,54,55	0
4	SO4	A	804	5/5	0.98	0.08	-2.77	48,48,49,50	0
2	MG	A	801	1/1	0.91	0.09	-	52,52,52,52	0
4	SO4	B	806	5/5	0.97	0.09	-	82,82,83,83	0
4	SO4	B	803	5/5	0.99	0.07	-	49,50,50,51	0
4	SO4	A	805	5/5	0.91	0.26	-	71,72,72,73	0
2	MG	B	801	1/1	0.80	0.10	-	50,50,50,50	0

6.5 Other polymers

There are no such residues in this entry.