Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 09:38 PM EDT

PDB ID	:	1TLT
Title	:	Crystal Structure of a Putative Oxidoreductase (VIRULENCE FACTOR mviM HOMOLOG)
Authors	:	Rajashankar, K.R.; Solorzano, V.; Kniewel, R.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-06-09
Resolution	:	2.70 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:

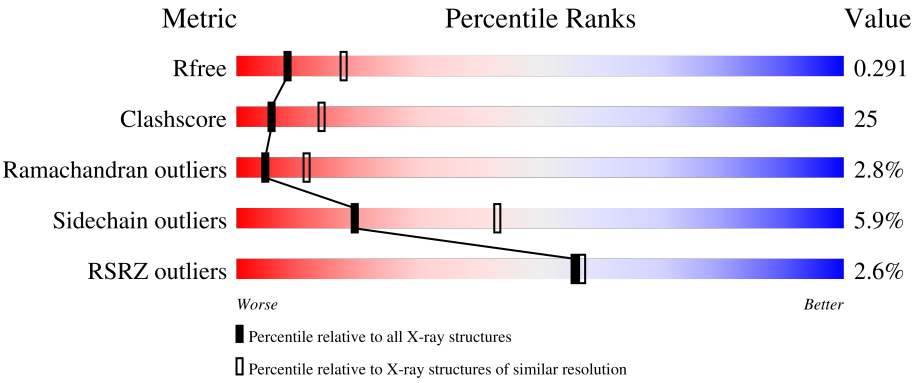
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	319	2% 58% 34% • 5%
1	B	319	3% 54% 36% 6% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4767 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 PUTATIVE OXIDOREDUCTASE (VIRULENCE FACTOR mviM HOMOLOG).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2341	1473	425	431	12			
1	B	305	Total	C	N	O	S	0	0	0
			2350	1478	426	434	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P75931
A	2	SER	-	cloning artifact	UNP P75931
A	3	LEU	-	cloning artifact	UNP P75931
A	310	GLU	-	expression tag	UNP P75931
A	311	GLY	-	expression tag	UNP P75931
A	312	GLY	-	expression tag	UNP P75931
A	313	SER	-	expression tag	UNP P75931
A	314	HIS	-	expression tag	UNP P75931
A	315	HIS	-	expression tag	UNP P75931
A	316	HIS	-	expression tag	UNP P75931
A	317	HIS	-	expression tag	UNP P75931
A	318	HIS	-	expression tag	UNP P75931
A	319	HIS	-	expression tag	UNP P75931
B	1	MET	-	cloning artifact	UNP P75931
B	2	SER	-	cloning artifact	UNP P75931
B	3	LEU	-	cloning artifact	UNP P75931
B	310	GLU	-	expression tag	UNP P75931
B	311	GLY	-	expression tag	UNP P75931
B	312	GLY	-	expression tag	UNP P75931
B	313	SER	-	expression tag	UNP P75931
B	314	HIS	-	expression tag	UNP P75931
B	315	HIS	-	expression tag	UNP P75931
B	316	HIS	-	expression tag	UNP P75931
B	317	HIS	-	expression tag	UNP P75931

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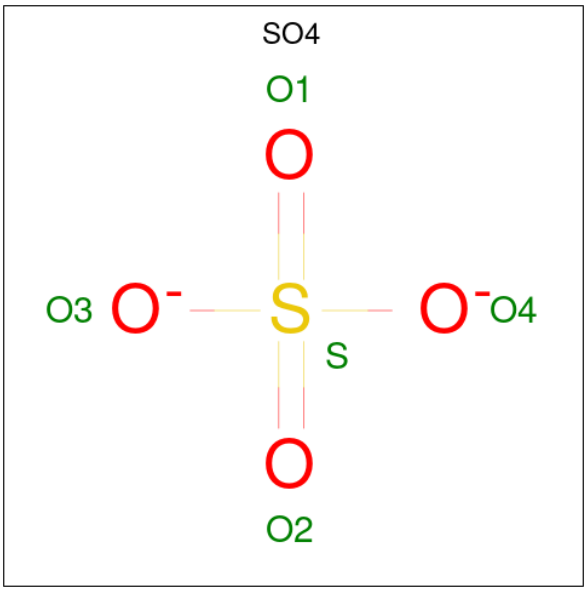
Chain	Residue	Modelled	Actual	Comment	Reference
B	318	HIS	-	expression tag	UNP P75931
B	319	HIS	-	expression tag	UNP P75931

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

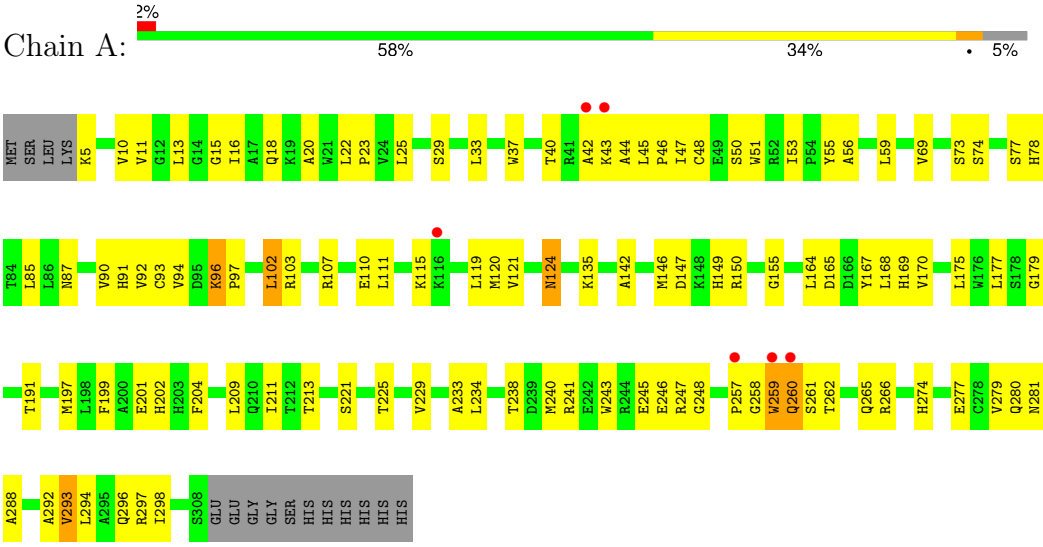
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	14	Total O 14 14	0	0

3 Residue-property plots (i)

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.

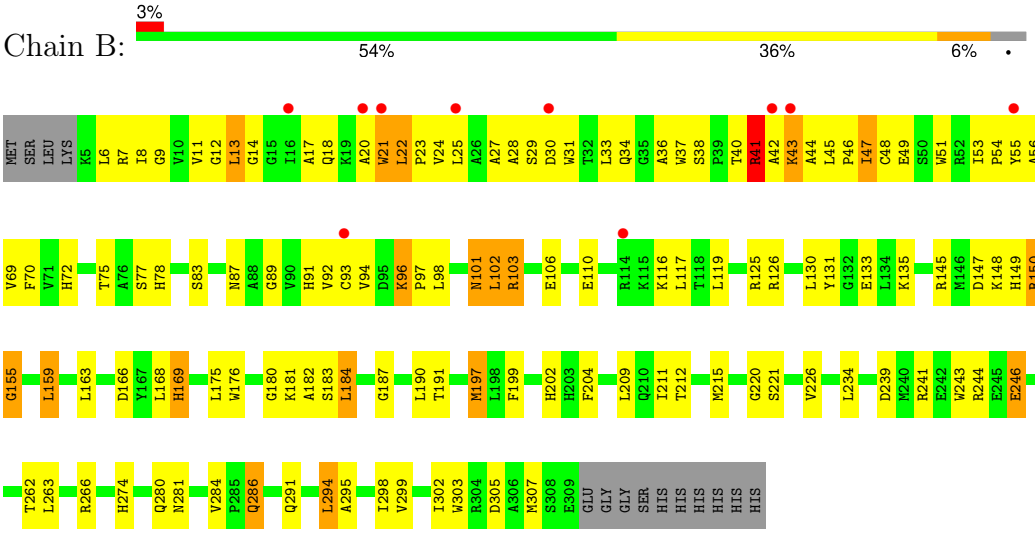
• Molecule 1: PUTATIVE OXIDOREDUCTASE (VIRULENCE FACTOR mviM HOMOLOG)

Chain A:



• Molecule 1: PUTATIVE OXIDOREDUCTASE (VIRULENCE FACTOR mviM HOMOLOG)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	96.86Å 96.86Å 380.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.91 – 2.70 19.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.91-2.70) 99.2 (19.91-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.294 0.242 , 0.291	Depositor DCC
R_{free} test set	1474 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4767	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0/2391	0.64	0/3248
1	B	0.54	0/2400	0.65	0/3260
All	All	0.53	0/4791	0.65	0/6508

There are no bond length outliers.

There are no bond angle outliers.

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	2341	0	2329	104	0
1	B	2350	0	2335	138	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
3	A	22	0	0	0	0
3	B	14	0	0	1	0
All	All	4767	0	4664	239	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 25.

All (239) 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:96:LYS:HB3	1:A:97:PRO:HD3	1.41	1.02
1:A:179:GLY:HA3	1:A:181:LYS:HE2	1.47	0.95
1:B:96:LYS:HB3	1:B:97:PRO:HD3	1.50	0.92
1:A:285:PRO:HG2	1:A:288:ALA:HB2	1.61	0.82
1:A:260:GLN:HE21	1:A:265:GLN:HE22	1.30	0.80
1:B:274:HIS:HE1	1:B:286:GLN:H	1.30	0.78
1:A:18:GLN:HA	1:A:22:LEU:HD12	1.69	0.75
1:A:43:LYS:C	1:A:46:PRO:HD2	2.07	0.75
1:A:43:LYS:O	1:A:46:PRO:HD2	1.88	0.72
1:A:280:GLN:HG3	1:A:281:ASN:ND2	2.05	0.71
1:A:16:ILE:HD12	1:A:16:ILE:H	1.54	0.71
1:A:96:LYS:HB3	1:A:97:PRO:CD	2.14	0.70
1:A:257:PRO:HG2	1:A:259:TRP:HB3	1.74	0.70
1:B:89:GLY:HA2	1:B:117:LEU:HD11	1.73	0.69
1:A:170:VAL:HG12	1:A:213:THR:HG22	1.73	0.69
1:B:204:PHE:HB2	1:B:211:ILE:HB	1.76	0.68
1:B:262:THR:O	1:B:266:ARG:HG2	1.94	0.68
1:B:17:ALA:HA	1:B:21:TRP:HB2	1.75	0.68
1:B:263:LEU:HD12	1:B:263:LEU:H	1.59	0.68
1:A:259:TRP:CH2	1:A:265:GLN:HG2	2.29	0.67
1:B:33:LEU:HD22	1:B:53:ILE:HD11	1.77	0.67
1:B:13:LEU:H	1:B:13:LEU:HD12	1.59	0.66
1:A:175:LEU:HD11	1:A:298:ILE:HD12	1.78	0.66
1:B:20:ALA:O	1:B:24:VAL:HG13	1.96	0.66
1:B:92:VAL:HB	1:B:119:LEU:CD2	2.25	0.66
1:B:133:GLU:OE2	1:B:254:LYS:HE2	1.95	0.65
1:B:135:LYS:HE2	1:B:176:TRP:O	1.96	0.65
1:B:48:CYS:HA	1:B:53:ILE:HG22	1.78	0.65
1:A:45:LEU:HD22	1:A:45:LEU:H	1.60	0.65
1:B:12:GLY:O	1:B:13:LEU:O	2.15	0.65
1:A:191:THR:HG22	1:A:197:MET:HA	1.79	0.64
1:B:47:ILE:HD12	1:B:47:ILE:H	1.60	0.64
1:B:96:LYS:HG2	1:B:168:LEU:HD23	1.79	0.63
1:B:29:SER:O	1:B:30:ASP:HB3	1.98	0.63
1:B:75:THR:HG23	1:B:97:PRO:HB2	1.81	0.63
1:B:103:ARG:HG2	1:B:103:ARG:HH11	1.62	0.63
1:A:96:LYS:HE3	1:A:169:HIS:CE1	2.34	0.63
1:A:102:LEU:HD22	1:A:296:GLN:HE21	1.64	0.63
1:A:274:HIS:HE1	1:A:286:GLN:H	1.47	0.62
1:A:43:LYS:HE2	1:A:43:LYS:HA	1.82	0.62
1:A:48:CYS:HB3	1:A:53:ILE:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:SER:HA	1:B:221:SER:H	1.66	0.60
1:B:24:VAL:HG23	1:B:25:LEU:HD22	1.84	0.60
1:B:103:ARG:CD	1:B:103:ARG:H	2.15	0.60
1:B:281:ASN:N	1:B:281:ASN:HD22	1.97	0.60
1:B:7:ARG:CD	1:B:34:GLN:HE21	2.14	0.59
1:A:42:ALA:C	1:A:44:ALA:H	2.06	0.59
1:A:260:GLN:HE21	1:A:265:GLN:NE2	1.98	0.58
1:B:101:ASN:HD21	1:B:103:ARG:HD3	1.69	0.58
1:A:40:THR:HG22	1:A:42:ALA:HB3	1.85	0.58
1:A:81:VAL:O	1:A:85:LEU:HD23	2.03	0.58
1:B:163:LEU:HD23	1:B:197:MET:HE3	1.84	0.58
1:B:184:LEU:HD11	1:B:302:ILE:HG12	1.86	0.57
1:A:13:LEU:N	1:A:13:LEU:HD12	2.19	0.57
1:B:103:ARG:HG2	1:B:103:ARG:NH1	2.19	0.56
1:B:150:ARG:HG2	1:B:153:SER:HB3	1.87	0.56
1:B:7:ARG:HB3	1:B:34:GLN:HB2	1.87	0.56
1:B:163:LEU:HD23	1:B:197:MET:CE	2.35	0.56
1:A:146:MET:SD	1:A:170:VAL:HA	2.46	0.56
1:A:181:LYS:HD3	1:A:181:LYS:N	2.21	0.55
1:A:37:TRP:HD1	1:A:56:ALA:O	1.89	0.55
1:A:45:LEU:HD22	1:A:45:LEU:N	2.21	0.55
1:A:45:LEU:HB2	1:A:46:PRO:HD3	1.89	0.55
1:B:17:ALA:O	1:B:22:LEU:HB2	2.06	0.55
1:A:103:ARG:O	1:A:107:ARG:HG3	2.06	0.55
1:B:8:ILE:HD13	1:B:31:TRP:HB2	1.89	0.54
1:A:59:LEU:HD22	1:A:85:LEU:HD21	1.90	0.54
1:A:121:VAL:HG23	1:A:292:ALA:HB1	1.89	0.54
1:B:45:LEU:N	1:B:46:PRO:CD	2.71	0.54
1:B:96:LYS:HB3	1:B:97:PRO:CD	2.30	0.54
1:A:246:GLU:HG2	1:B:221:SER:HB2	1.90	0.53
1:B:22:LEU:HB3	1:B:23:PRO:HD3	1.89	0.53
1:A:5:LYS:HE2	1:A:29:SER:O	2.07	0.53
1:A:225:THR:HG22	1:A:238:THR:HA	1.90	0.53
1:B:37:TRP:CG	1:B:38:SER:N	2.77	0.53
1:B:9:GLY:O	1:B:69:VAL:HG13	2.08	0.53
1:A:10:VAL:HG23	1:A:33:LEU:HD11	1.91	0.53
1:B:53:ILE:CD1	1:B:54:PRO:HD2	2.38	0.53
1:A:103:ARG:HB3	1:A:107:ARG:NH1	2.23	0.53
1:B:53:ILE:HD12	1:B:54:PRO:CD	2.39	0.53
1:B:298:ILE:HD12	1:B:298:ILE:N	2.24	0.53
1:A:221:SER:HB3	1:B:234:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:HG2	1:A:288:ALA:CB	2.37	0.53
1:B:103:ARG:H	1:B:103:ARG:HD2	1.74	0.53
1:B:106:GLU:O	1:B:110:GLU:HG3	2.09	0.53
1:A:48:CYS:SG	1:A:55:TYR:HD1	2.32	0.52
1:A:77:SER:O	1:A:81:VAL:HG23	2.09	0.52
1:B:53:ILE:HD12	1:B:54:PRO:HD2	1.91	0.52
1:B:101:ASN:C	1:B:101:ASN:ND2	2.61	0.52
1:B:92:VAL:HB	1:B:119:LEU:HD23	1.90	0.52
1:B:295:ALA:HA	1:B:298:ILE:HD13	1.91	0.52
1:A:22:LEU:HB2	1:A:23:PRO:HD3	1.91	0.52
1:B:274:HIS:CE1	1:B:286:GLN:H	2.20	0.52
1:A:40:THR:HG22	1:A:42:ALA:CB	2.40	0.51
1:A:43:LYS:O	1:A:47:ILE:HG13	2.10	0.51
1:A:241:ARG:HE	1:A:260:GLN:NE2	2.09	0.51
1:B:29:SER:O	1:B:30:ASP:CB	2.58	0.51
1:B:92:VAL:HG12	1:B:93:CYS:N	2.26	0.51
1:B:159:LEU:HD22	1:B:163:LEU:HG	1.93	0.51
1:A:40:THR:C	1:A:42:ALA:H	2.13	0.51
1:B:151:SER:HA	1:B:221:SER:N	2.26	0.51
1:B:44:ALA:HA	1:B:47:ILE:CD1	2.42	0.50
1:B:70:PHE:HB3	1:B:72:HIS:CE1	2.46	0.50
1:B:154:VAL:HG13	1:B:154:VAL:O	2.11	0.50
1:B:281:ASN:N	1:B:281:ASN:ND2	2.58	0.50
1:A:102:LEU:CD2	1:A:296:GLN:HG2	2.42	0.50
1:A:274:HIS:CE1	1:A:286:GLN:H	2.30	0.50
1:B:37:TRP:HB2	1:B:56:ALA:HB3	1.93	0.50
1:B:102:LEU:O	1:B:106:GLU:HG3	2.12	0.50
1:B:20:ALA:HA	1:B:263:LEU:HD23	1.93	0.49
1:B:44:ALA:HA	1:B:47:ILE:HD13	1.93	0.49
1:A:92:VAL:HG13	1:A:119:LEU:CD1	2.42	0.49
1:A:146:MET:SD	1:A:170:VAL:HG13	2.52	0.49
1:A:73:SER:O	1:A:74:SER:C	2.50	0.49
1:A:211:ILE:HD12	1:A:211:ILE:N	2.27	0.49
1:A:91:HIS:CD2	1:A:279:VAL:HG13	2.48	0.49
1:B:183:SER:O	1:B:204:PHE:HA	2.12	0.49
1:A:45:LEU:H	1:A:45:LEU:CD2	2.24	0.49
1:B:7:ARG:HG2	1:B:34:GLN:HE21	1.77	0.49
1:B:20:ALA:C	1:B:22:LEU:H	2.16	0.49
1:B:11:VAL:HA	1:B:37:TRP:O	2.12	0.49
1:A:78:HIS:O	1:A:82:VAL:HG23	2.12	0.48
1:B:20:ALA:O	1:B:24:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:TRP:CD2	1:B:72:HIS:CE1	3.02	0.48
1:B:209:LEU:HG	1:B:211:ILE:HD11	1.95	0.48
1:B:295:ALA:O	1:B:299:VAL:HG23	2.13	0.48
1:A:69:VAL:HG23	1:A:90:VAL:HG11	1.94	0.48
1:A:43:LYS:HE2	1:A:46:PRO:HG2	1.96	0.48
1:A:248:GLY:N	1:B:220:GLY:O	2.46	0.47
1:B:45:LEU:HG	1:B:49:GLU:OE2	2.14	0.47
1:B:103:ARG:HD2	1:B:103:ARG:N	2.30	0.47
1:A:259:TRP:O	1:A:259:TRP:CG	2.67	0.47
1:A:11:VAL:HG13	1:A:37:TRP:HE3	1.79	0.47
1:A:13:LEU:HD23	1:A:47:ILE:CG2	2.45	0.47
1:A:111:LEU:O	1:A:115:LYS:HB2	2.15	0.47
1:A:135:LYS:HB2	1:A:177:LEU:HD23	1.96	0.47
1:A:142:ALA:C	1:A:209:LEU:HD12	2.35	0.47
1:B:7:ARG:HB3	1:B:34:GLN:CB	2.44	0.47
1:B:7:ARG:CG	1:B:34:GLN:HE21	2.28	0.47
1:B:101:ASN:HD22	1:B:102:LEU:N	2.13	0.46
1:B:41:ARG:HB2	1:B:55:TYR:OH	2.15	0.46
1:B:40:THR:C	1:B:42:ALA:H	2.18	0.46
1:A:233:ALA:HB2	1:A:247:ARG:HG2	1.98	0.46
1:B:133:GLU:CD	1:B:254:LYS:HE2	2.35	0.46
1:B:36:ALA:HA	1:B:62:LEU:HD21	1.98	0.46
1:A:181:LYS:HD3	1:A:181:LYS:H	1.80	0.46
1:B:89:GLY:O	1:B:117:LEU:HD21	2.15	0.46
1:A:167:TYR:OH	1:A:202:HIS:HD2	1.98	0.46
1:A:229:VAL:HA	1:A:234:LEU:HD23	1.97	0.46
1:B:23:PRO:HG3	1:B:51:TRP:HH2	1.80	0.46
1:B:7:ARG:HD2	1:B:34:GLN:HE21	1.80	0.45
1:B:243:TRP:C	1:B:243:TRP:CD1	2.89	0.45
1:A:240:MET:HE3	1:A:266:ARG:NH1	2.31	0.45
1:A:124:ASN:HD22	1:A:124:ASN:H	1.65	0.45
1:A:20:ALA:O	1:A:23:PRO:HD2	2.17	0.45
1:B:12:GLY:O	1:B:13:LEU:C	2.54	0.45
1:B:7:ARG:C	1:B:8:ILE:HD12	2.37	0.45
1:A:96:LYS:HE3	1:A:169:HIS:NE2	2.31	0.45
1:B:77:SER:O	1:B:78:HIS:C	2.55	0.45
1:B:145:ARG:HG3	1:B:212:THR:HB	1.98	0.45
1:A:149:HIS:O	1:A:150:ARG:HD2	2.17	0.45
1:B:209:LEU:CD2	1:B:211:ILE:HD11	2.47	0.45
1:B:190:LEU:HB3	1:B:199:PHE:HB3	1.99	0.45
1:B:9:GLY:C	1:B:69:VAL:HG13	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LEU:O	1:B:298:ILE:CD1	2.64	0.44
1:B:303:TRP:CE2	1:B:307:MET:HG3	2.52	0.44
1:B:148:LYS:O	1:B:215:MET:HG3	2.17	0.44
1:B:182:ALA:HB1	1:B:204:PHE:HB3	1.98	0.44
1:B:103:ARG:CD	1:B:103:ARG:N	2.80	0.44
1:B:23:PRO:HG3	1:B:51:TRP:CH2	2.53	0.44
1:B:96:LYS:HD3	1:B:168:LEU:HB3	1.99	0.44
1:B:20:ALA:HA	1:B:263:LEU:CD2	2.48	0.44
1:B:133:GLU:OE1	1:B:254:LYS:NZ	2.51	0.44
1:B:125:ARG:NH1	1:B:169:HIS:CE1	2.86	0.44
1:B:43:LYS:O	1:B:47:ILE:HD11	2.18	0.43
1:B:126:ARG:NH1	1:B:291:GLN:OE1	2.46	0.43
1:B:305:ASP:C	1:B:307:MET:H	2.21	0.43
1:B:24:VAL:HG13	1:B:263:LEU:HD23	2.00	0.43
1:B:159:LEU:HG	1:B:191:THR:HG22	1.99	0.43
1:B:8:ILE:HD12	1:B:8:ILE:N	2.33	0.43
1:B:244:ARG:HG2	1:B:253:HIS:CD2	2.53	0.43
1:A:97:PRO:HG3	1:A:164:LEU:O	2.17	0.43
1:A:240:MET:CE	1:A:266:ARG:NH1	2.81	0.43
1:A:40:THR:CG2	1:A:42:ALA:HB3	2.48	0.43
1:B:21:TRP:HA	1:B:21:TRP:CE3	2.53	0.43
1:B:27:ALA:HA	3:B:330:HOH:O	2.19	0.43
1:B:83:SER:O	1:B:87:ASN:ND2	2.52	0.43
1:B:209:LEU:HD21	1:B:211:ILE:HD11	2.00	0.43
1:A:83:SER:O	1:A:87:ASN:ND2	2.52	0.43
1:A:44:ALA:HB1	1:A:55:TYR:CE1	2.53	0.42
1:B:96:LYS:HE3	1:B:169:HIS:CG	2.53	0.42
1:B:11:VAL:HG23	1:B:69:VAL:HG11	2.00	0.42
1:B:125:ARG:HH12	1:B:169:HIS:CE1	2.37	0.42
1:B:175:LEU:O	1:B:180:GLY:N	2.50	0.42
1:A:199:PHE:CZ	1:A:201:GLU:HB2	2.54	0.42
1:B:22:LEU:HA	1:B:25:LEU:HD23	2.01	0.42
1:B:246:GLU:HG3	1:B:251:VAL:HG22	1.99	0.42
1:A:23:PRO:HG3	1:A:51:TRP:HH2	1.85	0.42
1:B:147:ASP:HB3	1:B:149:HIS:NE2	2.34	0.42
1:A:258:GLY:C	1:A:260:GLN:H	2.21	0.42
1:A:287:THR:O	1:A:292:ALA:HB2	2.19	0.42
1:B:22:LEU:HA	1:B:22:LEU:HD12	1.88	0.42
1:A:293:VAL:HG22	1:A:293:VAL:O	2.19	0.42
1:B:209:LEU:CG	1:B:211:ILE:HD11	2.50	0.42
1:A:47:ILE:O	1:A:50:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:CD1	1:A:298:ILE:HD12	2.47	0.41
1:A:259:TRP:O	1:A:261:SER:N	2.54	0.41
1:B:133:GLU:OE1	1:B:254:LYS:HE2	2.19	0.41
1:A:183:SER:O	1:A:204:PHE:HA	2.20	0.41
1:B:41:ARG:HG3	1:B:41:ARG:HH11	1.86	0.41
1:B:131:TYR:CE2	1:B:226:VAL:HG21	2.55	0.41
1:A:92:VAL:HG22	1:A:93:CYS:N	2.35	0.41
1:B:68:ALA:HA	1:B:91:HIS:O	2.21	0.41
1:A:234:LEU:O	1:A:245:GLU:HA	2.20	0.41
1:A:257:PRO:C	1:A:259:TRP:N	2.74	0.41
1:B:130:LEU:HD22	1:B:243:TRP:CE3	2.56	0.41
1:B:239:ASP:C	1:B:241:ARG:H	2.24	0.41
1:A:13:LEU:N	1:A:13:LEU:CD1	2.81	0.41
1:A:42:ALA:C	1:A:44:ALA:N	2.72	0.41
1:A:281:ASN:N	1:A:281:ASN:HD22	2.18	0.41
1:B:101:ASN:ND2	1:B:102:LEU:N	2.68	0.41
1:B:154:VAL:O	1:B:155:GLY:O	2.38	0.41
1:A:102:LEU:HD22	1:A:296:GLN:NE2	2.32	0.41
1:A:201:GLU:HA	1:A:213:THR:O	2.20	0.41
1:B:6:LEU:HD12	1:B:6:LEU:N	2.37	0.41
1:A:297:ARG:HG3	1:A:297:ARG:HH11	1.86	0.40
1:A:243:TRP:CD1	1:A:243:TRP:C	2.94	0.40
1:A:261:SER:O	1:A:262:THR:C	2.56	0.40
1:B:62:LEU:HD13	1:B:62:LEU:O	2.20	0.40
1:B:78:HIS:CD2	1:B:97:PRO:O	2.74	0.40
1:A:96:LYS:HE2	1:A:165:ASP:O	2.21	0.40
1:A:257:PRO:C	1:A:259:TRP:H	2.24	0.40
1:B:13:LEU:HD12	1:B:13:LEU:N	2.32	0.40
1:B:239:ASP:C	1:B:241:ARG:N	2.73	0.40
1:B:280:GLN:HE21	1:B:280:GLN:HB2	1.47	0.40
1:A:25:LEU:O	1:A:33:LEU:HD22	2.21	0.40
1:A:120:MET:HB3	1:A:285:PRO:HG3	2.04	0.40
1:B:42:ALA:C	1:B:44:ALA:H	2.24	0.40
1:B:187:GLY:HA3	1:B:202:HIS:CD2	2.57	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	302/319 (95%)	271 (90%)	26 (9%)	5 (2%)	9 23
1	B	303/319 (95%)	256 (84%)	35 (12%)	12 (4%)	3 6
All	All	605/638 (95%)	527 (87%)	61 (10%)	17 (3%)	5 11

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	B	13	LEU
1	B	96	LYS
1	B	155	GLY
1	A	15	GLY
1	A	155	GLY
1	A	260	GLN
1	A	293	VAL
1	B	21	TRP
1	B	181	LYS
1	B	28	ALA
1	B	43	LYS
1	B	294	LEU
1	B	22	LEU
1	B	41	ARG
1	B	154	VAL
1	B	14	GLY

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	246/259 (95%)	235 (96%)	11 (4%)	27 55
1	B	247/259 (95%)	229 (93%)	18 (7%)	14 33
All	All	493/518 (95%)	464 (94%)	29 (6%)	19 43

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	A	102	LEU
1	A	110	GLU
1	A	124	ASN
1	A	147	ASP
1	A	168	LEU
1	A	181	LYS
1	A	259	TRP
1	A	277	GLU
1	A	286	GLN
1	A	294	LEU
1	B	18	GLN
1	B	41	ARG
1	B	47	ILE
1	B	94	VAL
1	B	98	LEU
1	B	101	ASN
1	B	102	LEU
1	B	103	ARG
1	B	116	LYS
1	B	150	ARG
1	B	159	LEU
1	B	166	ASP
1	B	169	HIS
1	B	184	LEU
1	B	197	MET
1	B	246	GLU
1	B	284	VAL
1	B	286	GLN

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	34	GLN
1	A	87	ASN
1	A	124	ASN
1	A	137	GLN
1	A	202	HIS
1	A	203	HIS
1	A	249	GLN
1	A	260	GLN
1	A	274	HIS
1	A	281	ASN
1	A	286	GLN
1	A	296	GLN
1	B	18	GLN
1	B	34	GLN
1	B	72	HIS
1	B	78	HIS
1	B	101	ASN
1	B	137	GLN
1	B	169	HIS
1	B	210	GLN
1	B	227	GLN
1	B	274	HIS
1	B	280	GLN
1	B	281	ASN
1	B	286	GLN
1	B	296	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	321	-	4,4,4	0.51	0	6,6,6	0.12	0
2	SO4	A	323	-	4,4,4	0.70	0	6,6,6	0.15	0
2	SO4	B	321	-	4,4,4	0.72	0	6,6,6	0.22	0
2	SO4	B	322	-	4,4,4	0.63	0	6,6,6	0.17	0
2	SO4	A	320	-	4,4,4	0.46	0	6,6,6	0.16	0
2	SO4	A	322	-	4,4,4	0.64	0	6,6,6	0.17	0
2	SO4	B	320	-	4,4,4	0.45	0	6,6,6	0.24	0
2	SO4	B	323	-	4,4,4	0.81	0	6,6,6	0.23	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	304/319 (95%)	-0.15	6 (1%) 65 67	30, 48, 61, 66	0
1	B	305/319 (95%)	-0.01	10 (3%) 46 46	35, 51, 64, 71	0
All	All	609/638 (95%)	-0.08	16 (2%) 56 57	30, 50, 63, 71	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	TRP	4.8
1	B	43	LYS	3.8
1	B	16	ILE	3.6
1	B	20	ALA	3.4
1	B	30	ASP	3.4
1	A	260	GLN	3.3
1	A	43	LYS	3.2
1	A	42	ALA	3.2
1	B	42	ALA	3.2
1	B	55	TYR	3.1
1	B	21	TRP	2.9
1	B	93	CYS	2.5
1	A	257	PRO	2.1
1	B	25	LEU	2.1
1	B	114	ARG	2.1
1	A	116	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	SO4	A	322	5/5	0.94	0.17	76,78,79,79	0
2	SO4	B	323	5/5	0.95	0.35	85,88,88,88	0
2	SO4	B	320	5/5	0.97	0.14	66,66,67,67	0
2	SO4	B	321	5/5	0.97	0.12	81,82,83,83	0
2	SO4	B	322	5/5	0.97	0.15	74,75,75,75	0
2	SO4	A	323	5/5	0.97	0.10	74,76,77,77	0
2	SO4	A	321	5/5	0.98	0.15	68,68,69,69	0
2	SO4	A	320	5/5	0.99	0.13	58,58,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.