Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:10 pm BST

PDB ID	:	2VA8
Title	:	DNA Repair Helicase Hel308
Authors	:	Johnson, K.A.; Richards, J.; Liu, H.; McMahon, S.; Oke, M.; Carter, L.; Naismith, J.H.; White, M.F.
Deposited on	:	2007-08-30
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

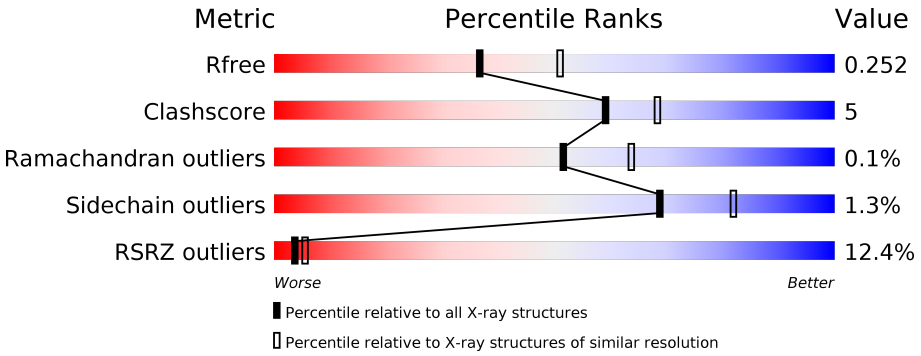
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	715	11% 87% 10%
1	B	715	13% 84% 12%

2 Entry composition

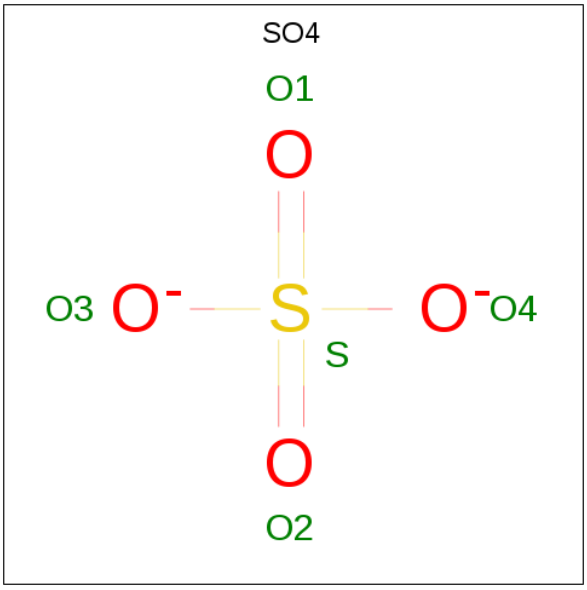
There are 3 unique types of molecules in this entry. The entry contains 11297 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SKI2-TYPE HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5550	3551	936	1049	14			
1	B	695	Total	C	N	O	S	0	0	0
			5566	3563	938	1051	14			

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



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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.

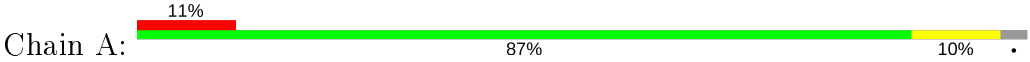
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	62	Total O 62 62	0	0
3	B	84	Total O 84 84	0	0

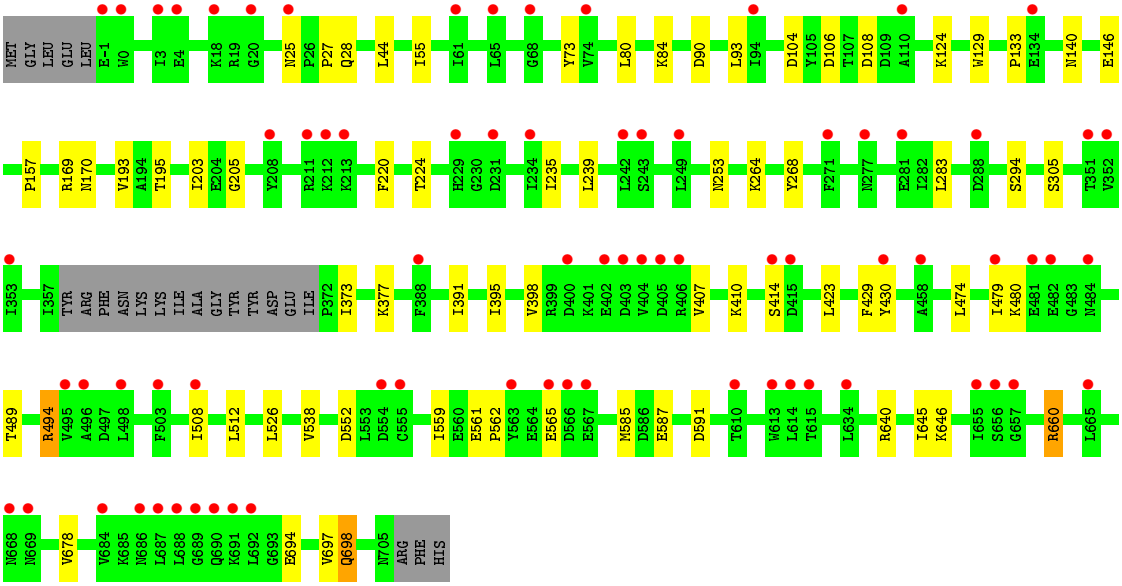
3 Residue-property plots (i)

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 (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: SKI2-TYPE HELICASE

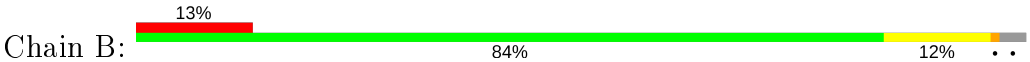
Chain A:

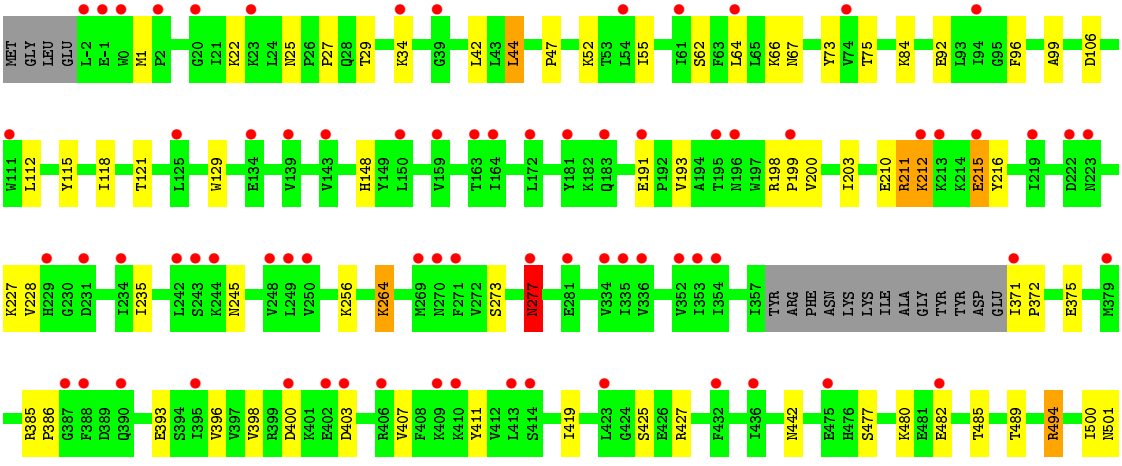


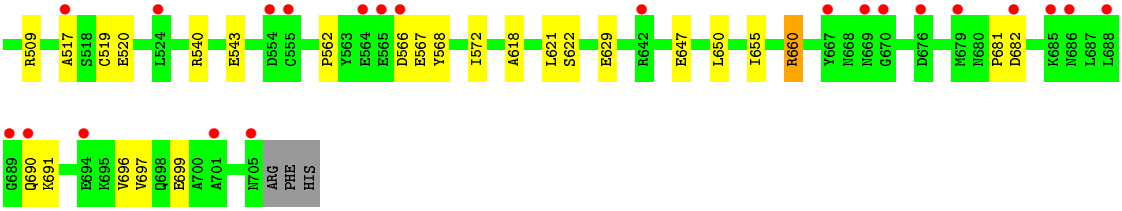


- Molecule 1: SKI2-TYPE HELICASE

Chain B:






R509
A517
S518
C519
E520
L524
R540
E543
D554
C555
P562
Y563
E564
E565
D566
E567
Y568
I572
A618
L621
S622
E629
R642
E647
L650
I655
R660
Y667
N668
N669
G670
D676
M679
N680
P681
D682
K685
N686
L687
L688
G689
Q690
K691
E694
K695
V696
V697
Q698
E699
A700
A701
N705
ARG
PHE
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.66Å 138.08Å 107.55Å 90.00° 94.65° 90.00°	Depositor
Resolution (Å)	107.21 – 2.30 29.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (107.21-2.30) 99.8 (29.99-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.68 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.259 0.206 , 0.252	Depositor DCC
R_{free} test set	3995 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11297	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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	0.50	0/5647	0.59	2/7628 (0.0%)
1	B	0.61	10/5663 (0.2%)	0.62	2/7651 (0.0%)
All	All	0.56	10/11310 (0.1%)	0.60	4/15279 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	273	SER	CB-OG	9.03	1.53	1.42
1	B	211	ARG	CZ-NH2	7.61	1.43	1.33
1	B	212	LYS	CE-NZ	7.08	1.66	1.49
1	B	216	TYR	C-N	6.56	1.49	1.34
1	B	216	TYR	CE1-CZ	6.23	1.46	1.38
1	B	277	ASN	CG-ND2	5.83	1.47	1.32
1	B	227	LYS	C-O	5.82	1.34	1.23
1	B	216	TYR	CG-CD2	5.75	1.46	1.39
1	B	215	GLU	CG-CD	5.39	1.60	1.51
1	B	228	VAL	C-N	5.23	1.46	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	494	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	B	215	GLU	OE1-CD-OE2	-5.39	116.84	123.30
1	A	494	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	494	ARG	NE-CZ-NH2	5.16	122.88	120.30

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	5550	0	5659	43	0
1	B	5566	0	5680	65	0
2	A	10	0	0	0	0
2	B	25	0	0	0	0
3	A	62	0	0	1	0
3	B	84	0	0	1	0
All	All	11297	0	11339	106	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 5.

All (106) 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:480:LYS:HE3	1:A:489:THR:HG22	1.46	0.97
1:A:25:ASN:HB3	1:A:27:PRO:HD2	1.47	0.94
1:B:62:SER:O	1:B:66:LYS:HG2	1.70	0.90
1:B:372:PRO:HG2	1:B:375:GLU:HG3	1.60	0.82
1:B:198:ARG:HD2	1:B:200:VAL:O	1.80	0.81
1:A:106:ASP:OD1	1:A:494:ARG:NH1	2.15	0.79
1:A:526:LEU:HA	1:A:559:ILE:HD11	1.64	0.77
1:B:34:LYS:HD3	1:B:193:VAL:HG22	1.67	0.76
1:A:235:ILE:HD11	1:A:264:LYS:HG2	1.67	0.75
1:B:106:ASP:OD1	1:B:494:ARG:NH1	2.18	0.75
1:B:25:ASN:HB3	1:B:27:PRO:HD2	1.71	0.72
1:B:517:ALA:HB2	1:B:629:GLU:HG2	1.71	0.72
1:B:500:ILE:HD11	1:B:621:LEU:HD11	1.73	0.70
1:B:372:PRO:HG2	1:B:375:GLU:CG	2.20	0.69
1:A:283:LEU:HD11	1:A:305:SER:HB3	1.73	0.69
1:B:482:GLU:O	1:B:485:THR:HB	1.95	0.65
1:B:1:MET:H	1:B:29:THR:HG21	1.63	0.64
1:B:112:LEU:HD22	1:B:118:ILE:HG12	1.79	0.64
1:A:585:MET:HG2	1:A:640:ARG:HB3	1.80	0.63
1:B:52:LYS:HA	1:B:55:ILE:HD12	1.81	0.62
1:B:73:TYR:CE2	1:B:84:LYS:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:PRO:CG	1:B:375:GLU:HG3	2.29	0.59
1:A:157:PRO:HB3	1:A:423:LEU:HD23	1.84	0.59
1:B:25:ASN:O	1:B:29:THR:HG23	2.04	0.57
1:B:398:VAL:HG11	1:B:403:ASP:HB3	1.87	0.57
1:B:647:GLU:O	1:B:650:LEU:HG	2.04	0.56
1:B:371:ILE:HG23	1:B:411:TYR:OH	2.06	0.56
3:A:2044:HOH:O	1:B:256:LYS:HG2	2.06	0.55
1:B:480:LYS:HE3	1:B:489:THR:HG22	1.89	0.54
1:A:694:GLU:O	1:A:698:GLN:NE2	2.41	0.54
1:B:211:ARG:HB3	1:B:212:LYS:HZ2	1.71	0.54
1:A:587:GLU:HA	1:A:660:ARG:HH21	1.73	0.53
1:B:211:ARG:CB	1:B:212:LYS:HZ2	2.21	0.53
1:B:210:GLU:HB2	1:B:215:GLU:HG3	1.91	0.53
1:B:398:VAL:HG12	1:B:400:ASP:H	1.74	0.52
1:B:198:ARG:HG2	1:B:199:PRO:HD2	1.91	0.52
1:A:538:VAL:O	1:B:540:ARG:HD2	2.09	0.52
1:A:80:LEU:O	1:A:84:LYS:HG2	2.10	0.52
1:B:211:ARG:HB2	1:B:212:LYS:NZ	2.25	0.52
1:B:427:ARG:HG2	1:B:501:ASN:ND2	2.24	0.52
1:A:108:ASP:HB2	1:A:133:PRO:HB3	1.93	0.51
1:A:373:ILE:O	1:A:377:LYS:HG2	2.10	0.51
1:B:106:ASP:CG	1:B:494:ARG:HH12	2.12	0.51
1:B:562:PRO:HB3	1:B:567:GLU:HB3	1.93	0.50
1:A:430:TYR:N	1:A:430:TYR:CD1	2.79	0.50
1:A:73:TYR:CE2	1:A:84:LYS:HG3	2.47	0.50
1:A:157:PRO:HB3	1:A:423:LEU:CD2	2.42	0.50
1:B:148:HIS:HA	1:B:419:ILE:HD11	1.94	0.50
1:B:203:ILE:HD11	1:B:393:GLU:HG2	1.94	0.49
1:A:640:ARG:NH2	1:A:646:LYS:HD3	2.27	0.49
1:B:403:ASP:O	1:B:407:VAL:HG23	2.11	0.49
1:B:64:LEU:O	1:B:67:ASN:O	2.30	0.49
1:A:552:ASP:OD1	1:B:264:LYS:HE3	2.12	0.49
1:B:92:GLU:HA	1:B:96:PHE:O	2.13	0.48
1:B:520:GLU:H	1:B:520:GLU:CD	2.17	0.48
1:B:211:ARG:CB	1:B:212:LYS:NZ	2.77	0.48
1:A:106:ASP:CG	1:A:494:ARG:HH12	2.14	0.48
1:A:678:VAL:HA	1:A:697:VAL:HG13	1.96	0.48
1:B:480:LYS:HG3	1:B:489:THR:HG22	1.96	0.47
1:B:396:VAL:HG11	1:B:407:VAL:HG11	1.95	0.47
1:A:430:TYR:N	1:A:430:TYR:HD1	2.13	0.47
1:A:205:GLY:O	1:A:395:ILE:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:VAL:CG1	1:A:407:VAL:HG21	2.46	0.46
1:A:90:ASP:O	1:A:93:LEU:HD12	2.15	0.46
1:B:277:ASN:OD1	1:B:277:ASN:N	2.49	0.46
1:A:645:ILE:HG22	1:A:660:ARG:HG3	1.98	0.46
1:B:568:TYR:CE1	1:B:572:ILE:HD11	2.51	0.46
1:B:562:PRO:CB	1:B:567:GLU:HB3	2.46	0.45
1:B:690:GLN:H	1:B:690:GLN:CD	2.19	0.45
1:B:442:ASN:HB3	1:B:485:THR:HG23	1.98	0.45
1:B:99:ALA:HB2	1:B:115:TYR:CD1	2.52	0.45
1:A:398:VAL:HG11	1:A:407:VAL:HG21	1.98	0.44
1:B:75:THR:O	1:B:121:THR:HA	2.16	0.44
1:B:682:ASP:OD1	1:B:682:ASP:N	2.49	0.44
1:A:410:LYS:O	1:A:414:SER:OG	2.36	0.44
1:B:655:ILE:HG21	1:B:696:VAL:HG13	2.00	0.44
1:B:42:LEU:HD23	1:B:191:GLU:HB3	2.00	0.44
1:A:104:ASP:O	1:A:124:LYS:NZ	2.40	0.44
1:A:561:GLU:HA	1:A:562:PRO:HD3	1.89	0.43
1:B:148:HIS:HA	1:B:419:ILE:CD1	2.47	0.43
1:A:294:SER:OG	1:A:591:ASP:OD1	2.36	0.43
1:B:1:MET:N	1:B:29:THR:HG21	2.33	0.43
1:B:477:SER:HB2	1:B:509:ARG:HH12	1.82	0.43
1:B:681:PRO:HA	1:B:697:VAL:HG21	2.01	0.43
1:B:44:LEU:HD22	1:B:55:ILE:HG21	2.00	0.43
1:B:385:ARG:HA	1:B:386:PRO:HD3	1.87	0.43
1:A:480:LYS:CE	1:A:489:THR:HG22	2.33	0.42
1:B:543:GLU:HG3	1:B:572:ILE:HG21	2.01	0.42
1:A:28:GLN:HG2	1:A:55:ILE:HG13	2.02	0.42
1:A:508:ILE:O	1:A:512:LEU:HG	2.20	0.41
1:A:140:ASN:HA	1:A:169:ARG:HG2	2.02	0.41
1:B:44:LEU:CD2	1:B:55:ILE:HD13	2.50	0.41
1:A:80:LEU:HD13	1:A:146:GLU:OE2	2.21	0.41
1:A:27:PRO:HB3	1:A:195:THR:HG21	2.02	0.41
1:B:398:VAL:CG1	1:B:403:ASP:HB3	2.50	0.41
1:B:568:TYR:CE1	1:B:572:ILE:CD1	3.02	0.41
1:A:474:LEU:HD23	1:A:479:ILE:HG13	2.02	0.41
1:B:235:ILE:HD11	1:B:264:LYS:HG2	2.03	0.41
1:A:169:ARG:HB3	1:A:170:ASN:H	1.55	0.41
1:A:220:PHE:HB2	1:A:224:THR:HB	2.02	0.41
1:B:690:GLN:HG2	1:B:691:LYS:H	1.85	0.41
1:A:239:LEU:HD11	1:A:268:TYR:HB3	2.03	0.40
1:A:44:LEU:HD23	1:A:193:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:ARG:HG2	3:B:2075:HOH:O	2.21	0.40
1:B:618:ALA:O	1:B:622:SER:HB2	2.22	0.40
1:A:203:ILE:HG23	1:A:391:ILE:HD11	2.04	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	689/715 (96%)	666 (97%)	23 (3%)	0	100	100
1	B	691/715 (97%)	671 (97%)	18 (3%)	2 (0%)	41	50
All	All	1380/1430 (96%)	1337 (97%)	41 (3%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	245	ASN
1	B	47	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	605/624 (97%)	599 (99%)	6 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	607/624 (97%)	597 (98%)	10 (2%)	62 78
All	All	1212/1248 (97%)	1196 (99%)	16 (1%)	69 82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	TRP
1	A	253	ASN
1	A	429	PHE
1	A	565	GLU
1	A	660	ARG
1	A	698	GLN
1	B	22	LYS
1	B	44	LEU
1	B	129	TRP
1	B	264	LYS
1	B	277	ASN
1	B	425	SER
1	B	519	CYS
1	B	566	ASP
1	B	660	ARG
1	B	699	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	698	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 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	1707	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	B	1706	-	4,4,4	0.29	0	6,6,6	0.13	0
2	SO4	B	1709	-	4,4,4	0.11	0	6,6,6	0.18	0
2	SO4	B	1707	-	4,4,4	0.17	0	6,6,6	0.37	0
2	SO4	B	1710	-	4,4,4	0.17	0	6,6,6	0.22	0
2	SO4	B	1708	-	4,4,4	0.12	0	6,6,6	0.22	0
2	SO4	A	1706	-	4,4,4	0.15	0	6,6,6	0.19	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	693/715 (96%)	0.82	76 (10%) 5 7	38, 45, 53, 62	0
1	B	695/715 (97%)	0.99	96 (13%) 2 4	37, 46, 52, 69	0
All	All	1388/1430 (97%)	0.91	172 (12%) 4 5	37, 45, 53, 69	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	PHE	10.1
1	B	243	SER	9.4
1	B	213	LYS	6.5
1	A	684	VAL	6.3
1	B	679	MET	5.8
1	A	213	LYS	5.6
1	A	212	LYS	5.5
1	B	482	GLU	5.0
1	A	414	SER	4.8
1	B	248	VAL	4.8
1	A	243	SER	4.7
1	A	691	LYS	4.6
1	B	555	CYS	4.6
1	B	2	PRO	4.5
1	A	669	ASN	4.5
1	B	686	ASN	4.5
1	B	249	LEU	4.4
1	B	705	ASN	4.2
1	B	222	ASP	4.2
1	B	554	ASP	4.1
1	B	271	PHE	4.0
1	A	211	ARG	4.0
1	B	212	LYS	4.0
1	B	403	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	181	TYR	4.0
1	A	277	ASN	3.9
1	A	208	TYR	3.9
1	A	554	ASP	3.8
1	B	223	ASN	3.8
1	B	-1	GLU	3.8
1	B	0	TRP	3.8
1	B	688	LEU	3.8
1	B	517	ALA	3.7
1	A	403	ASP	3.7
1	B	335	ILE	3.6
1	A	110	ALA	3.6
1	A	690	GLN	3.6
1	A	61	ILE	3.6
1	B	353	ILE	3.6
1	B	388	PHE	3.6
1	B	669	ASN	3.5
1	B	371	ILE	3.5
1	A	665	LEU	3.4
1	B	682	ASP	3.4
1	B	219	ILE	3.4
1	A	415	ASP	3.4
1	B	196	ASN	3.3
1	B	565	GLU	3.3
1	B	400	ASP	3.3
1	B	564	GLU	3.3
1	B	34	LYS	3.3
1	A	234	ILE	3.2
1	A	508	ILE	3.2
1	A	402	GLU	3.2
1	B	352	VAL	3.2
1	A	668	ASN	3.2
1	A	281	GLU	3.1
1	A	563	TYR	3.1
1	B	39	GLY	3.1
1	B	-2	LEU	3.1
1	B	231	ASP	3.1
1	B	215	GLU	3.1
1	B	277	ASN	3.0
1	A	503	PHE	3.0
1	B	670	GLY	3.0
1	A	614	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	191	GLU	2.9
1	A	555	CYS	2.9
1	B	250	VAL	2.9
1	B	690	GLN	2.9
1	B	242	LEU	2.9
1	A	3	ILE	2.9
1	B	229	HIS	2.9
1	B	667	TYR	2.9
1	A	566	ASP	2.9
1	A	479	ILE	2.8
1	B	269	MET	2.8
1	A	242	LEU	2.7
1	B	270	ASN	2.7
1	A	94	ILE	2.7
1	B	566	ASP	2.7
1	A	498	LEU	2.7
1	A	687	LEU	2.7
1	B	150	LEU	2.7
1	B	159	VAL	2.7
1	B	354	ILE	2.6
1	A	688	LEU	2.6
1	A	134	GLU	2.6
1	B	183	GLN	2.6
1	A	655	ILE	2.6
1	A	65	LEU	2.6
1	B	281	GLU	2.6
1	B	475	GLU	2.6
1	A	352	VAL	2.6
1	A	400	ASP	2.6
1	A	405	ASP	2.6
1	A	458	ALA	2.6
1	A	689	GLY	2.6
1	B	74	VAL	2.5
1	B	336	VAL	2.5
1	A	613	TRP	2.5
1	A	406	ARG	2.5
1	B	125	LEU	2.5
1	A	495	VAL	2.5
1	B	111	TRP	2.5
1	A	496	ALA	2.5
1	A	231	ASP	2.5
1	A	567	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	351	THR	2.5
1	A	4	GLU	2.5
1	A	481	GLU	2.5
1	A	656	SER	2.4
1	B	334	VAL	2.4
1	A	353	ILE	2.4
1	B	94	ILE	2.4
1	A	692	LEU	2.4
1	B	172	LEU	2.4
1	B	387	GLY	2.4
1	B	676	ASP	2.4
1	B	163	THR	2.4
1	B	244	LYS	2.4
1	B	61	ILE	2.4
1	A	20	GLY	2.4
1	A	229	HIS	2.3
1	A	249	LEU	2.3
1	B	410	LYS	2.3
1	B	234	ILE	2.3
1	B	413	LEU	2.3
1	A	74	VAL	2.3
1	A	388	PHE	2.3
1	B	689	GLY	2.3
1	B	395	ILE	2.3
1	B	54	LEU	2.3
1	B	409	LYS	2.3
1	B	423	LEU	2.3
1	A	0	TRP	2.3
1	A	18	LYS	2.3
1	A	615	THR	2.3
1	B	402	GLU	2.3
1	B	64	LEU	2.2
1	B	195	THR	2.2
1	A	-1	GLU	2.2
1	A	565	GLU	2.2
1	B	406	ARG	2.2
1	A	25	ASN	2.2
1	B	23	LYS	2.2
1	B	701	ALA	2.2
1	A	686	ASN	2.2
1	B	642	ARG	2.2
1	B	379	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	199	PRO	2.2
1	A	288	ASP	2.2
1	B	685	LYS	2.2
1	B	436	ILE	2.2
1	B	694	GLU	2.1
1	B	390	GLN	2.1
1	B	164	ILE	2.1
1	A	484	ASN	2.1
1	B	414	SER	2.1
1	B	432	PHE	2.1
1	A	634	LEU	2.1
1	A	482	GLU	2.1
1	B	134	GLU	2.1
1	A	404	VAL	2.1
1	B	20	GLY	2.1
1	B	139	VAL	2.1
1	A	610	THR	2.0
1	B	143	VAL	2.0
1	A	430	TYR	2.0
1	B	524	LEU	2.0
1	A	68	GLY	2.0
1	A	657	GLY	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. 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	B	1710	5/5	0.95	0.37	58,59,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	1706	5/5	0.97	0.17	53,54,55,55	0
2	SO4	B	1707	5/5	0.98	0.30	47,48,49,49	0
2	SO4	A	1707	5/5	0.98	0.18	45,45,47,47	0
2	SO4	B	1708	5/5	0.98	0.17	41,42,45,46	0
2	SO4	B	1706	5/5	0.98	0.17	39,40,42,43	0
2	SO4	B	1709	5/5	0.99	0.20	45,45,45,46	0

6.5 Other polymers

There are no such residues in this entry.