Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:55 AM GMT

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

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

with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865

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.
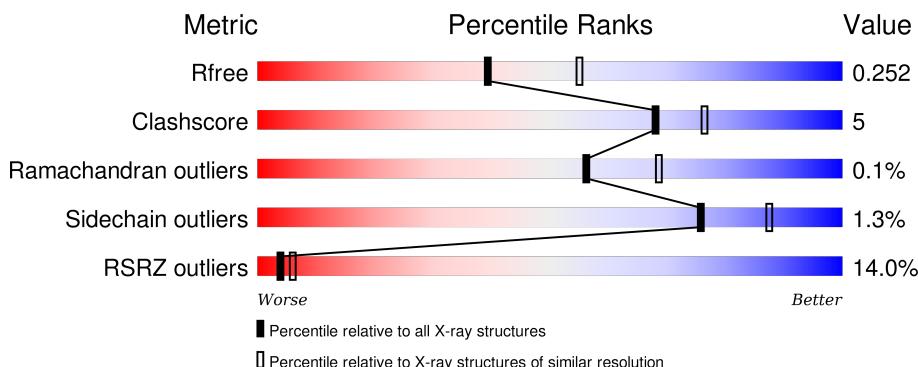
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	
1	B	715	
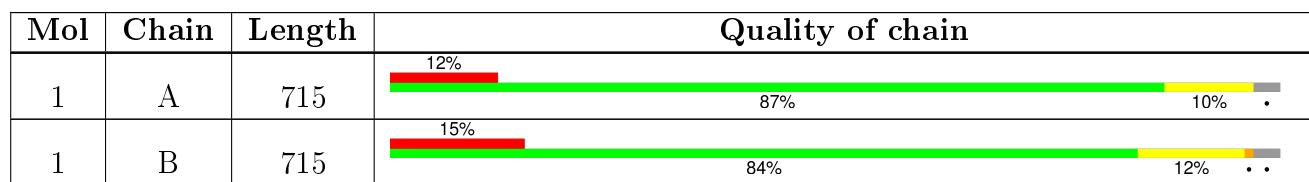
2 Entry composition (i)

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 5550	C 3551	N 936	O 1049	S 14	0	0	0
1	B	695	Total 5566	C 3563	N 938	O 1051	S 14	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
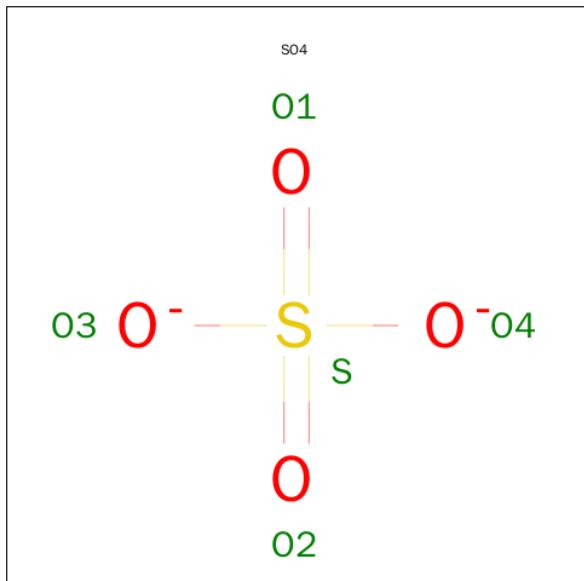
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

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

- Molecule 3 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

- Molecule 1: SKI2-TYPE HELICASE

K480 E481 E482 T485 T489 R494 I500 N501 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 R702 L703 L704 N705 ARG PHE HIS
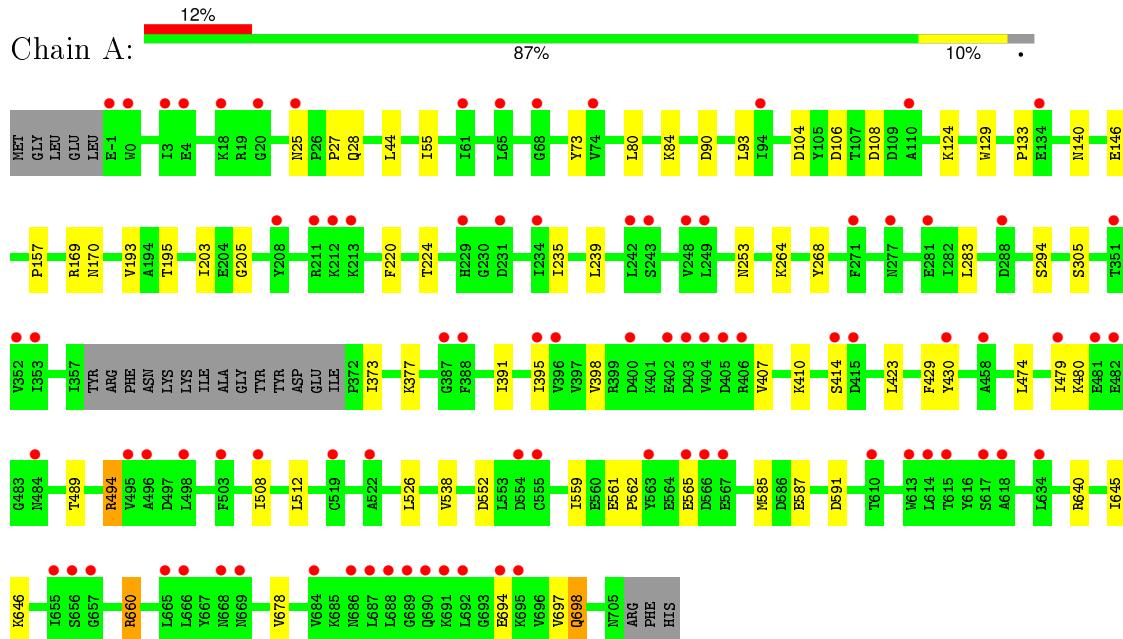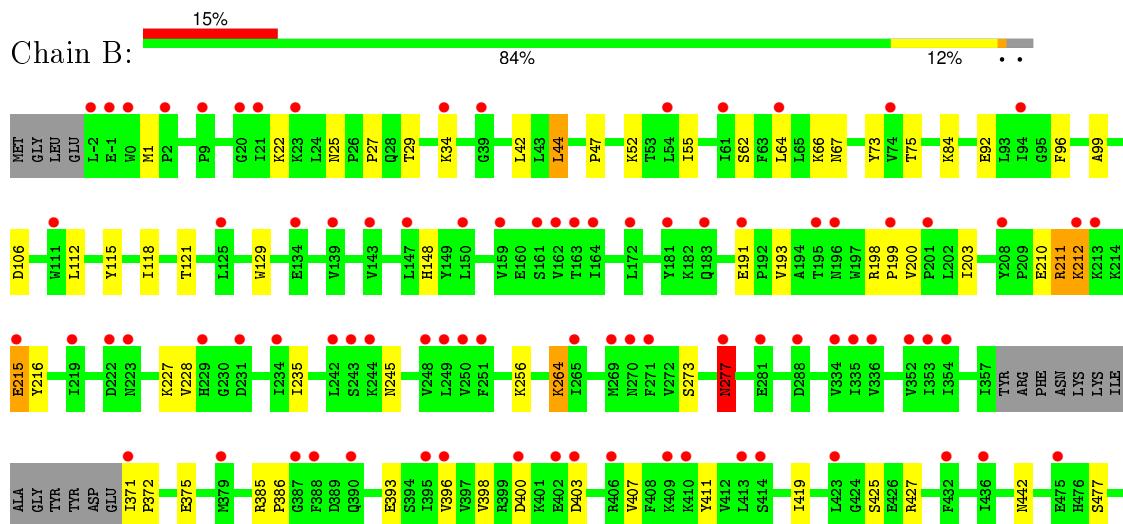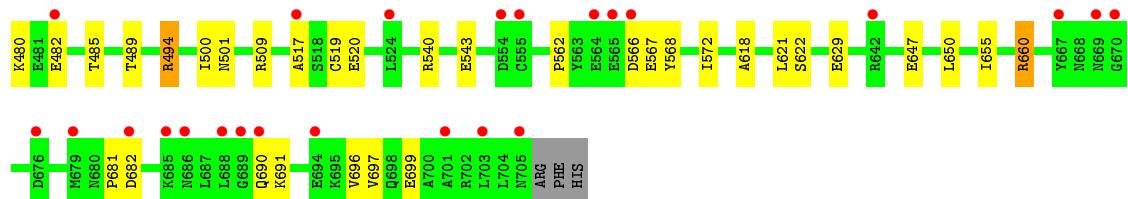
4   Data and refinement statistics (i)

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 (5.31%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	0 of 79292 reflections	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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:90:ASP:O	1:A:93:LEU:HD12	2.15	0.46
1:A:398:VAL:CG1	1:A:407:VAL:HG21	2.46	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:B:44:LEU:CD2	1:B:55:ILE:HD13	2.50	0.41
1:A:140:ASN:HA	1:A:169:ARG:HG2	2.02	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:A:80:LEU:HD13	1:A:146:GLU:OE2	2.21	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:B:690:GLN:HG2	1:B:691:LYS:H	1.85	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:660:ARG:HG2	3:B:2075:HOH:O	2.21	0.40
1:A:239:LEU:HD11	1:A:268:TYR:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD23	1:A:193:VAL:HB	2.03	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 (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	689/715 (96%)	666 (97%)	23 (3%)	0	100	100
1	B	691/715 (97%)	671 (97%)	18 (3%)	2 (0%)	46	57
All	All	1380/1430 (96%)	1337 (97%)	41 (3%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	245	ASN
1	B	47	PRO

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	605/624 (97%)	599 (99%)	6 (1%)	82	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	607/624 (97%)	597 (98%)	10 (2%)	70	84
All	All	1212/1248 (97%)	1196 (99%)	16 (1%)	76	87

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 (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)

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	1706	-	4,4,4	0.32	0	6,6,6	0.15	0
2	SO4	A	1707	-	4,4,4	0.30	0	6,6,6	0.22	0
2	SO4	B	1706	-	4,4,4	0.53	0	6,6,6	0.14	0
2	SO4	B	1707	-	4,4,4	0.24	0	6,6,6	0.31	0
2	SO4	B	1708	-	4,4,4	0.27	0	6,6,6	0.31	0
2	SO4	B	1709	-	4,4,4	0.30	0	6,6,6	0.21	0
2	SO4	B	1710	-	4,4,4	0.19	0	6,6,6	0.16	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
2	SO4	A	1706	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1707	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1706	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1707	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1708	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1709	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1710	-	-	0/0/0/0	0/0/0/0

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 ⓘ

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(Å²)	Q<0.9
1	A	693/715 (96%)	0.90	87 (12%)	5	8	38, 45, 53, 62	0
1	B	695/715 (97%)	1.08	108 (15%)	3	4	37, 46, 52, 69	0
All	All	1388/1430 (97%)	0.99	195 (14%)	4	6	37, 45, 53, 69	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	PHE	10.4
1	B	243	SER	9.6
1	B	213	LYS	6.8
1	A	684	VAL	6.6
1	B	679	MET	6.1
1	A	213	LYS	5.9
1	A	212	LYS	5.7
1	B	482	GLU	5.1
1	B	248	VAL	5.0
1	A	243	SER	4.9
1	A	414	SER	4.9
1	A	691	LYS	4.8
1	B	555	CYS	4.8
1	B	2	PRO	4.7
1	A	669	ASN	4.6
1	B	686	ASN	4.6
1	B	249	LEU	4.6
1	B	705	ASN	4.4
1	B	222	ASP	4.4
1	B	554	ASP	4.3
1	A	208	TYR	4.1
1	B	181	TYR	4.1
1	B	271	PHE	4.1
1	B	403	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	277	ASN	4.1
1	A	211	ARG	4.1
1	B	212	LYS	4.1
1	A	554	ASP	4.0
1	B	-1	GLU	4.0
1	B	223	ASN	4.0
1	B	0	TRP	4.0
1	B	517	ALA	3.9
1	B	688	LEU	3.9
1	A	403	ASP	3.9
1	A	690	GLN	3.9
1	B	335	ILE	3.8
1	A	110	ALA	3.8
1	A	61	ILE	3.8
1	B	353	ILE	3.8
1	B	388	PHE	3.7
1	B	371	ILE	3.6
1	A	665	LEU	3.6
1	B	219	ILE	3.6
1	B	669	ASN	3.6
1	B	196	ASN	3.5
1	B	682	ASP	3.5
1	A	415	ASP	3.5
1	B	400	ASP	3.4
1	B	565	GLU	3.4
1	A	234	ILE	3.4
1	A	402	GLU	3.4
1	A	508	ILE	3.4
1	B	564	GLU	3.4
1	B	352	VAL	3.4
1	B	34	LYS	3.3
1	B	-2	LEU	3.3
1	A	563	TYR	3.3
1	A	668	ASN	3.3
1	B	39	GLY	3.3
1	A	281	GLU	3.3
1	B	231	ASP	3.2
1	B	215	GLU	3.2
1	B	277	ASN	3.2
1	B	250	VAL	3.1
1	A	614	LEU	3.1
1	B	670	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	503	PHE	3.1
1	A	555	CYS	3.1
1	B	191	GLU	3.0
1	A	479	ILE	3.0
1	B	229	HIS	3.0
1	B	690	GLN	3.0
1	B	242	LEU	3.0
1	A	566	ASP	3.0
1	A	3	ILE	3.0
1	B	667	TYR	3.0
1	A	242	LEU	2.9
1	B	269	MET	2.9
1	A	94	ILE	2.8
1	A	688	LEU	2.8
1	B	270	ASN	2.8
1	B	159	VAL	2.8
1	B	354	ILE	2.8
1	B	566	ASP	2.8
1	A	498	LEU	2.8
1	A	687	LEU	2.8
1	A	65	LEU	2.8
1	A	655	ILE	2.8
1	B	150	LEU	2.8
1	A	689	GLY	2.8
1	A	400	ASP	2.7
1	A	134	GLU	2.7
1	A	405	ASP	2.7
1	A	352	VAL	2.7
1	B	74	VAL	2.7
1	B	281	GLU	2.7
1	B	336	VAL	2.7
1	B	183	GLN	2.7
1	A	613	TRP	2.7
1	A	458	ALA	2.7
1	B	475	GLU	2.7
1	A	406	ARG	2.6
1	A	495	VAL	2.6
1	B	334	VAL	2.6
1	A	496	ALA	2.6
1	A	692	LEU	2.6
1	B	125	LEU	2.6
1	A	231	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	351	THR	2.6
1	B	111	TRP	2.6
1	A	353	ILE	2.6
1	A	567	GLU	2.6
1	B	61	ILE	2.6
1	A	656	SER	2.6
1	B	172	LEU	2.6
1	A	4	GLU	2.5
1	A	481	GLU	2.5
1	B	94	ILE	2.5
1	B	387	GLY	2.5
1	B	163	THR	2.5
1	B	676	ASP	2.5
1	A	229	HIS	2.5
1	B	54	LEU	2.5
1	B	234	ILE	2.5
1	A	388	PHE	2.5
1	A	20	GLY	2.5
1	A	249	LEU	2.5
1	A	74	VAL	2.5
1	B	244	LYS	2.5
1	B	395	ILE	2.4
1	B	689	GLY	2.4
1	A	0	TRP	2.4
1	A	615	THR	2.4
1	B	195	THR	2.4
1	B	413	LEU	2.4
1	B	423	LEU	2.4
1	A	565	GLU	2.4
1	B	64	LEU	2.4
1	B	410	LYS	2.4
1	B	701	ALA	2.4
1	B	409	LYS	2.4
1	A	-1	GLU	2.4
1	B	23	LYS	2.4
1	A	25	ASN	2.3
1	B	436	ILE	2.3
1	B	199	PRO	2.3
1	A	686	ASN	2.3
1	A	18	LYS	2.3
1	B	402	GLU	2.3
1	A	288	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	379	MET	2.3
1	B	406	ARG	2.3
1	B	685	LYS	2.3
1	B	642	ARG	2.3
1	B	694	GLU	2.3
1	B	164	ILE	2.2
1	A	404	VAL	2.2
1	B	390	GLN	2.2
1	B	432	PHE	2.2
1	B	139	VAL	2.2
1	B	143	VAL	2.2
1	A	634	LEU	2.2
1	A	484	ASN	2.2
1	B	396	VAL	2.2
1	B	414	SER	2.2
1	A	610	THR	2.2
1	B	20	GLY	2.1
1	B	201	PRO	2.1
1	A	519	CYS	2.1
1	B	134	GLU	2.1
1	A	396	VAL	2.1
1	B	524	LEU	2.1
1	A	482	GLU	2.1
1	A	68	GLY	2.1
1	A	657	GLY	2.1
1	A	395	ILE	2.1
1	A	430	TYR	2.1
1	B	147	LEU	2.1
1	A	522	ALA	2.1
1	A	617	SER	2.1
1	B	703	LEU	2.1
1	B	9	PRO	2.1
1	A	618	ALA	2.1
1	B	288	ASP	2.1
1	B	161	SER	2.1
1	A	694	GLU	2.0
1	B	162	VAL	2.1
1	B	208	TYR	2.0
1	B	21	ILE	2.0
1	A	666	LEU	2.0
1	A	695	LYS	2.0
1	A	387	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	265	ILE	2.0
1	A	248	VAL	2.0
1	B	251	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(Å²)	Q<0.9
2	SO4	B	1708	5/5	0.98	0.17	1.60	41,42,45,46	0
2	SO4	A	1707	5/5	0.98	0.18	1.18	45,45,47,47	0
2	SO4	B	1709	5/5	0.99	0.20	0.21	45,45,45,46	0
2	SO4	B	1706	5/5	0.98	0.17	0.17	39,40,42,43	0
2	SO4	B	1710	5/5	0.95	0.37	-	58,59,60,61	0
2	SO4	B	1707	5/5	0.98	0.30	-	47,48,49,49	0
2	SO4	A	1706	5/5	0.97	0.17	-	53,54,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.