Full wwPDB X-ray Structure Validation Report (i)

Sep 27, 2022 – 10:50 am BST

PDB ID	:	7ZMQ
Title	:	Crystal structure of human RECQL5 helicase APO form in complex with engineered nanobody (Gluebody) G2*-006
Authors	:	Ye, M.; Makola, M.; Newman, J.A.; Fairhead, M.; MacLean, E.; Krojer, T.; Aitkenhead, H.; Bountra, C.; Gileadi, O.; von Delft, F.
Deposited on	:	2022-04-19
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 (i) 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 (i)) were used in the production of this report:

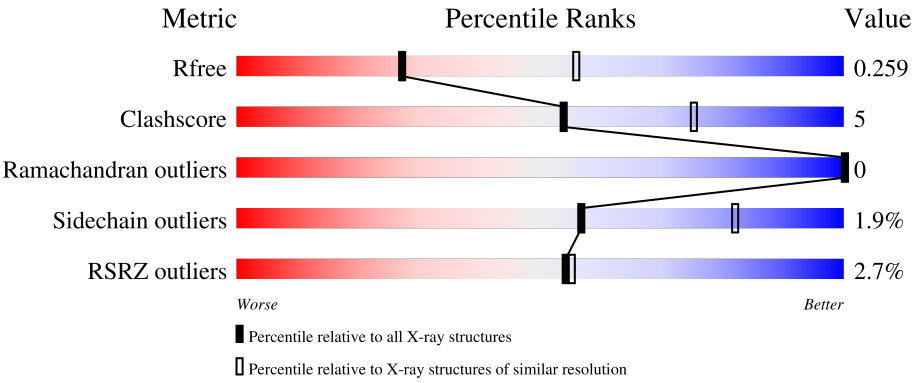
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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	445	2% 84% 14% ·
1	B	445	5% 86% 13% ·
2	C	127	85% 13% ·
2	K	127	82% 15% · ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8929 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 ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	5	0
			3467	2188	622	633	24			
1	B	442	Total	C	N	O	S	0	5	0
			3467	2188	624	631	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	SER	-	expression tag	UNP O94762
A	10	MET	-	expression tag	UNP O94762
B	9	SER	-	expression tag	UNP O94762
B	10	MET	-	expression tag	UNP O94762

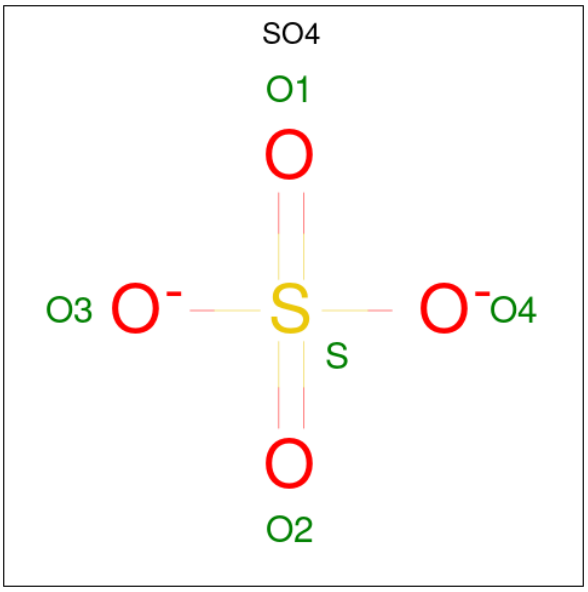
- Molecule 2 is a protein called Gluebody G2*-006.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	124	Total	C	N	O	S	0	1	0
			955	594	164	193	4			
2	C	124	Total	C	N	O	S	0	2	0
			966	600	168	194	4			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

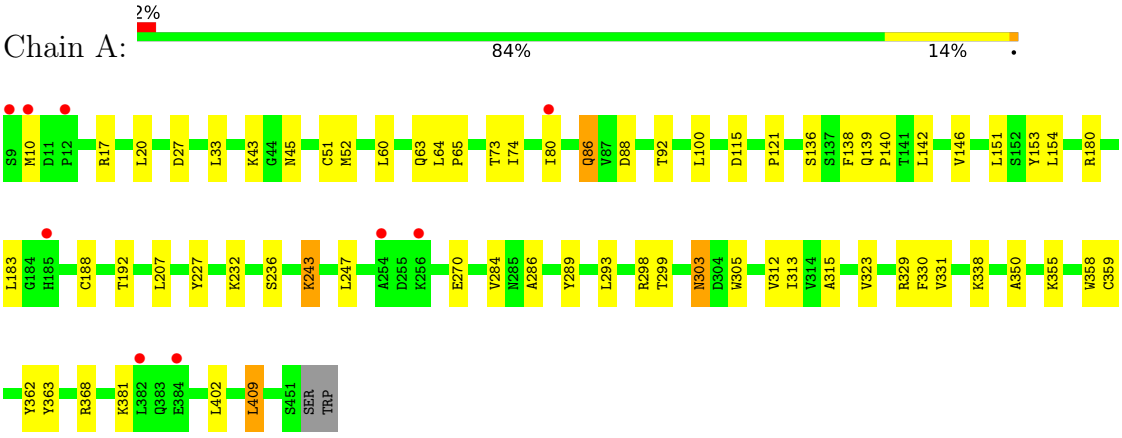
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0
5	B	14	Total O 14 14	0	0
5	K	9	Total O 9 9	0	0
5	C	11	Total O 11 11	0	0

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.

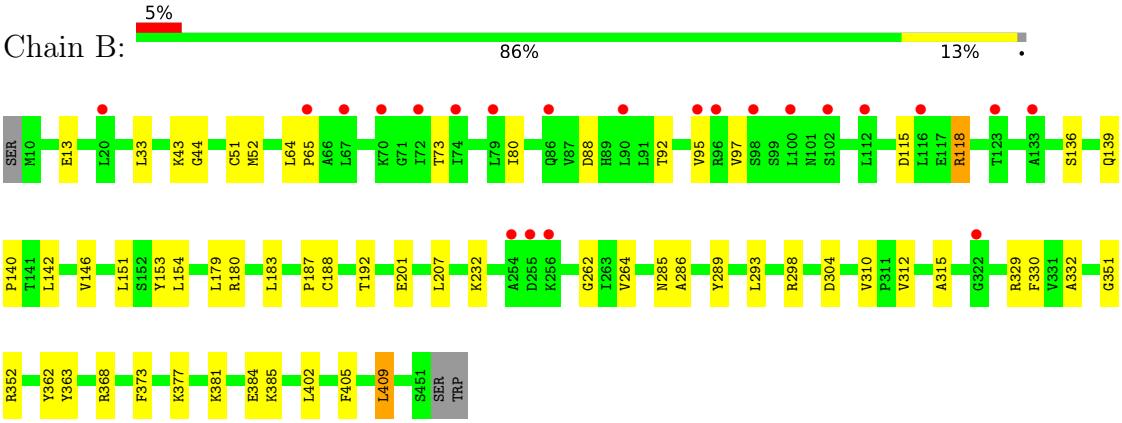
• Molecule 1: ATP-dependent DNA helicase Q5

Chain A:



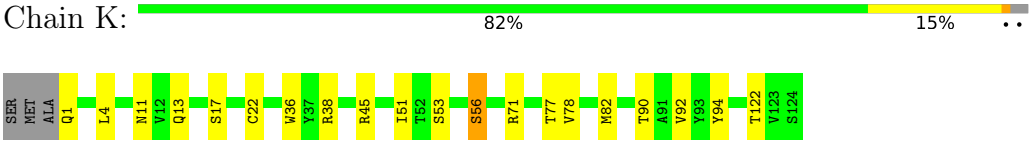
• Molecule 1: ATP-dependent DNA helicase Q5

Chain B:



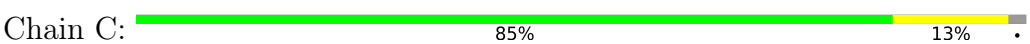
• Molecule 2: Gluebody G2*-006

Chain K:



• Molecule 2: Gluebody G2*-006

Chain C:




SER
MET
ALA
Q1
N7
N11
S17
C22
W36
I51
S56
Y59
K64
R71
D72
N73
T77
V78
M82
T90
T122
V123
S124

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	115.13Å 199.09Å 174.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.67 – 2.70 99.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.67-2.70) 99.9 (99.66-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.225 , 0.258 0.227 , 0.259	Depositor DCC
R_{free} test set	2899 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.002 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8929	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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, ZN

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	0.69	0/3543	0.85	0/4789
1	B	0.71	2/3543 (0.1%)	0.85	3/4788 (0.1%)
2	C	0.71	0/989	0.88	0/1342
2	K	0.72	0/978	0.88	0/1328
All	All	0.71	2/9053 (0.0%)	0.86	3/12247 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118[A]	ARG	C-O	7.73	1.38	1.23
1	B	118[B]	ARG	C-O	7.73	1.38	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	285	ASN	CB-CA-C	5.51	121.42	110.40
1	B	118[A]	ARG	CA-C-O	5.06	130.73	120.10
1	B	118[B]	ARG	CA-C-O	5.06	130.73	120.10

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	3467	0	3481	39	0
1	B	3467	0	3487	35	0
2	C	966	0	914	9	0
2	K	955	0	902	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	18	0	0	1	0
5	B	14	0	0	2	0
5	C	11	0	0	0	0
5	K	9	0	0	1	0
All	All	8929	0	8784	94	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 (94) 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:363:TYR:OH	1:B:368:ARG:HD3	1.86	0.76
1:B:151:LEU:HD21	1:B:183:LEU:HD13	1.69	0.74
2:K:45:ARG:HD2	2:K:94:TYR:OH	1.89	0.73
1:B:154:LEU:HD22	1:B:183:LEU:HD12	1.74	0.69
1:B:136:SER:HA	1:B:139:GLN:HG2	1.75	0.68
1:A:363:TYR:OH	1:A:368:ARG:HD3	1.97	0.65
1:A:136:SER:HA	1:A:139:GLN:HG2	1.79	0.65
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.83	0.61
2:K:45:ARG:CD	2:K:94:TYR:OH	2.49	0.60
1:B:64:LEU:HB3	1:B:65:PRO:HD3	1.84	0.60
1:A:142:LEU:O	1:A:146:VAL:HG23	2.03	0.58
1:B:142:LEU:O	1:B:146:VAL:HG23	2.04	0.58
1:B:73:THR:HG23	1:B:153:TYR:HB2	1.86	0.58
1:B:142:LEU:HD21	1:B:179:LEU:CD1	2.35	0.57
1:B:232:LYS:HD2	1:B:362:TYR:HB3	1.87	0.55
2:C:90:THR:HG23	2:C:122:THR:HA	1.88	0.55
1:A:299:THR:O	1:A:303:ASN:HB2	2.07	0.55
1:A:180:ARG:HG2	1:A:207:LEU:O	2.07	0.55
1:B:64:LEU:C	1:B:64:LEU:HD23	2.28	0.54
1:B:329:ARG:HH22	1:B:351:GLY:HA2	1.71	0.54
2:C:71[B]:ARG:NE	2:C:73:ASN:HD21	2.06	0.54
1:A:64:LEU:C	1:A:64:LEU:HD23	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:HG2	1:B:207:LEU:O	2.08	0.53
2:C:59:TYR:HB2	2:C:64:LYS:HG3	1.91	0.53
1:A:286:ALA:HA	1:A:312:VAL:O	2.10	0.52
1:B:262:GLY:HA3	1:B:330:PHE:CE2	2.45	0.50
1:A:338:LYS:HD2	5:A:616:HOH:O	2.11	0.50
1:A:20:LEU:HD13	1:A:60:LEU:HD21	1.93	0.50
2:K:53:SER:HA	2:K:71:ARG:NH2	2.26	0.50
1:A:289:TYR:CZ	1:A:298:ARG:HD2	2.46	0.50
2:K:17:SER:HA	2:K:82:MET:O	2.12	0.50
2:C:17:SER:HA	2:C:82:MET:O	2.12	0.50
1:A:180:ARG:HD3	1:A:188:CYS:HB2	1.93	0.49
1:A:73:THR:HG23	1:A:153:TYR:HB2	1.94	0.49
1:B:286:ALA:HA	1:B:312:VAL:O	2.14	0.48
1:A:151:LEU:HD12	1:A:183:LEU:HD22	1.96	0.48
1:A:115:ASP:O	1:A:121:PRO:HB3	2.14	0.47
1:B:289:TYR:CZ	1:B:298:ARG:HD2	2.48	0.47
1:A:88:ASP:O	1:A:92:THR:HG23	2.14	0.47
1:B:329:ARG:NH2	1:B:351:GLY:HA2	2.30	0.47
1:B:88:ASP:O	1:B:92:THR:HG23	2.15	0.46
1:A:293:LEU:O	1:A:298:ARG:NH1	2.49	0.46
1:A:154:LEU:O	1:A:188:CYS:HA	2.15	0.46
1:B:115:ASP:HA	1:B:118[B]:ARG:HD3	1.98	0.46
1:A:232:LYS:HD2	1:A:362:TYR:HB3	1.97	0.45
1:B:293:LEU:O	1:B:298:ARG:NH1	2.50	0.45
2:K:4:LEU:HD12	2:K:4:LEU:HA	1.85	0.45
1:A:139:GLN:N	1:A:140:PRO:HD2	2.32	0.45
1:A:305:TRP:HZ3	1:A:323:VAL:HG11	1.81	0.44
1:A:51:CYS:HA	1:A:192:THR:O	2.18	0.44
1:A:409:LEU:H	1:A:409:LEU:HD13	1.83	0.44
1:B:409:LEU:HD13	1:B:409:LEU:H	1.83	0.44
1:A:331:VAL:HG23	1:A:350:ALA:HB2	2.00	0.43
2:K:90:THR:HG23	2:K:122:THR:HA	2.00	0.43
1:A:17:ARG:NH1	1:A:27:ASP:O	2.51	0.43
2:K:38:ARG:HA	2:K:92:VAL:O	2.19	0.43
2:K:22:CYS:HB2	2:K:36:TRP:CZ2	2.53	0.43
1:A:329:ARG:NH2	1:A:355:LYS:HD3	2.34	0.43
1:B:44:GLY:O	1:B:187:PRO:HG3	2.19	0.43
1:B:154:LEU:O	1:B:188:CYS:HA	2.19	0.43
1:A:33:LEU:HD23	1:A:52:MET:HE3	2.00	0.43
1:B:373:PHE:CE1	1:B:377:LYS:HD2	2.53	0.43
1:B:139:GLN:N	1:B:140:PRO:HD2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:HE22	1:A:86:GLN:HG2	1.83	0.42
2:C:22:CYS:O	2:C:77:THR:HA	2.19	0.42
1:B:201:GLU:CB	5:B:611:HOH:O	2.67	0.42
1:A:45:ASN:OD1	1:A:45:ASN:N	2.43	0.42
1:A:74:ILE:HG13	1:A:151:LEU:HD22	2.01	0.42
1:A:289:TYR:O	1:A:315:ALA:HA	2.18	0.42
1:B:384:GLU:HG3	1:B:385:LYS:N	2.35	0.42
1:B:201:GLU:HB3	5:B:611:HOH:O	2.19	0.42
1:B:289:TYR:O	1:B:315:ALA:HA	2.19	0.42
2:K:22:CYS:O	2:K:77:THR:HA	2.19	0.42
1:A:227:TYR:HA	1:A:359:CYS:O	2.20	0.42
1:B:51:CYS:HA	1:B:192:THR:O	2.20	0.42
1:B:264:VAL:HA	1:B:332:ALA:O	2.20	0.41
2:K:51:ILE:HA	2:K:56:SER:O	2.20	0.41
2:K:1:GLN:NE2	5:K:201:HOH:O	2.49	0.41
1:A:100:LEU:CD2	1:A:138:PHE:CD1	3.03	0.41
2:K:13:GLN:OE1	2:C:7:ASN:ND2	2.54	0.41
2:C:22:CYS:HB2	2:C:36:TRP:CZ2	2.55	0.41
2:C:51:ILE:HA	2:C:56:SER:O	2.20	0.41
2:C:71[B]:ARG:HH21	2:C:71[B]:ARG:HG2	1.85	0.41
1:B:33:LEU:HD23	1:B:52:MET:HE2	2.03	0.41
1:A:270:GLU:H	1:A:270:GLU:CD	2.24	0.41
1:A:289:TYR:HB2	1:A:313:ILE:HD11	2.03	0.41
1:A:402:LEU:HD12	1:A:402:LEU:HA	1.91	0.41
1:A:243:LYS:HG2	1:A:284:VAL:HG23	2.02	0.40
1:B:95:VAL:O	1:B:97:VAL:HG12	2.21	0.40
1:B:304:ASP:HB3	1:B:310:VAL:HG23	2.04	0.40
1:A:247:LEU:CD2	1:A:284:VAL:HG22	2.51	0.40
1:B:13:GLU:OE2	1:B:43:LYS:HG3	2.20	0.40
1:A:330:PHE:HA	1:A:358:TRP:O	2.22	0.40
1:B:402:LEU:O	1:B:405:PHE:HB3	2.21	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	446/445 (100%)	433 (97%)	13 (3%)	0	100	100
1	B	445/445 (100%)	429 (96%)	16 (4%)	0	100	100
2	C	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
2	K	123/127 (97%)	120 (98%)	3 (2%)	0	100	100
All	All	1138/1144 (100%)	1103 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	370/373 (99%)	361 (98%)	9 (2%)	49	77
1	B	370/373 (99%)	366 (99%)	4 (1%)	73	90
2	C	100/100 (100%)	98 (98%)	2 (2%)	55	81
2	K	99/100 (99%)	96 (97%)	3 (3%)	41	70
All	All	939/946 (99%)	921 (98%)	18 (2%)	57	82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	43	LYS
1	A	80	ILE
1	A	86	GLN
1	A	236	SER
1	A	243	LYS
1	A	303	ASN
1	A	381	LYS
1	A	409	LEU
1	B	80	ILE

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Mol	Chain	Res	Type
1	B	352	ARG
1	B	381	LYS
1	B	409	LEU
2	K	11	ASN
2	K	56	SER
2	K	78	VAL
2	C	11	ASN
2	C	78	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	86	GLN
1	A	285	ASN
1	A	302	GLN
1	B	34	GLN
1	B	139	GLN
1	B	285	ASN
2	K	3	GLN
2	K	7	ASN
2	K	39	GLN
2	K	81	GLN
2	C	39	GLN
2	C	81	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	SO4	B	503	-	4,4,4	0.37	0	6,6,6	0.15	0
4	SO4	B	502	-	4,4,4	0.33	0	6,6,6	0.20	0
4	SO4	A	503	-	4,4,4	0.36	0	6,6,6	0.15	0
4	SO4	A	502	-	4,4,4	0.32	0	6,6,6	0.20	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	443/445 (99%)	0.33	9 (2%) 65 67	30, 56, 113, 216	0
1	B	442/445 (99%)	0.44	22 (4%) 28 27	34, 64, 136, 179	0
2	C	124/127 (97%)	0.31	0 100 100	40, 52, 85, 101	0
2	K	124/127 (97%)	0.25	0 100 100	35, 47, 80, 108	0
All	All	1133/1144 (99%)	0.36	31 (2%) 54 55	30, 56, 124, 216	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	MET	11.9
1	B	255	ASP	5.2
1	B	86	GLN	4.9
1	B	79	LEU	4.1
1	B	254	ALA	3.8
1	B	100	LEU	3.5
1	A	382	LEU	3.4
1	B	116	LEU	3.3
1	B	96	ARG	3.3
1	A	185	HIS	3.2
1	B	102	SER	3.2
1	A	12	PRO	3.1
1	B	123	THR	3.0
1	A	256	LYS	3.0
1	B	70	LYS	3.0
1	A	9	SER	2.9
1	B	256	LYS	2.8
1	B	112	LEU	2.8
1	A	254	ALA	2.6
1	B	90	LEU	2.6
1	B	133	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	65	PRO	2.5
1	A	384	GLU	2.3
1	B	67	LEU	2.2
1	A	80	ILE	2.1
1	B	74	ILE	2.1
1	B	95	VAL	2.1
1	B	72	ILE	2.1
1	B	98	SER	2.0
1	B	322	GLY	2.0
1	B	20	LEU	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 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
4	SO4	B	502	5/5	0.90	0.16	75,77,92,96	0
4	SO4	A	503	5/5	0.97	0.17	66,67,70,73	0
4	SO4	B	503	5/5	0.98	0.14	54,56,62,65	0
4	SO4	A	502	5/5	0.99	0.17	44,44,57,57	0
3	ZN	B	501	1/1	0.99	0.19	56,56,56,56	0
3	ZN	A	501	1/1	1.00	0.19	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.