



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:15 PM UTC

PDB ID : 7ZMQ / pdb_00007zmq
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

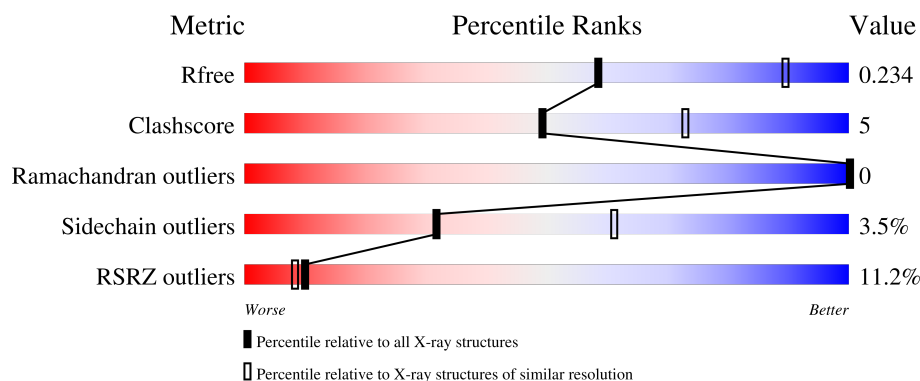
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	445	9% 82% 17% .
1	B	445	16% 85% 14% ..
2	C	127	8% 83% 13% ..
2	K	127	4% 80% 17% ..

2 Entry composition

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 (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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

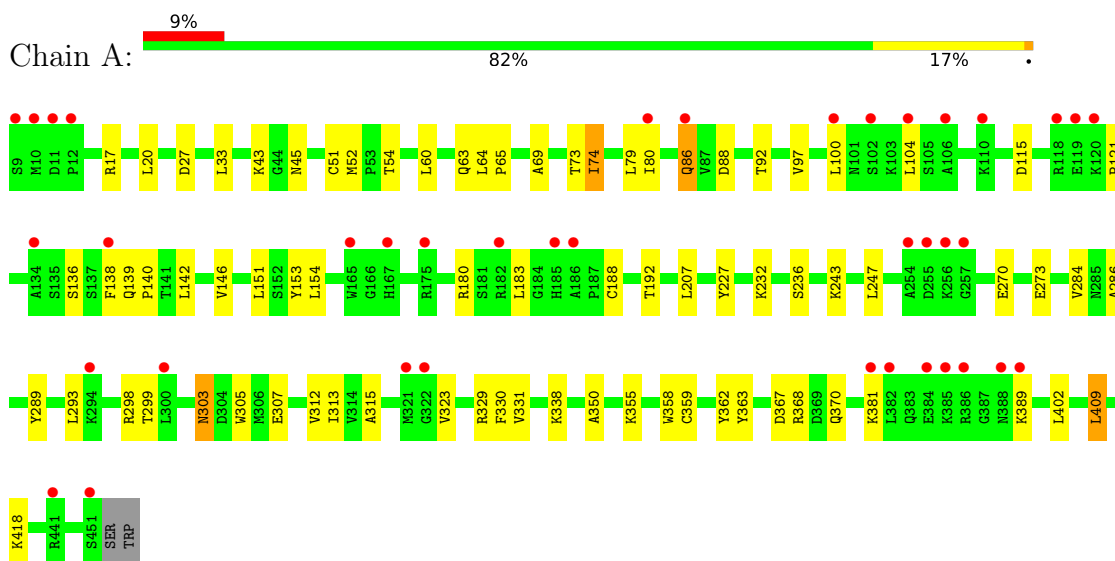
- Molecule 5 is water.

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

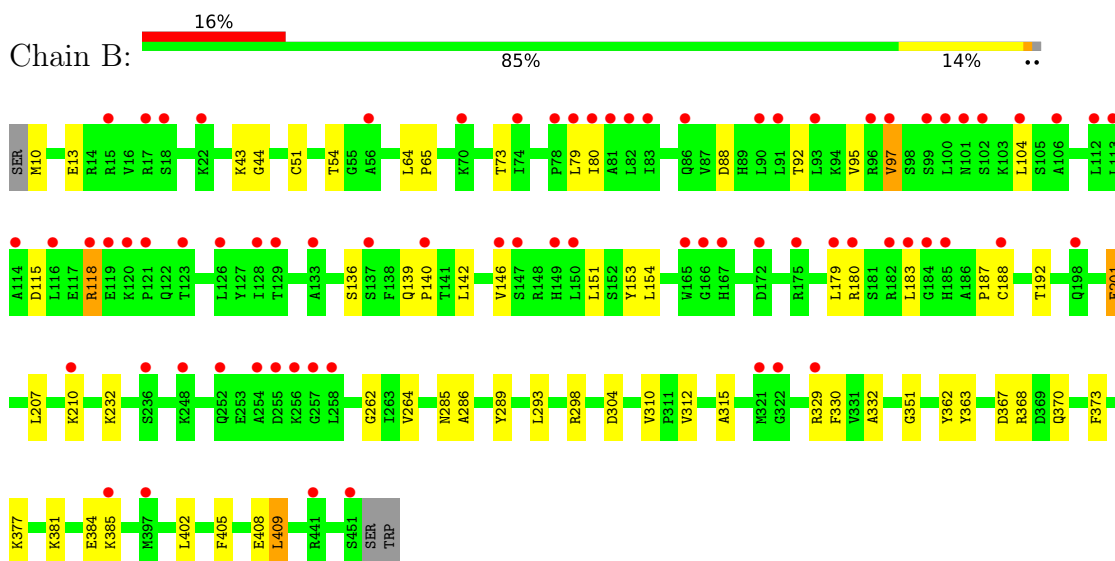
3 Residue-property plots [i](#)

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.

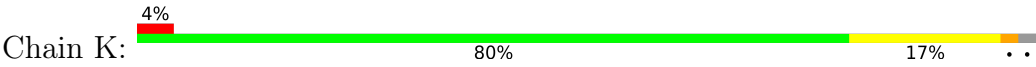
- Molecule 1: ATP-dependent DNA helicase Q5



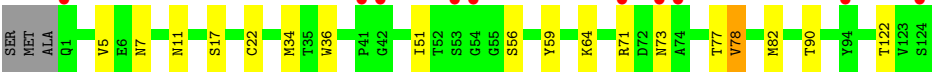
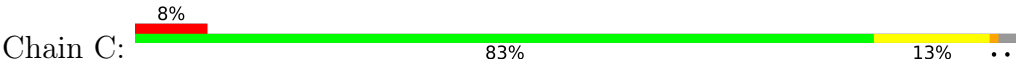
- Molecule 1: ATP-dependent DNA helicase Q5



- Molecule 2: Gluebody G2*-006



● Molecule 2: Gluebody G2*-006



4 Data and refinement statistics

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 99.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.67-2.70) 99.9 (99.67-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.225 , 0.258 (Not available) , 0.234	Depositor DCC
R_{free} test set	2899 reflections (5.25%)	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)	0.30 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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	0.93	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	1.03	0/3543	1.48	6/4789 (0.1%)
1	B	1.07	2/3543 (0.1%)	1.50	11/4788 (0.2%)
2	C	1.03	0/989	1.32	0/1342
2	K	1.03	0/978	1.34	2/1328 (0.2%)
All	All	1.05	2/9053 (0.0%)	1.46	19/12247 (0.2%)

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	11.92	1.38	1.23
1	B	118[B]	ARG	C-O	11.92	1.38	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118[A]	ARG	CA-C-O	8.67	130.73	121.19
1	B	118[B]	ARG	CA-C-O	8.67	130.73	121.19
1	B	118[A]	ARG	N-CA-C	8.17	122.08	110.23
1	B	118[B]	ARG	N-CA-C	8.17	122.08	110.23
1	B	285	ASN	CB-CA-C	7.07	121.42	110.67
1	B	54	THR	CB-CA-C	6.30	118.82	110.06
1	A	54	THR	CB-CA-C	6.19	118.67	110.06
1	B	367	ASP	CB-CA-C	-6.10	101.31	110.88
1	A	367	ASP	CB-CA-C	-5.93	101.57	110.88
1	B	118[A]	ARG	O-C-N	-5.93	115.58	122.87
1	B	118[B]	ARG	O-C-N	-5.93	115.58	122.87
1	B	201	GLU	CB-CG-CD	5.39	121.77	112.60
1	B	367	ASP	CA-CB-CG	5.26	117.86	112.60
2	K	8	GLY	CA-C-N	5.17	126.08	120.44
2	K	8	GLY	C-N-CA	5.17	126.08	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ALA	CA-C-N	5.13	127.16	120.28
1	A	69	ALA	C-N-CA	5.13	127.16	120.28
1	A	79	LEU	CA-C-N	5.10	127.66	120.42
1	A	79	LEU	C-N-CA	5.10	127.66	120.42

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	34	0
2	C	966	0	914	10	0
2	K	955	0	902	13	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	95	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 (95) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:64:LEU:C	1:B:64:LEU:HD23	2.28	0.59
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:A:64:LEU:C	1:A:64:LEU:HD23	2.27	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: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: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
2:C:34:MET:HE3	2:C:78:VAL:HG13	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:H	1:A:270:GLU:CD	2.24	0.45
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:34:MET:HE3	2:K:78:VAL:HG13	1.99	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: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
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:A:33:LEU:HD23	1:A:52:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	355 (96%)	15 (4%)	27	56
1	B	370/373 (99%)	360 (97%)	10 (3%)	39	69
2	C	100/100 (100%)	97 (97%)	3 (3%)	36	66
2	K	99/100 (99%)	95 (96%)	4 (4%)	28	56
All	All	939/946 (99%)	907 (97%)	32 (3%)	32	62

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	74	ILE
1	A	80	ILE
1	A	86	GLN
1	A	97	VAL
1	A	104	LEU
1	A	236	SER
1	A	273	GLU
1	A	303	ASN
1	A	307	GLU
1	A	370	GLN
1	A	381	LYS
1	A	389	LYS
1	A	409	LEU
1	A	418	LYS
1	B	10	MET
1	B	79	LEU
1	B	80	ILE
1	B	97	VAL
1	B	104	LEU
1	B	210	LYS
1	B	370	GLN
1	B	381	LYS
1	B	408	GLU
1	B	409	LEU
2	K	5	VAL
2	K	11	ASN
2	K	56	SER
2	K	78	VAL
2	C	5	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	63	GLN
1	A	86	GLN
1	A	139	GLN
1	A	285	ASN
1	B	86	GLN
1	B	285	ASN
2	K	3	GLN
2	K	7	ASN
2	K	13	GLN
2	K	39	GLN
2	C	7	ASN
2	C	39	GLN
2	C	120	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 oligosaccharides 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	0.34	0	6,6,6	0.17	0
4	SO4	B	502	-	4,4,4	0.30	0	6,6,6	0.21	0
4	SO4	A	503	-	4,4,4	0.30	0	6,6,6	0.17	0
4	SO4	A	502	-	4,4,4	0.28	0	6,6,6	0.18	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 [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(Å ²)	Q<0.9
1	A	443/445 (99%)	0.46	39 (8%) 15 13	22, 56, 113, 216	5 (1%)
1	B	442/445 (99%)	0.81	73 (16%) 4 4	29, 64, 136, 179	5 (1%)
2	C	124/127 (97%)	0.37	10 (8%) 18 15	26, 51, 85, 101	2 (1%)
2	K	124/127 (97%)	0.11	5 (4%) 42 38	25, 47, 80, 108	1 (0%)
All	All	1133/1144 (99%)	0.55	127 (11%) 10 8	22, 56, 124, 216	13 (1%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	PRO	6.8
1	A	185	HIS	6.7
1	A	10	MET	5.2
1	B	254	ALA	5.0
1	B	165	TRP	4.9
1	B	86	GLN	4.9
1	B	80	ILE	4.9
2	K	74	ALA	4.8
1	A	254	ALA	4.8
1	B	185	HIS	4.4
1	B	79	LEU	4.3
1	B	113	LEU	4.3
2	K	73	ASN	4.1
1	A	175[A]	ARG	4.1
1	A	9	SER	4.1
1	B	116	LEU	3.9
1	A	451	SER	3.9
1	B	104	LEU	3.8
1	B	167[A]	HIS	3.8
1	A	104	LEU	3.8
1	B	100	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	149	HIS	3.6
1	A	86	GLN	3.6
1	B	256	LYS	3.5
1	A	389	LYS	3.5
1	B	106	ALA	3.5
1	A	322	GLY	3.5
1	B	257	GLY	3.4
1	B	258	LEU	3.4
1	B	112	LEU	3.4
1	A	321	MET	3.3
1	B	175[A]	ARG	3.3
1	B	133	ALA	3.3
1	B	70	LYS	3.2
1	A	165	TRP	3.1
1	A	388	ASN	3.1
2	C	74	ALA	3.0
1	B	179	LEU	3.0
1	A	385	LYS	2.9
2	C	41	PRO	2.9
1	B	441[A]	ARG	2.9
1	B	74	ILE	2.9
1	A	257	GLY	2.9
1	A	300	LEU	2.9
1	A	80	ILE	2.9
1	B	123	THR	2.9
1	A	381	LYS	2.8
1	A	118[A]	ARG	2.8
1	A	110	LYS	2.8
1	B	188	CYS	2.8
1	B	78	PRO	2.8
1	B	146	VAL	2.8
1	A	386	ARG	2.8
1	B	118[A]	ARG	2.8
1	B	385	LYS	2.8
1	A	256	LYS	2.7
1	A	167[A]	HIS	2.7
1	A	102	SER	2.7
2	C	54	GLY	2.7
2	C	71[A]	ARG	2.7
2	C	124	SER	2.7
1	B	90	LEU	2.7
1	B	137	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	321	MET	2.6
1	B	119	GLU	2.6
2	C	1	GLN	2.6
1	B	126	LEU	2.6
1	B	56	ALA	2.6
1	A	11	ASP	2.5
2	C	42	GLY	2.5
1	B	101	ASN	2.5
1	B	329	ARG	2.5
1	B	172	ASP	2.5
1	B	180	ARG	2.5
2	C	94	TYR	2.5
1	B	82	LEU	2.4
1	B	99	SER	2.4
2	C	53	SER	2.4
1	B	210	LYS	2.4
1	A	106	ALA	2.4
1	A	186	ALA	2.4
1	A	182	ARG	2.4
1	B	121	PRO	2.4
1	B	322	GLY	2.4
1	B	97	VAL	2.4
1	B	114	ALA	2.4
2	K	71	ARG	2.4
1	B	91	LEU	2.4
1	B	17	ARG	2.4
1	B	83	ILE	2.4
1	B	81	ALA	2.3
1	B	183	LEU	2.3
2	C	73	ASN	2.3
1	B	397	MET	2.3
1	A	119	GLU	2.3
1	A	120	LYS	2.3
1	B	120	LYS	2.3
1	B	184	GLY	2.3
1	B	128	ILE	2.2
1	A	441[A]	ARG	2.2
1	B	18	SER	2.2
1	B	255	ASP	2.2
2	K	72	ASP	2.2
1	B	102	SER	2.2
1	B	93	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	198[A]	GLN	2.2
1	B	252	GLN	2.2
1	B	129	THR	2.2
1	B	96	ARG	2.2
1	B	236	SER	2.2
1	A	294	LYS	2.1
1	B	166	GLY	2.1
1	A	138	PHE	2.1
1	A	134	ALA	2.1
1	A	384	GLU	2.1
1	A	255	ASP	2.1
1	B	147	SER	2.1
1	B	451	SER	2.1
1	A	100	LEU	2.1
1	B	150	LEU	2.1
1	B	182	ARG	2.0
2	K	124	SER	2.0
1	B	22	LYS	2.0
1	B	15	ARG	2.0
1	B	248	LYS	2.0
1	B	140	PRO	2.0
1	A	382	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
4	SO4	B	502	5/5	0.88	0.11	75,77,92,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	503	5/5	0.96	0.08	66,67,70,73	0
4	SO4	B	503	5/5	0.97	0.08	54,56,62,65	0
4	SO4	A	502	5/5	0.98	0.07	44,44,57,57	0
3	ZN	A	501	1/1	1.00	0.02	47,47,47,47	0
3	ZN	B	501	1/1	1.00	0.01	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.