



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:39 AM UTC

PDB ID : 7ZMV / pdb_00007zmv
Title : Crystal structure of human RECQL5 helicase APO form in complex with engineered nanobody (Gluebody) G5-006
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 : 2.00 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

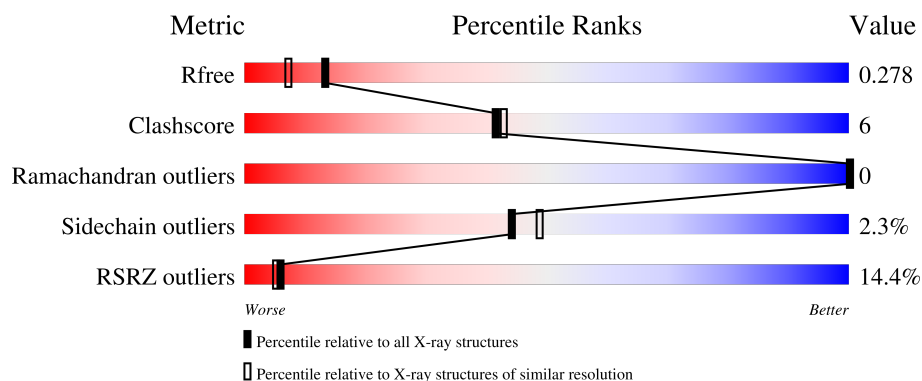
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



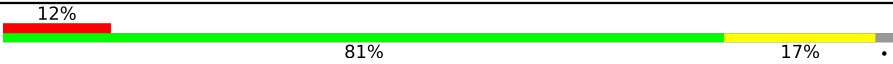
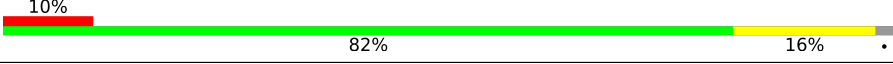
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	 14% 83% 15% ..
1	B	445	 13% 85% 13% ..
1	C	445	 14% 86% 13% ..
1	D	445	 17% 84% 15% .
2	E	127	 13% 83% 15% .

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Mol	Chain	Length	Quality of chain
2	F	127	 12% 81% 17% •
2	G	127	 15% 77% 20% •
2	K	127	 10% 82% 16% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18647 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	440	Total	C	N	O	S	0	5	0
			3455	2182	623	627	23			
1	B	440	Total	C	N	O	S	0	4	0
			3445	2177	618	627	23			
1	C	440	Total	C	N	O	S	0	5	0
			3452	2181	621	627	23			
1	D	440	Total	C	N	O	S	0	5	0
			3459	2185	624	627	23			

There are 8 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
C	9	SER	-	expression tag	UNP O94762
C	10	MET	-	expression tag	UNP O94762
D	9	SER	-	expression tag	UNP O94762
D	10	MET	-	expression tag	UNP O94762

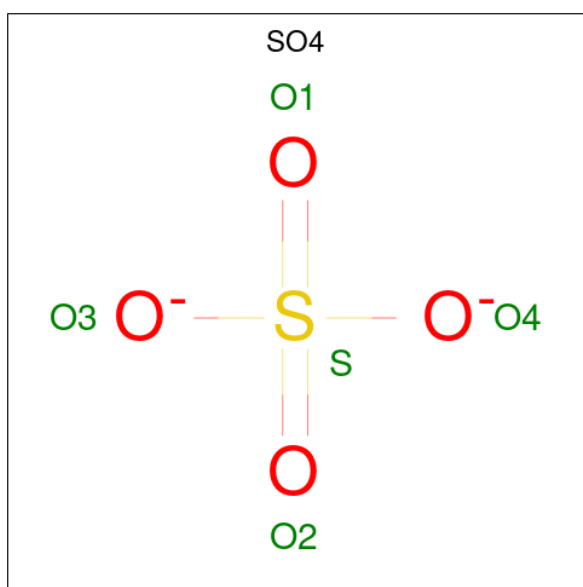
- Molecule 2 is a protein called Gluebody G5-006.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	124	Total	C	N	O	S	0	1	0
			946	586	161	193	6			
2	E	124	Total	C	N	O	S	0	1	0
			946	586	161	193	6			
2	F	124	Total	C	N	O	S	0	1	0
			946	586	161	193	6			
2	G	124	Total	C	N	O	S	0	1	0
			946	586	161	193	6			

- 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		
3	C	1	Total	Zn	0	0
			1	1		
3	D	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	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	187	Total	O	0	0
			187	187		

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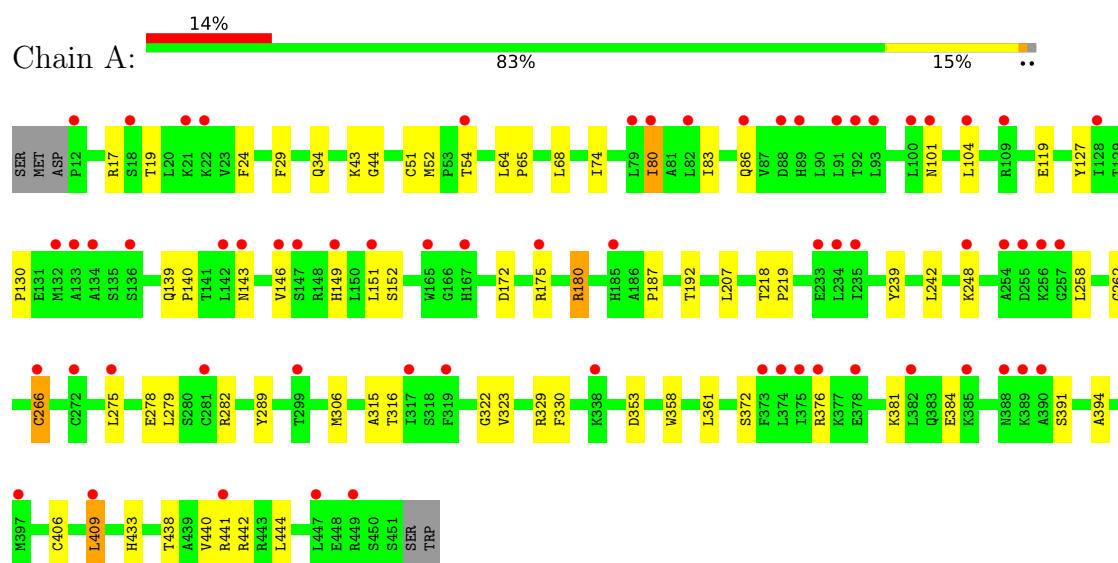
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	186	Total 186	O 186	0	0
5	C	193	Total 193	O 193	0	0
5	D	186	Total 186	O 186	0	0
5	K	78	Total 78	O 78	0	0
5	E	60	Total 60	O 60	0	0
5	F	72	Total 72	O 72	0	0
5	G	66	Total 66	O 66	0	0

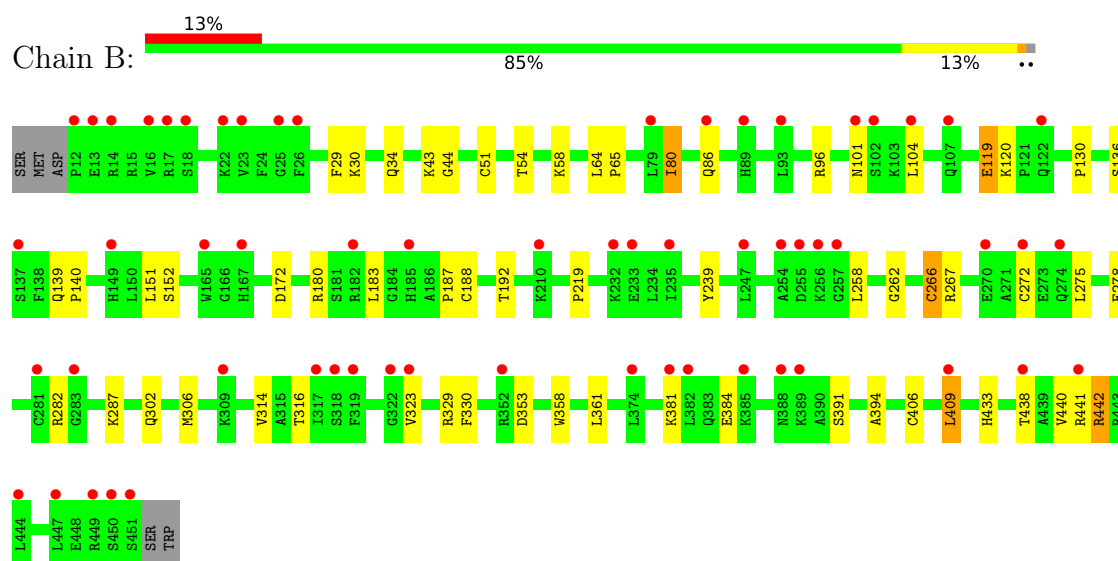
3 Residue-property plots [i](#)

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.

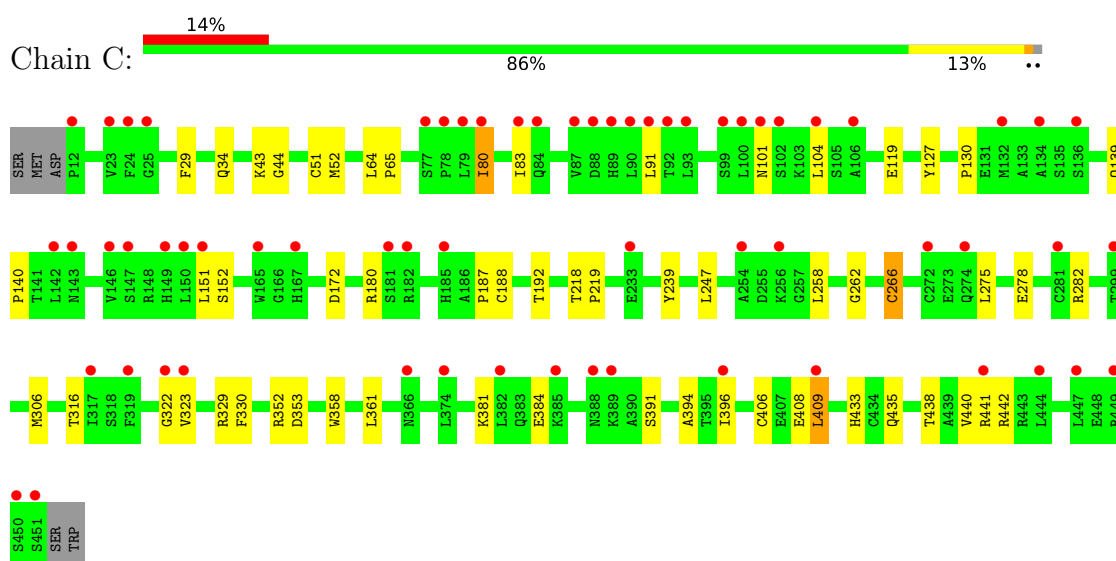
• Molecule 1: ATP-dependent DNA helicase Q5



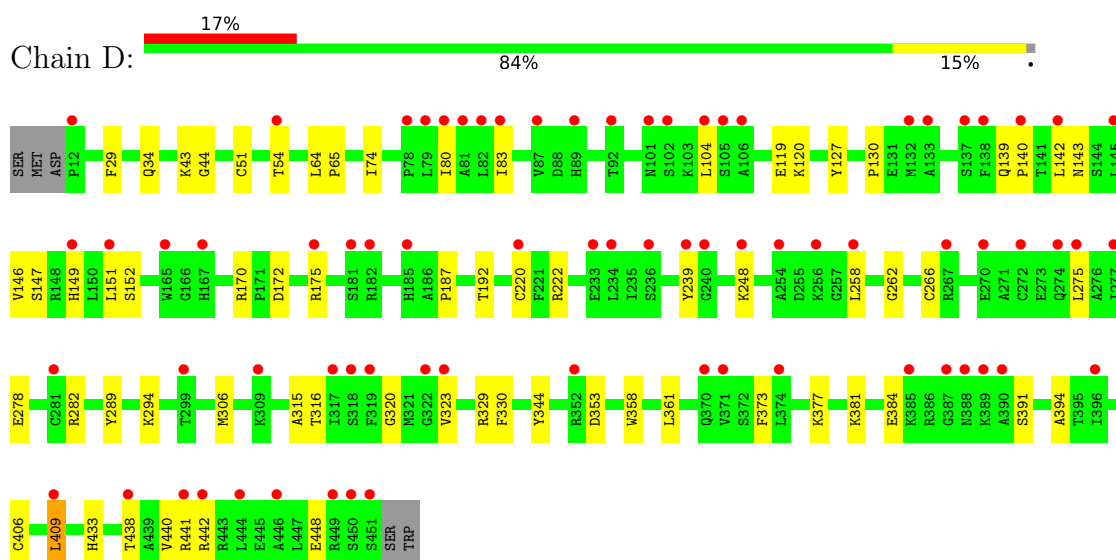
• Molecule 1: ATP-dependent DNA helicase Q5



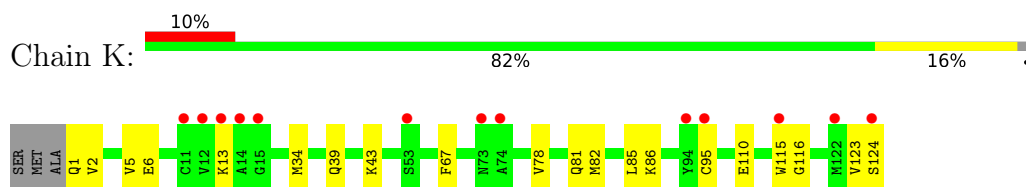
• Molecule 1: ATP-dependent DNA helicase Q5



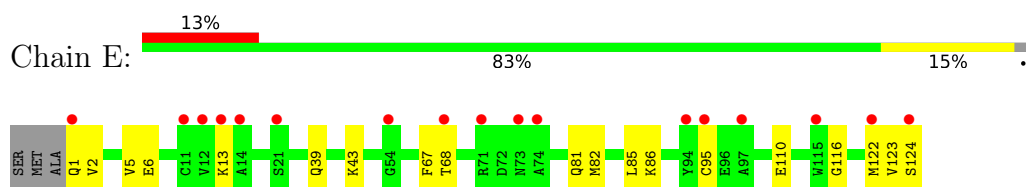
• Molecule 1: ATP-dependent DNA helicase Q5



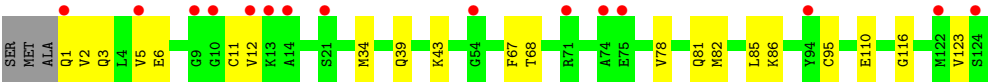
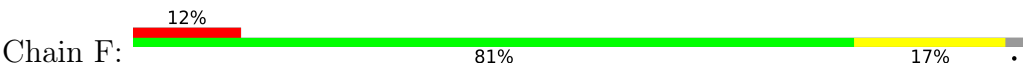
• Molecule 2: Gluebody G5-006



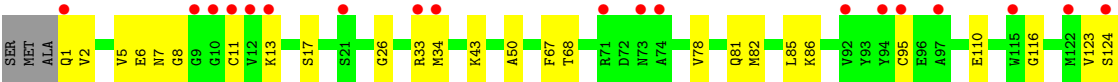
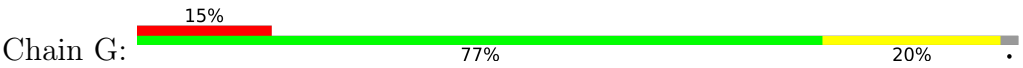
• Molecule 2: Gluebody G5-006



• Molecule 2: Gluebody G5-006



● Molecule 2: Gluebody G5-006



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.59Å 89.97Å 164.13Å 90.00° 110.06° 90.00°	Depositor
Resolution (Å)	77.69 – 2.00 77.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (77.69-2.00) 97.6 (77.69-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.243 , 0.275 0.247 , 0.278	Depositor DCC
R_{free} test set	10399 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18647	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3908e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.03	0/3531	1.39	6/4770 (0.1%)
1	B	1.04	0/3518	1.40	5/4753 (0.1%)
1	C	1.02	0/3535	1.39	4/4774 (0.1%)
1	D	1.03	0/3535	1.38	4/4774 (0.1%)
2	E	0.98	0/968	1.29	0/1314
2	F	1.00	0/968	1.28	0/1314
2	G	1.01	0/968	1.28	1/1314 (0.1%)
2	K	1.00	0/968	1.29	0/1314
All	All	1.03	0/17991	1.37	20/24327 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	PRO	CA-C-N	5.72	127.95	120.28
1	A	219	PRO	C-N-CA	5.72	127.95	120.28
2	G	26	GLY	CA-C-O	-5.70	117.05	122.13
1	C	219	PRO	CA-C-N	5.70	127.91	120.28
1	C	219	PRO	C-N-CA	5.70	127.91	120.28
1	D	119	GLU	N-CA-C	-5.54	101.45	109.59
1	B	119	GLU	N-CA-C	-5.46	101.56	109.59
1	B	266	CYS	CA-C-O	-5.38	115.32	121.40
1	A	119	GLU	N-CA-C	-5.37	101.70	109.59
1	C	119	GLU	N-CA-C	-5.33	101.75	109.59
1	A	54	THR	CB-CA-C	5.29	116.31	109.80
1	B	219	PRO	CA-C-N	5.26	127.33	120.28
1	B	219	PRO	C-N-CA	5.26	127.33	120.28
1	D	54	THR	CB-CA-C	5.17	116.16	109.80
1	A	180	ARG	CG-CD-NE	5.14	123.32	112.00
1	A	266	CYS	CA-C-O	-5.13	115.60	121.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	CYS	CA-C-O	-5.11	115.62	121.40
1	B	58	LYS	CB-CA-C	-5.03	102.76	110.81
1	D	222	ARG	CA-C-N	5.03	127.02	120.28
1	D	222	ARG	C-N-CA	5.03	127.02	120.28

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	3455	0	3486	48	0
1	B	3445	0	3473	39	0
1	C	3452	0	3479	40	0
1	D	3459	0	3497	41	0
2	E	946	0	887	12	0
2	F	946	0	887	14	0
2	G	946	0	887	17	0
2	K	946	0	887	15	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	187	0	0	8	0
5	B	186	0	0	6	0
5	C	193	0	0	9	0
5	D	186	0	0	6	0
5	E	60	0	0	1	0
5	F	72	0	0	2	0
5	G	66	0	0	2	0
5	K	78	0	0	5	0
All	All	18647	0	17483	225	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 6.

All (225) 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:D:143:ASN:O	1:D:146:VAL:HG22	1.60	1.00
1:A:306:MET:HE1	1:A:323:VAL:HG11	1.45	0.98
1:D:248:LYS:HG2	5:D:647:HOH:O	1.62	0.97
1:C:352:ARG:HD3	5:C:660:HOH:O	1.71	0.90
1:B:442:ARG:HG3	5:B:730:HOH:O	1.71	0.89
2:F:11:CYS:HG	2:G:11:CYS:HG	0.83	0.81
1:B:54:THR:HG22	5:B:750:HOH:O	1.84	0.77
1:A:143:ASN:HB3	5:A:740:HOH:O	1.88	0.72
1:B:119:GLU:O	1:B:120:LYS:HG2	1.90	0.71
1:C:408:GLU:HG3	5:C:632:HOH:O	1.90	0.70
1:A:172:ASP:OD1	1:A:175[B]:ARG:NH2	2.24	0.69
1:C:306:MET:HE1	1:C:323:VAL:HG11	1.75	0.68
1:D:74:ILE:HG13	1:D:151:LEU:HD11	1.74	0.67
1:D:120:LYS:HE3	5:D:743:HOH:O	1.96	0.66
1:D:438:THR:HG22	1:D:441[A]:ARG:NH2	2.10	0.66
2:E:13:LYS:HA	2:E:124:SER:OG	1.95	0.66
1:A:438:THR:HG22	1:A:441[A]:ARG:NH2	2.12	0.65
1:C:438:THR:HG22	1:C:441[A]:ARG:NH2	2.12	0.65
2:G:33:ARG:HD2	2:G:50:ALA:HB1	1.78	0.64
1:C:396:ILE:HD12	5:C:730:HOH:O	1.99	0.63
1:A:74:ILE:HG13	1:A:151:LEU:HD11	1.81	0.62
1:A:306:MET:HE1	1:A:323:VAL:CG1	2.27	0.62
2:G:67:PHE:CE2	2:G:82:MET:HE3	2.35	0.62
1:A:24:PHE:HB3	5:A:617:HOH:O	2.01	0.61
1:B:96:ARG:HD3	5:B:764:HOH:O	1.99	0.61
1:A:146:VAL:HG21	5:A:700:HOH:O	2.00	0.60
1:A:17:ARG:HD2	5:A:761:HOH:O	2.01	0.60
1:C:396:ILE:CD1	5:C:730:HOH:O	2.48	0.60
2:E:5:VAL:HG12	5:E:234:HOH:O	2.00	0.60
1:C:91:LEU:HD23	5:C:666:HOH:O	2.01	0.59
2:F:67:PHE:CE2	2:F:82:MET:HE3	2.38	0.59
1:C:306:MET:HE1	1:C:323:VAL:CG1	2.32	0.59
2:E:67:PHE:CE2	2:E:82:MET:HE3	2.37	0.58
2:K:67:PHE:CE2	2:K:82:MET:HE3	2.38	0.58
1:B:239:TYR:HE1	1:B:275:LEU:HD13	1.69	0.58
1:B:119:GLU:C	1:B:120:LYS:HG2	2.29	0.58
2:G:13:LYS:HA	2:G:124:SER:OG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:NH2	1:A:353:ASP:OD2	2.37	0.57
1:A:239:TYR:HE1	1:A:275:LEU:HD13	1.68	0.57
2:K:115:TRP:CZ2	5:K:256:HOH:O	2.51	0.57
1:C:239:TYR:HE1	1:C:275:LEU:HD13	1.69	0.56
1:C:329:ARG:NH2	1:C:353:ASP:OD2	2.37	0.56
1:B:329:ARG:NH2	1:B:353:ASP:OD2	2.38	0.56
2:K:115:TRP:CH2	5:K:256:HOH:O	2.58	0.56
2:G:67:PHE:CZ	2:G:82:MET:HE3	2.40	0.56
1:A:278:GLU:OE1	1:A:282:ARG:NH1	2.39	0.55
1:A:322:GLY:HA3	5:A:621:HOH:O	2.05	0.55
1:B:64:LEU:HD23	1:B:64:LEU:C	2.32	0.55
1:B:119:GLU:O	1:B:120:LYS:CG	2.54	0.55
1:D:329:ARG:NH2	1:D:353:ASP:OD2	2.39	0.55
5:K:265:HOH:O	2:E:122:MET:HB2	2.06	0.55
1:A:64:LEU:C	1:A:64:LEU:HD23	2.32	0.55
1:C:278:GLU:OE1	1:C:282:ARG:NH1	2.40	0.54
1:C:64:LEU:C	1:C:64:LEU:HD23	2.32	0.54
2:G:43:LYS:HE3	5:G:263:HOH:O	2.07	0.54
1:B:278:GLU:OE1	1:B:282:ARG:NH1	2.39	0.54
2:G:5:VAL:HG12	5:G:232:HOH:O	2.07	0.54
1:B:29:PHE:HD1	1:B:34:GLN:HE21	1.54	0.54
2:G:82:MET:HE2	2:G:85:LEU:HD21	1.90	0.54
1:D:29:PHE:HD1	1:D:34:GLN:HE21	1.54	0.54
1:C:361:LEU:HD13	1:C:406:CYS:SG	2.48	0.54
1:A:143:ASN:CB	5:A:740:HOH:O	2.52	0.53
2:E:39:GLN:NE2	2:E:43:LYS:O	2.41	0.53
1:C:409:LEU:HA	5:C:670:HOH:O	2.08	0.53
1:D:64:LEU:C	1:D:64:LEU:HD23	2.33	0.53
2:F:39:GLN:NE2	2:F:43:LYS:O	2.41	0.53
1:D:142:LEU:O	1:D:146:VAL:HG13	2.08	0.53
1:B:438:THR:HG22	1:B:441[A]:ARG:NH2	2.24	0.53
1:D:278:GLU:OE1	1:D:282:ARG:NH1	2.40	0.53
1:D:361:LEU:HD13	1:D:406:CYS:SG	2.49	0.53
2:K:39:GLN:NE2	2:K:43:LYS:O	2.42	0.53
1:C:130:PRO:HB2	1:C:172:ASP:HB3	1.91	0.53
1:C:180:ARG:HD3	1:C:188:CYS:HB2	1.91	0.53
2:K:86:LYS:C	2:K:123:VAL:HG11	2.34	0.52
1:A:409:LEU:HD13	5:A:678:HOH:O	2.09	0.52
2:F:86:LYS:C	2:F:123:VAL:HG11	2.35	0.52
1:A:29:PHE:HD1	1:A:34:GLN:HE21	1.57	0.52
1:D:170:ARG:HD3	5:D:715:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:VAL:HG23	5:D:640:HOH:O	2.10	0.51
2:K:5:VAL:HG12	5:K:229:HOH:O	2.09	0.51
1:D:146:VAL:HG23	1:D:147:SER:N	2.25	0.51
2:G:86:LYS:C	2:G:123:VAL:HG11	2.35	0.51
1:D:239:TYR:HE1	1:D:275:LEU:HD13	1.73	0.51
1:C:29:PHE:HD1	1:C:34:GLN:HE21	1.57	0.51
1:D:130:PRO:HB2	1:D:172:ASP:HB3	1.92	0.51
2:K:67:PHE:CZ	2:K:82:MET:HE3	2.46	0.50
1:A:239:TYR:CE1	1:A:275:LEU:HD13	2.46	0.50
1:B:381:LYS:O	1:B:384:GLU:HG2	2.12	0.50
2:E:67:PHE:CZ	2:E:82:MET:HE3	2.46	0.50
2:E:82:MET:HE2	2:E:85:LEU:HD21	1.94	0.50
1:C:239:TYR:CE1	1:C:275:LEU:HD13	2.47	0.50
1:D:149:HIS:HA	5:D:673:HOH:O	2.11	0.50
2:E:86:LYS:C	2:E:123:VAL:HG11	2.36	0.49
2:G:34:MET:HG2	2:G:78:VAL:HG21	1.93	0.49
1:B:130:PRO:HB2	1:B:172:ASP:HB3	1.94	0.49
1:D:172:ASP:OD1	1:D:175[B]:ARG:NH2	2.46	0.49
2:G:6:GLU:OE2	2:G:116:GLY:HA3	2.12	0.49
1:B:239:TYR:CE1	1:B:275:LEU:HD13	2.47	0.49
1:A:130:PRO:HB2	1:A:172:ASP:HB3	1.95	0.49
1:C:435:GLN:HG3	5:C:747:HOH:O	2.11	0.49
2:E:6:GLU:OE2	2:E:116:GLY:HA3	2.13	0.49
1:A:381:LYS:O	1:A:384:GLU:HG2	2.12	0.49
1:B:30:LYS:NZ	5:B:604:HOH:O	2.44	0.49
1:A:149:HIS:CD2	5:A:737:HOH:O	2.66	0.49
2:F:67:PHE:CZ	2:F:82:MET:HE3	2.47	0.48
2:F:6:GLU:OE2	2:F:116:GLY:HA3	2.13	0.48
1:B:151:LEU:HD12	1:B:183:LEU:HD22	1.96	0.48
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.96	0.48
1:B:361:LEU:HD13	1:B:406:CYS:SG	2.54	0.48
1:C:329:ARG:HH22	1:C:353:ASP:CG	2.22	0.48
1:D:381:LYS:O	1:D:384:GLU:HG2	2.14	0.48
1:B:287:LYS:HE2	5:B:760:HOH:O	2.14	0.47
1:C:381:LYS:O	1:C:384:GLU:HG2	2.14	0.47
1:D:146:VAL:CG2	1:D:147:SER:N	2.76	0.47
1:B:329:ARG:HH22	1:B:353:ASP:CG	2.22	0.47
2:K:6:GLU:OE2	2:K:116:GLY:HA3	2.13	0.47
2:K:82:MET:HE2	2:K:85:LEU:HD21	1.96	0.47
1:C:266:CYS:SG	1:C:275:LEU:HD23	2.55	0.47
1:A:329:ARG:HH22	1:A:353:ASP:CG	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LEU:HB3	1:D:65:PRO:HD3	1.97	0.47
1:A:266:CYS:SG	1:A:275:LEU:HD23	2.55	0.46
1:B:266:CYS:SG	1:B:275:LEU:HD23	2.54	0.46
2:F:82:MET:HE2	2:F:85:LEU:HD21	1.97	0.46
1:A:361:LEU:HD13	1:A:406:CYS:SG	2.55	0.46
1:B:51:CYS:HA	1:B:192:THR:O	2.15	0.46
2:K:67:PHE:HA	2:K:81:GLN:O	2.16	0.46
1:C:83:ILE:HG23	1:C:127:TYR:HB3	1.97	0.46
1:C:352:ARG:CD	5:C:660:HOH:O	2.45	0.46
2:F:67:PHE:HA	2:F:81:GLN:O	2.16	0.46
1:A:180:ARG:HG2	1:A:207:LEU:O	2.16	0.46
1:B:262:GLY:HA3	1:B:330:PHE:CE2	2.51	0.46
1:B:302:GLN:NE2	1:B:323:VAL:HG21	2.31	0.46
1:D:83:ILE:HG23	1:D:127:TYR:HB3	1.96	0.46
2:E:1:GLN:HG2	2:E:2:VAL:N	2.31	0.45
1:A:372:SER:O	1:A:376:ARG:HG2	2.15	0.45
1:A:433:HIS:HA	1:A:440:VAL:HG21	1.99	0.45
1:B:409:LEU:C	1:B:409:LEU:HD22	2.42	0.45
1:B:433:HIS:HA	1:B:440:VAL:HG21	1.99	0.45
1:A:409:LEU:C	1:A:409:LEU:HD22	2.42	0.45
1:C:152:SER:O	1:C:187:PRO:HD2	2.16	0.45
1:D:266:CYS:SG	1:D:275:LEU:HD23	2.57	0.45
1:D:51:CYS:HA	1:D:192:THR:O	2.16	0.45
1:D:330:PHE:HA	1:D:358:TRP:O	2.17	0.45
1:A:152:SER:O	1:A:187:PRO:HD2	2.16	0.45
1:C:64:LEU:HB3	1:C:65:PRO:HD3	1.98	0.45
1:A:262:GLY:HA3	1:A:330:PHE:CE2	2.52	0.45
1:B:64:LEU:HB3	1:B:65:PRO:HD3	1.99	0.45
1:D:239:TYR:CE1	1:D:275:LEU:HD13	2.50	0.45
1:C:409:LEU:C	1:C:409:LEU:HD22	2.41	0.44
1:D:152:SER:O	1:D:187:PRO:HD2	2.17	0.44
1:B:80:ILE:CD1	1:B:101:ASN:HB2	2.47	0.44
1:B:330:PHE:HA	1:B:358:TRP:O	2.16	0.44
2:E:67:PHE:HA	2:E:81:GLN:O	2.17	0.44
1:C:262:GLY:HA3	1:C:330:PHE:CE2	2.52	0.44
1:C:433:HIS:HA	1:C:440:VAL:HG21	1.98	0.44
1:D:329:ARG:HH22	1:D:353:ASP:CG	2.23	0.44
1:A:51:CYS:HA	1:A:192:THR:O	2.17	0.44
1:D:175[B]:ARG:NH2	5:D:609:HOH:O	2.49	0.44
1:D:409:LEU:HD22	1:D:409:LEU:C	2.42	0.44
1:D:433:HIS:HA	1:D:440:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLY:O	1:B:187:PRO:HG3	2.18	0.44
1:C:51:CYS:HA	1:C:192:THR:O	2.17	0.44
1:D:262:GLY:HA3	1:D:330:PHE:CE2	2.53	0.43
1:B:272:CYS:SG	1:B:314:VAL:O	2.76	0.43
2:G:34:MET:HG2	2:G:78:VAL:HG11	2.00	0.43
2:F:5:VAL:HG12	5:F:240:HOH:O	2.18	0.43
1:A:44:GLY:O	1:A:187:PRO:HG3	2.18	0.43
1:A:391:SER:O	1:A:394:ALA:HB3	2.19	0.43
1:B:139:GLN:N	1:B:140:PRO:HD2	2.33	0.43
1:C:391:SER:O	1:C:394:ALA:HB3	2.19	0.43
2:G:7:ASN:CG	2:G:8:GLY:N	2.76	0.43
1:A:180:ARG:HH11	1:A:180:ARG:HD2	1.67	0.43
1:A:330:PHE:HA	1:A:358:TRP:O	2.18	0.43
1:B:267:ARG:HD3	5:B:655:HOH:O	2.19	0.43
2:G:1:GLN:HG2	2:G:2:VAL:N	2.33	0.43
1:C:139:GLN:N	1:C:140:PRO:HD2	2.34	0.43
1:D:316:THR:O	1:D:320:GLY:N	2.46	0.43
2:G:67:PHE:HA	2:G:81:GLN:O	2.18	0.43
2:F:12:VAL:HG11	2:F:85:LEU:HD13	2.01	0.42
1:B:306:MET:HE2	1:B:306:MET:HB2	1.91	0.42
1:C:262:GLY:HA3	1:C:330:PHE:CZ	2.54	0.42
1:C:330:PHE:HA	1:C:358:TRP:O	2.19	0.42
1:B:152:SER:O	1:B:187:PRO:HD2	2.18	0.42
1:A:139:GLN:N	1:A:140:PRO:HD2	2.34	0.42
1:B:391:SER:O	1:B:394:ALA:HB3	2.20	0.42
1:C:322:GLY:HA2	5:C:763:HOH:O	2.18	0.42
1:A:83:ILE:HG23	1:A:127:TYR:HB3	2.02	0.42
2:F:1:GLN:HG2	2:F:2:VAL:N	2.33	0.42
2:F:3:GLN:HG3	5:F:262:HOH:O	2.20	0.42
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.93	0.42
1:D:220:CYS:HB2	1:D:344:TYR:CE1	2.54	0.42
2:K:13:LYS:HA	2:K:124:SER:OG	2.20	0.42
1:A:262:GLY:HA3	1:A:330:PHE:CZ	2.55	0.42
1:D:44:GLY:O	1:D:187:PRO:HG3	2.20	0.42
1:B:180:ARG:HD3	1:B:188:CYS:HB2	2.01	0.42
1:A:266:CYS:O	1:A:316:THR:HA	2.20	0.42
1:B:262:GLY:HA3	1:B:330:PHE:CZ	2.55	0.42
1:D:139:GLN:N	1:D:140:PRO:HD2	2.35	0.42
1:C:44:GLY:O	1:C:187:PRO:HG3	2.19	0.41
1:C:80:ILE:CD1	1:C:101:ASN:HB2	2.51	0.41
1:C:247:LEU:HD23	1:C:247:LEU:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:CYS:O	1:C:316:THR:HA	2.21	0.41
1:D:373:PHE:CE1	1:D:377:LYS:HD2	2.55	0.41
2:K:1:GLN:HG3	2:K:2:VAL:N	2.34	0.41
1:D:266:CYS:O	1:D:316:THR:HA	2.20	0.41
2:G:67:PHE:CZ	2:G:82:MET:CE	3.03	0.41
1:D:306:MET:HE2	1:D:306:MET:HB2	1.92	0.41
2:F:34:MET:HG2	2:F:78:VAL:HG21	2.02	0.41
2:G:17:SER:HA	2:G:82:MET:O	2.21	0.41
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.94	0.41
1:A:289:TYR:O	1:A:315:ALA:HA	2.21	0.41
1:A:306:MET:HE2	1:A:306:MET:HB2	1.85	0.41
1:A:19:THR:OG1	1:A:68:LEU:HD21	2.21	0.41
1:A:80:ILE:CD1	1:A:101:ASN:HB2	2.50	0.41
1:B:266:CYS:O	1:B:316:THR:HA	2.20	0.41
2:K:115:TRP:CE2	5:K:256:HOH:O	2.74	0.41
2:E:67:PHE:CZ	2:E:82:MET:CE	3.04	0.41
1:C:52:MET:HG2	1:C:218:THR:OG1	2.21	0.41
2:K:34:MET:HG2	2:K:78:VAL:HG21	2.03	0.41
2:K:67:PHE:CZ	2:K:82:MET:CE	3.04	0.41
1:A:52:MET:HG2	1:A:218:THR:OG1	2.21	0.40
1:A:242:LEU:CD2	1:A:275:LEU:HD11	2.51	0.40
2:F:67:PHE:CZ	2:F:82:MET:CE	3.05	0.40
1:D:289:TYR:O	1:D:315:ALA:HA	2.21	0.40
1:D:391:SER:O	1:D:394:ALA: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	443/445 (100%)	432 (98%)	11 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	442/445 (99%)	433 (98%)	9 (2%)	0	100	100
1	C	443/445 (100%)	430 (97%)	13 (3%)	0	100	100
1	D	443/445 (100%)	430 (97%)	13 (3%)	0	100	100
2	E	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
2	F	123/127 (97%)	120 (98%)	3 (2%)	0	100	100
2	G	123/127 (97%)	118 (96%)	5 (4%)	0	100	100
2	K	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
All	All	2263/2288 (99%)	2201 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	369/373 (99%)	361 (98%)	8 (2%)	45	50
1	B	368/373 (99%)	360 (98%)	8 (2%)	45	50
1	C	370/373 (99%)	363 (98%)	7 (2%)	50	56
1	D	370/373 (99%)	362 (98%)	8 (2%)	45	50
2	E	98/100 (98%)	95 (97%)	3 (3%)	35	37
2	F	98/100 (98%)	95 (97%)	3 (3%)	35	37
2	G	98/100 (98%)	95 (97%)	3 (3%)	35	37
2	K	98/100 (98%)	96 (98%)	2 (2%)	48	54
All	All	1869/1892 (99%)	1827 (98%)	42 (2%)	44	50

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	80	ILE

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Mol	Chain	Res	Type
1	A	86	GLN
1	A	104	LEU
1	A	248	LYS
1	A	258	LEU
1	A	409	LEU
1	A	442	ARG
1	B	43	LYS
1	B	80	ILE
1	B	86	GLN
1	B	104	LEU
1	B	136	SER
1	B	258	LEU
1	B	409	LEU
1	B	442	ARG
1	C	43	LYS
1	C	80	ILE
1	C	104	LEU
1	C	151	LEU
1	C	258	LEU
1	C	409	LEU
1	C	442	ARG
1	D	43	LYS
1	D	80	ILE
1	D	104	LEU
1	D	258	LEU
1	D	294	LYS
1	D	409	LEU
1	D	442	ARG
1	D	448	GLU
2	K	95	CYS
2	K	110	GLU
2	E	68	THR
2	E	95	CYS
2	E	110	GLU
2	F	68	THR
2	F	95	CYS
2	F	110	GLU
2	G	68	THR
2	G	95	CYS
2	G	110	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	86	GLN
1	A	285	ASN
1	B	34	GLN
1	B	139	GLN
1	B	285	ASN
1	B	302	GLN
1	C	34	GLN
1	C	208	HIS
1	C	285	ASN
1	D	34	GLN
1	D	285	ASN
1	D	302	GLN
2	K	3	GLN
2	K	73	ASN
2	K	120	GLN
2	E	3	GLN
2	F	3	GLN
2	F	81	GLN
2	G	3	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 8 ligands modelled in this entry, 4 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	A	502	-	4,4,4	0.26	0	6,6,6	0.09	0
4	SO4	B	502	-	4,4,4	0.35	0	6,6,6	0.24	0
4	SO4	D	502	-	4,4,4	0.08	0	6,6,6	0.26	0
4	SO4	C	502	-	4,4,4	0.36	0	6,6,6	0.25	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, 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	440/445 (98%)	1.07	64 (14%) 6 5	23, 51, 82, 107	5 (1%)
1	B	440/445 (98%)	0.87	60 (13%) 7 6	19, 48, 77, 109	4 (0%)
1	C	440/445 (98%)	0.89	63 (14%) 6 5	20, 49, 81, 114	4 (0%)
1	D	440/445 (98%)	0.98	74 (16%) 4 4	20, 51, 83, 104	5 (1%)
2	E	124/127 (97%)	0.65	17 (13%) 6 6	26, 42, 66, 105	1 (0%)
2	F	124/127 (97%)	0.71	15 (12%) 8 8	27, 41, 70, 103	1 (0%)
2	G	124/127 (97%)	0.82	19 (15%) 5 4	28, 43, 69, 113	1 (0%)
2	K	124/127 (97%)	0.62	13 (10%) 11 10	27, 42, 66, 108	1 (0%)
All	All	2256/2288 (98%)	0.90	325 (14%) 6 5	19, 47, 80, 114	22 (0%)

All (325) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	12	PRO	7.5
1	D	12	PRO	7.3
1	A	12	PRO	7.0
1	C	12	PRO	6.7
2	F	10	GLY	6.7
2	G	10	GLY	6.6
1	B	409	LEU	6.1
1	D	79	LEU	5.8
1	D	409	LEU	5.6
1	D	317	ILE	5.5
1	C	317	ILE	5.4
1	A	409	LEU	5.3
1	A	165	TRP	5.3
2	F	9	GLY	5.0
1	C	319	PHE	4.9
1	A	79	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	409	LEU	4.7
1	D	104	LEU	4.7
1	A	382	LEU	4.6
1	C	79	LEU	4.6
2	K	124	SER	4.3
1	B	374	LEU	4.3
2	G	74	ALA	4.2
1	D	165	TRP	4.1
1	B	79	LEU	4.1
1	A	319	PHE	4.1
1	B	319	PHE	4.1
1	D	185	HIS	4.1
1	D	80	ILE	4.0
1	C	165	TRP	4.0
2	K	14	ALA	4.0
1	A	317	ILE	4.0
1	B	165	TRP	3.9
1	C	80	ILE	3.9
2	E	124	SER	3.9
2	F	74	ALA	3.9
2	K	13	LYS	3.9
1	A	185	HIS	3.8
1	D	319	PHE	3.8
1	B	185	HIS	3.8
1	D	374	LEU	3.8
1	C	167[A]	HIS	3.7
1	D	254	ALA	3.7
2	G	95	CYS	3.7
1	A	374	LEU	3.7
2	G	122	MET	3.7
1	C	89	HIS	3.7
2	E	12	VAL	3.7
2	G	94	TYR	3.7
1	C	102	SER	3.7
1	C	441[A]	ARG	3.7
1	A	167[A]	HIS	3.6
2	G	124	SER	3.6
1	A	390	ALA	3.6
1	D	133	ALA	3.6
1	C	322	GLY	3.6
2	F	124	SER	3.6
1	C	104	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	185	HIS	3.6
2	F	14	ALA	3.5
1	B	281	CYS	3.5
2	G	33	ARG	3.5
1	A	254	ALA	3.5
2	G	9	GLY	3.5
2	K	122	MET	3.5
1	B	13	GLU	3.4
2	E	14	ALA	3.4
1	B	167[A]	HIS	3.4
1	D	167[A]	HIS	3.4
1	C	272	CYS	3.4
1	D	132	MET	3.4
1	C	281	CYS	3.3
1	D	451	SER	3.3
1	C	254	ALA	3.3
2	K	74	ALA	3.3
1	B	104	LEU	3.3
2	E	1	GLN	3.3
1	B	233	GLU	3.3
2	G	34	MET	3.3
1	B	256	LYS	3.3
2	E	13	LYS	3.3
1	A	136	SER	3.3
1	B	255	ASP	3.3
1	B	102	SER	3.2
2	K	95	CYS	3.2
1	B	441[A]	ARG	3.2
1	C	182	ARG	3.2
2	F	122	MET	3.2
2	E	74	ALA	3.2
1	C	444	LEU	3.2
1	D	277	ILE	3.2
1	A	281	CYS	3.2
1	B	388	ASN	3.2
1	D	175[A]	ARG	3.1
1	D	441[A]	ARG	3.1
1	A	378	GLU	3.1
2	G	21	SER	3.1
1	A	389	LYS	3.1
1	D	82	LEU	3.1
1	A	266	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	12	VAL	3.1
1	A	149	HIS	3.1
1	B	254	ALA	3.1
1	D	323	VAL	3.1
1	C	389	LYS	3.0
1	C	134	ALA	3.0
1	C	451	SER	3.0
1	A	441[A]	ARG	3.0
1	C	256	LYS	3.0
2	G	1	GLN	2.9
1	B	449	ARG	2.9
2	E	97	ALA	2.9
1	D	281	CYS	2.9
1	C	149	HIS	2.9
1	A	86	GLN	2.9
1	D	101	ASN	2.9
1	C	100	LEU	2.9
1	D	142	LEU	2.9
1	D	272	CYS	2.9
1	D	309	LYS	2.9
2	F	13	LYS	2.9
1	A	146	VAL	2.9
1	B	323	VAL	2.9
2	G	12	VAL	2.9
1	B	86	GLN	2.9
2	G	73	ASN	2.9
1	D	444	LEU	2.8
2	F	1	GLN	2.8
1	A	109	ARG	2.8
1	C	87	VAL	2.8
1	A	80	ILE	2.8
1	A	299	THR	2.8
1	D	78	PRO	2.8
1	D	371	VAL	2.8
2	E	95	CYS	2.8
1	D	256	LYS	2.8
1	C	449	ARG	2.8
1	D	318	SER	2.8
1	A	275	LEU	2.8
1	C	142	LEU	2.8
1	C	447	LEU	2.8
1	D	220	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	K	12	VAL	2.8
1	B	257	GLY	2.7
1	C	106	ALA	2.7
1	D	234	LEU	2.7
1	A	89	HIS	2.7
1	B	451	SER	2.7
1	D	81	ALA	2.7
1	B	93	LEU	2.7
1	C	101	ASN	2.7
1	D	233	GLU	2.7
1	A	235	ILE	2.7
1	C	83	ILE	2.7
1	C	181	SER	2.7
1	A	272	CYS	2.7
1	A	134	ALA	2.6
1	A	373	PHE	2.6
1	C	78	PRO	2.6
1	B	317	ILE	2.6
1	B	247	LEU	2.6
1	A	255	ASP	2.6
1	B	137	SER	2.6
1	D	102	SER	2.6
1	D	389	LYS	2.6
2	F	5	VAL	2.6
2	K	11	CYS	2.6
1	A	257	GLY	2.6
1	A	397	MET	2.6
1	A	234	LEU	2.6
1	C	150	LEU	2.6
1	D	140	PRO	2.6
1	B	25	GLY	2.6
1	D	299	THR	2.6
1	A	104	LEU	2.6
1	A	142	LEU	2.6
1	C	151	LEU	2.6
1	C	374	LEU	2.6
2	G	115	TRP	2.6
1	A	233	GLU	2.5
2	E	122	MET	2.5
1	C	143	ASN	2.5
1	A	147	SER	2.5
1	B	450	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	K	15	GLY	2.5
1	D	149	HIS	2.5
1	D	385	LYS	2.5
1	D	388	ASN	2.5
1	D	105	SER	2.5
1	A	22	LYS	2.5
1	B	22	LYS	2.5
1	B	322	GLY	2.5
1	B	23	VAL	2.5
2	E	71	ARG	2.5
1	C	388	ASN	2.5
2	E	94	TYR	2.5
1	B	438	THR	2.5
2	G	97	ALA	2.5
1	B	14	ARG	2.5
1	B	17	ARG	2.5
2	F	71	ARG	2.5
1	C	136	SER	2.4
1	C	299	THR	2.4
1	A	133	ALA	2.4
1	C	132	MET	2.4
1	A	248	LYS	2.4
1	B	447	LEU	2.4
1	C	93	LEU	2.4
1	D	145	LEU	2.4
1	A	101	ASN	2.4
1	C	450	SER	2.4
2	F	94	TYR	2.4
1	B	389	LYS	2.4
1	B	89	HIS	2.4
1	C	382	LEU	2.4
1	B	283	GLY	2.4
1	B	274	GLN	2.4
1	D	54	THR	2.4
1	D	352	ARG	2.4
1	D	89	HIS	2.4
1	C	91	LEU	2.4
2	E	73	ASN	2.4
1	C	88	ASP	2.4
1	C	23	VAL	2.4
1	D	83	ILE	2.4
1	A	385	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	318	SER	2.4
1	B	385	LYS	2.4
1	D	267	ARG	2.4
2	E	21	SER	2.4
1	A	91	LEU	2.3
1	C	366	ASN	2.3
1	D	387	GLY	2.3
1	A	376	ARG	2.3
1	A	449	ARG	2.3
1	B	352	ARG	2.3
1	D	270	GLU	2.3
1	C	84	GLN	2.3
2	E	115	TRP	2.3
1	B	444	LEU	2.3
1	D	275	LEU	2.3
1	D	236	SER	2.3
1	D	450	SER	2.3
1	B	16	VAL	2.3
1	D	87	VAL	2.3
2	F	75	GLU	2.3
1	D	274	GLN	2.3
1	A	82	LEU	2.3
2	F	54	GLY	2.3
2	G	71	ARG	2.3
1	B	381	LYS	2.3
2	G	13	LYS	2.3
1	A	18	SER	2.3
1	B	18	SER	2.3
2	F	21	SER	2.3
1	B	272	CYS	2.3
1	D	182	ARG	2.3
1	C	385	LYS	2.3
1	A	447	LEU	2.3
1	B	382	LEU	2.3
2	K	115	TRP	2.3
1	C	146	VAL	2.2
1	C	323	VAL	2.2
2	E	68	THR	2.2
1	A	143	ASN	2.2
1	A	21	LYS	2.2
1	D	240	GLY	2.2
1	D	322	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	239	TYR	2.2
2	K	53	SER	2.2
1	A	175[A]	ARG	2.2
1	C	24	PHE	2.2
1	A	54	THR	2.2
1	A	128	ILE	2.2
1	A	388	ASN	2.2
1	B	210	LYS	2.2
1	D	92	THR	2.2
1	D	248	LYS	2.2
2	K	73	ASN	2.2
1	A	132	MET	2.2
1	D	137	SER	2.2
1	D	449	ARG	2.2
1	B	235	ILE	2.2
1	D	151	LEU	2.2
1	C	147	SER	2.2
1	B	309	LYS	2.2
1	A	93	LEU	2.1
1	B	182	ARG	2.1
1	D	258	LEU	2.1
2	G	11	CYS	2.1
1	C	77	SER	2.1
1	A	338	LYS	2.1
2	K	94	TYR	2.1
1	A	88	ASP	2.1
1	A	256	LYS	2.1
1	C	99	SER	2.1
1	A	92	THR	2.1
1	B	122	GLN	2.1
1	C	92	THR	2.1
1	B	149	HIS	2.1
1	C	25	GLY	2.1
1	D	396	ILE	2.1
1	D	442	ARG	2.1
1	D	390	ALA	2.1
1	D	446	ALA	2.1
1	A	151	LEU	2.1
1	D	181	SER	2.1
1	B	270	GLU	2.1
2	E	54	GLY	2.1
1	A	375	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	232	LYS	2.1
1	C	396	ILE	2.1
1	B	26	PHE	2.1
2	G	92	VAL	2.1
1	B	107	GLN	2.0
1	C	233	GLU	2.0
1	D	138	PHE	2.0
1	D	106	ALA	2.0
1	B	101	ASN	2.0
1	A	100	LEU	2.0
1	C	90	LEU	2.0
1	C	274	GLN	2.0
1	D	370	GLN	2.0
2	E	11	CYS	2.0
1	D	438	THR	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	A	502	5/5	0.82	0.12	62,74,82,85	0
4	SO4	C	502	5/5	0.82	0.12	48,61,76,78	0
4	SO4	B	502	5/5	0.83	0.11	55,57,66,74	0
4	SO4	D	502	5/5	0.84	0.10	49,52,65,68	0
3	ZN	A	501	1/1	0.99	0.03	47,47,47,47	0
3	ZN	B	501	1/1	0.99	0.03	44,44,44,44	0
3	ZN	C	501	1/1	0.99	0.03	42,42,42,42	0
3	ZN	D	501	1/1	0.99	0.02	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.