



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:57 PM UTC

PDB ID : 7ZML / pdb_00007zml
Title : Crystal structure of human RECQL5 helicase APO form in complex with engineered nanobody (Gluebody) G1-001
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 : 2.79 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:

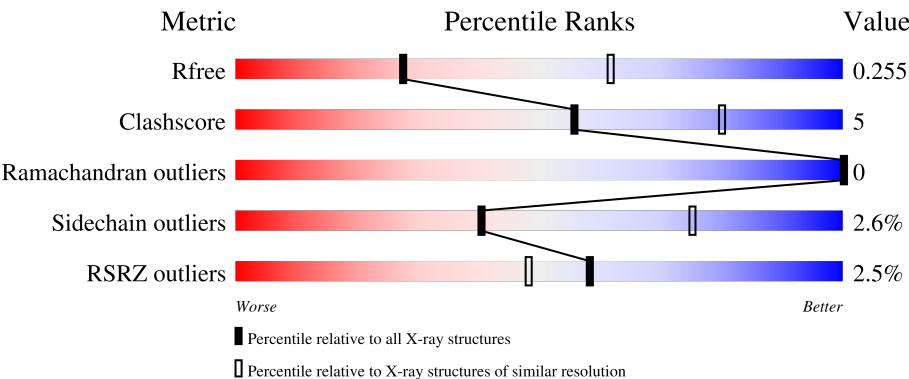
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	
1	B	445	
1	C	445	
1	D	445	
2	E	132	

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Mol	Chain	Length	Quality of chain
2	F	132	
2	G	132	
2	K	132	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17730 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	441	Total	C	N	O	S	0	4	0
			3452	2180	622	627	23			
1	B	441	Total	C	N	O	S	0	4	0
			3409	2155	605	626	23			
1	C	441	Total	C	N	O	S	0	5	0
			3432	2169	612	628	23			
1	D	440	Total	C	N	O	S	0	5	0
			3452	2180	623	626	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

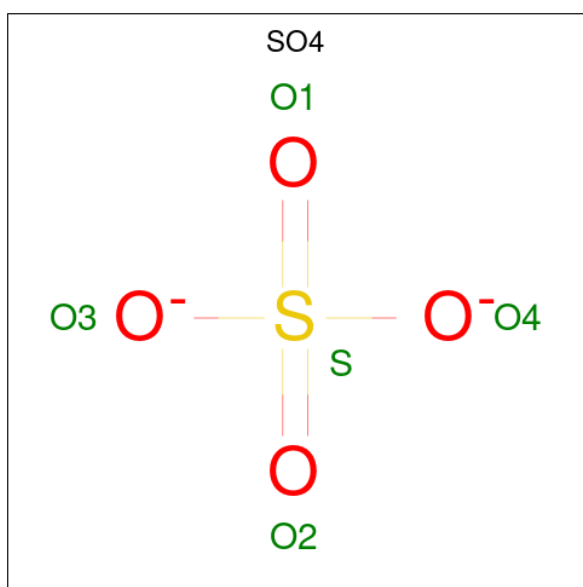
- Molecule 2 is a protein called Gluebody G1-001.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	131	Total	C	N	O	S	0	0	0
			996	623	169	200	4			
2	E	128	Total	C	N	O	S	0	0	0
			965	599	166	196	4			
2	F	130	Total	C	N	O	S	0	0	0
			985	614	168	199	4			
2	G	131	Total	C	N	O	S	0	0	0
			996	623	169	200	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		
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	3	Total	O	0	0
			3	3		

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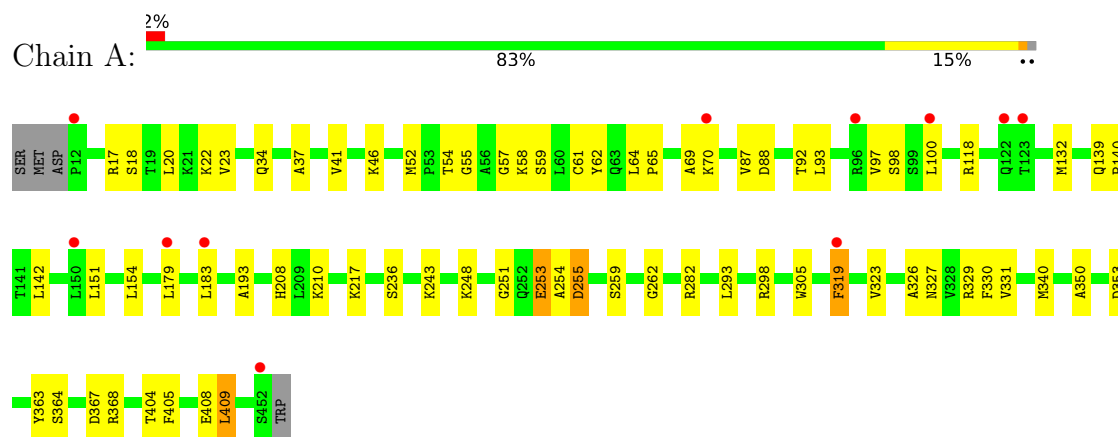
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	6	Total 6	O 6	0	0
5	C	2	Total 2	O 2	0	0
5	D	2	Total 2	O 2	0	0
5	K	1	Total 1	O 1	0	0
5	E	3	Total 3	O 3	0	0
5	G	2	Total 2	O 2	0	0

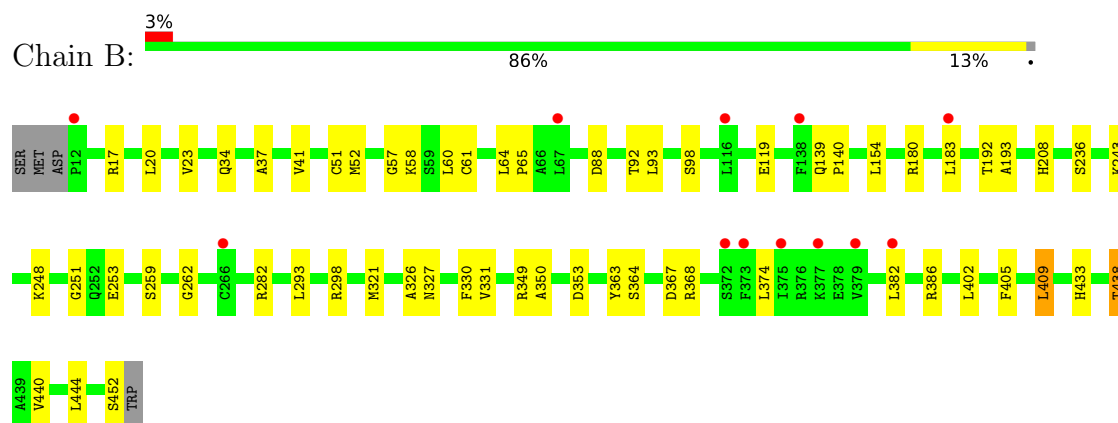
3 Residue-property plots [i](#)

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.

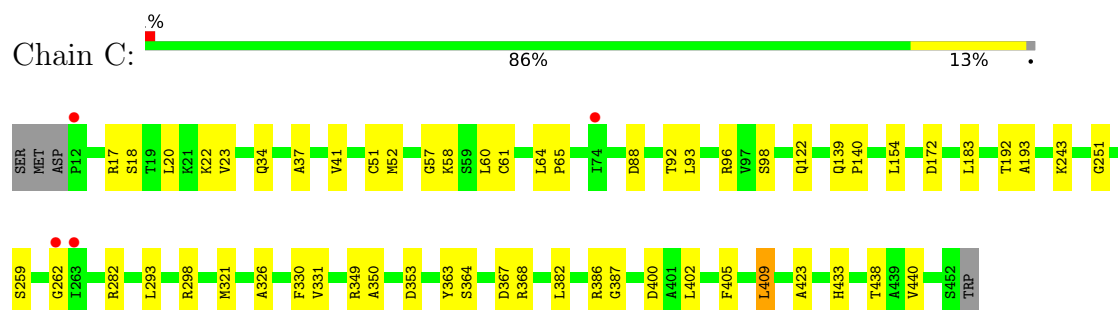
• Molecule 1: ATP-dependent DNA helicase Q5



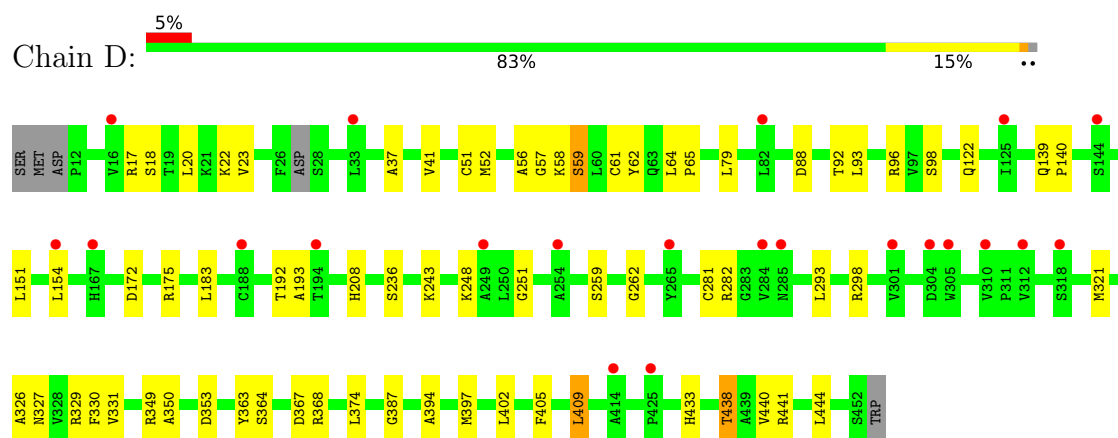
• Molecule 1: ATP-dependent DNA helicase Q5



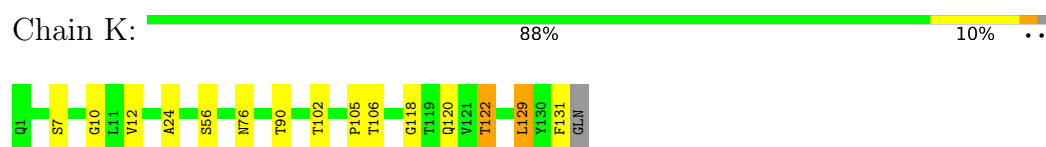
• Molecule 1: ATP-dependent DNA helicase Q5



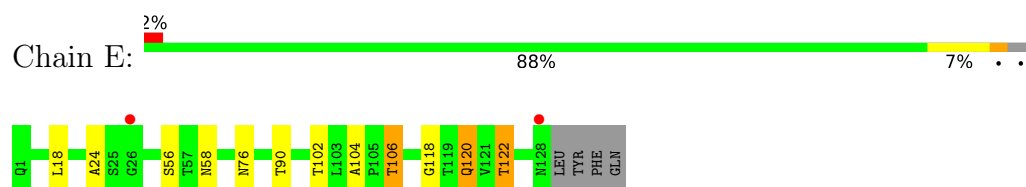
- Molecule 1: ATP-dependent DNA helicase Q5



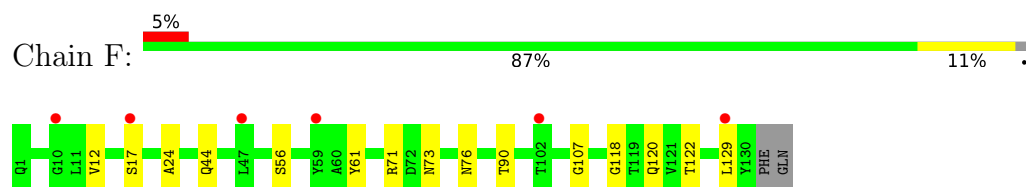
- Molecule 2: Gluebody G1-001



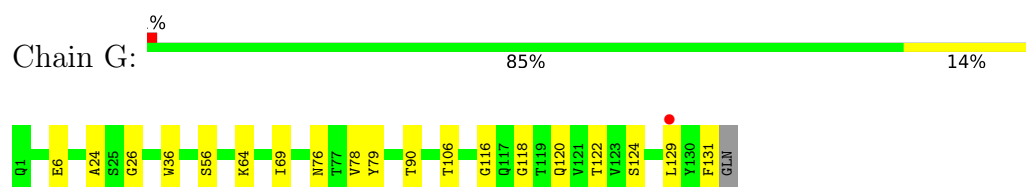
- Molecule 2: Gluebody G1-001



- Molecule 2: Gluebody G1-001



- Molecule 2: Gluebody G1-001



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.74Å 185.53Å 101.01Å 90.00° 107.47° 90.00°	Depositor
Resolution (Å)	96.35 – 2.79 96.35 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.6 (96.35-2.79) 99.6 (96.35-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.224 , 0.261 (Not available) , 0.255	Depositor DCC
R_{free} test set	3147 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.7	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	17730	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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

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	1.01	0/3528	1.51	6/4766 (0.1%)
1	B	1.01	0/3504	1.50	2/4738 (0.0%)
1	C	1.01	0/3525	1.49	1/4764 (0.0%)
1	D	1.00	0/3526	1.48	1/4761 (0.0%)
2	E	0.99	0/983	1.31	2/1332 (0.2%)
2	F	0.99	0/1004	1.30	2/1361 (0.1%)
2	G	0.99	0/1016	1.30	2/1377 (0.1%)
2	K	0.99	0/1016	1.31	3/1377 (0.2%)
All	All	1.00	0/18102	1.45	19/24476 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ASP	CA-CB-CG	7.72	120.32	112.60
1	C	172	ASP	CA-CB-CG	6.99	119.59	112.60
1	B	119	GLU	N-CA-C	-6.93	100.93	110.35
2	E	118	GLY	CA-C-O	-6.52	117.98	122.22
2	F	118	GLY	CA-C-O	-6.04	118.30	122.22
2	K	118	GLY	CA-C-O	-5.92	118.37	122.22
2	G	118	GLY	CA-C-O	-5.83	118.25	122.45
1	A	319	PHE	CA-C-O	-5.78	114.33	120.92
2	F	44	GLN	CB-CA-C	5.65	118.85	109.53
1	B	452	SER	CA-C-O	5.62	130.36	120.80
1	A	210	LYS	CB-CA-C	5.59	118.97	109.80
1	D	59	SER	CA-C-O	-5.36	114.84	120.63
2	G	26	GLY	CA-C-O	-5.35	117.11	121.76
1	A	254	ALA	CA-C-N	5.30	127.70	120.54
1	A	254	ALA	C-N-CA	5.30	127.70	120.54
2	K	12	VAL	CA-C-N	5.20	128.23	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	12	VAL	C-N-CA	5.20	128.23	120.95
2	E	58	ASN	CB-CA-C	5.18	117.60	110.34
1	A	54	THR	CA-CB-OG1	-5.16	101.86	109.60

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	3452	0	3484	41	0
1	B	3409	0	3399	33	0
1	C	3432	0	3439	33	0
1	D	3452	0	3481	39	0
2	E	965	0	918	5	0
2	F	985	0	938	6	0
2	G	996	0	947	13	0
2	K	996	0	947	8	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	2	0
4	B	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	1	0
5	A	3	0	0	1	0
5	B	6	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	G	2	0	0	0	0
5	K	1	0	0	0	0
All	All	17730	0	17553	167	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 (167) 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:243:LYS:HD3	1:D:282:ARG:HB3	1.69	0.74
1:A:142:LEU:CD2	1:A:179:LEU:HD11	2.18	0.73
1:B:208:HIS:ND1	1:D:387:GLY:HA3	2.06	0.70
1:D:52:MET:O	1:D:193:ALA:HA	1.92	0.69
2:E:90:THR:HG23	2:E:122:THR:HA	1.76	0.68
1:A:57:GLY:N	4:A:502:SO4:O4	2.26	0.68
1:A:243:LYS:HD3	1:A:282:ARG:HB3	1.74	0.68
1:A:142:LEU:HD21	1:A:179:LEU:HD11	1.76	0.66
1:B:243:LYS:HD3	1:B:282:ARG:HB3	1.78	0.66
1:A:88:ASP:O	1:A:92:THR:HG23	1.98	0.64
2:F:90:THR:HG23	2:F:122:THR:HA	1.79	0.64
1:C:88:ASP:O	1:C:92:THR:HG23	2.00	0.62
1:D:88:ASP:O	1:D:92:THR:HG23	2.00	0.61
1:B:88:ASP:O	1:B:92:THR:HG23	2.00	0.61
2:G:36:TRP:HD1	2:G:69:ILE:HD13	1.65	0.61
1:B:409:LEU:HD13	1:B:409:LEU:H	1.67	0.60
2:G:90:THR:HG23	2:G:122:THR:HA	1.82	0.59
1:D:59:SER:HA	1:D:62:TYR:CE2	2.37	0.59
1:D:64:LEU:HB3	1:D:65:PRO:HD3	1.85	0.59
2:G:69:ILE:HD11	2:G:78:VAL:CG2	2.33	0.59
2:K:90:THR:HG23	2:K:122:THR:HA	1.83	0.58
1:C:64:LEU:HB3	1:C:65:PRO:HD3	1.84	0.58
1:B:64:LEU:HB3	1:B:65:PRO:HD3	1.84	0.58
1:B:262:GLY:HA3	1:B:330:PHE:CE2	2.40	0.57
1:A:52:MET:O	1:A:193:ALA:HA	2.04	0.57
1:D:438:THR:HG22	1:D:441[A]:ARG:NH2	2.20	0.57
1:B:154:LEU:HD22	1:B:183:LEU:HD12	1.86	0.56
1:C:409:LEU:H	1:C:409:LEU:HD13	1.70	0.56
1:C:262:GLY:HA3	1:C:330:PHE:CE2	2.41	0.56
1:A:409:LEU:H	1:A:409:LEU:HD13	1.71	0.56
1:D:409:LEU:H	1:D:409:LEU:HD13	1.71	0.56
2:F:71:ARG:HD2	2:F:73:ASN:OD1	2.05	0.56
1:A:262:GLY:HA3	1:A:330:PHE:CE2	2.41	0.55
1:C:57:GLY:N	4:C:502:SO4:O1	2.37	0.55
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.88	0.55
1:D:251:GLY:H	1:D:259:SER:H	1.55	0.55
1:D:262:GLY:HA3	1:D:330:PHE:CE2	2.41	0.55
1:A:251:GLY:H	1:A:259:SER:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:ARG:NH2	1:D:353:ASP:OD2	2.38	0.54
1:A:55:GLY:O	4:A:502:SO4:O4	2.25	0.54
1:B:52:MET:O	1:B:193:ALA:HA	2.06	0.54
1:B:139:GLN:N	1:B:140:PRO:HD2	2.23	0.54
1:A:34:GLN:HA	1:A:52:MET:HE1	1.91	0.53
1:C:139:GLN:N	1:C:140:PRO:HD2	2.24	0.53
1:A:139:GLN:N	1:A:140:PRO:HD2	2.24	0.53
1:A:154:LEU:HD22	1:A:183:LEU:HD12	1.90	0.53
1:D:139:GLN:N	1:D:140:PRO:HD2	2.23	0.53
1:C:23:VAL:O	1:C:93:LEU:HD22	2.09	0.53
1:D:23:VAL:O	1:D:93:LEU:HD22	2.08	0.53
1:A:58:LYS:O	1:A:61:CYS:HB2	2.10	0.52
1:D:154:LEU:HD22	1:D:183:LEU:HD12	1.92	0.52
1:A:329:ARG:NH2	1:A:353:ASP:OD2	2.39	0.52
1:C:52:MET:O	1:C:193:ALA:HA	2.09	0.52
1:D:331:VAL:HG23	1:D:350:ALA:HB2	1.92	0.52
1:B:251:GLY:H	1:B:259:SER:H	1.58	0.52
1:A:217:LYS:O	2:F:107:GLY:HA3	2.10	0.51
1:B:34:GLN:HA	1:B:52:MET:HE1	1.91	0.51
1:C:34:GLN:HA	1:C:52:MET:HE1	1.92	0.51
2:K:10:GLY:HA2	2:G:131:PHE:CZ	2.46	0.50
1:C:58:LYS:O	1:C:61:CYS:HB2	2.13	0.49
1:C:331:VAL:HG23	1:C:350:ALA:HB2	1.94	0.49
1:A:23:VAL:O	1:A:93:LEU:HD22	2.12	0.49
1:C:154:LEU:HD22	1:C:183:LEU:HD12	1.94	0.49
1:C:251:GLY:H	1:C:259:SER:H	1.61	0.49
1:D:326:ALA:HB1	1:D:353:ASP:HB3	1.95	0.49
1:B:331:VAL:HG23	1:B:350:ALA:HB2	1.94	0.48
1:D:172:ASP:CG	1:D:175[B]:ARG:HH22	2.22	0.48
1:A:208:HIS:ND1	1:C:387:GLY:HA3	2.27	0.48
1:B:58:LYS:O	1:B:61:CYS:HB2	2.12	0.48
1:B:382:LEU:HD13	1:B:386:ARG:NH1	2.28	0.48
1:C:243:LYS:HD3	1:C:282:ARG:HB3	1.95	0.48
1:B:57:GLY:N	4:B:502:SO4:O1	2.39	0.48
1:D:58:LYS:O	1:D:61:CYS:HB2	2.12	0.48
1:A:331:VAL:HG23	1:A:350:ALA:HB2	1.95	0.48
2:G:24:ALA:HB3	2:G:76:ASN:HB3	1.96	0.48
1:C:400:ASP:OD1	2:F:61:TYR:OH	2.26	0.48
2:E:120:GLN:OE1	2:E:122:THR:HG23	2.13	0.48
1:B:326:ALA:HB1	1:B:353:ASP:HB3	1.96	0.47
1:C:364:SER:O	1:C:367:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:120:GLN:OE1	2:K:122:THR:HG23	2.14	0.47
2:G:124:SER:HB3	2:G:129:LEU:HD22	1.95	0.47
1:C:326:ALA:HB1	1:C:353:ASP:HB3	1.96	0.47
1:D:364:SER:O	1:D:367:ASP:HB2	2.14	0.47
1:A:326:ALA:HB1	1:A:353:ASP:HB3	1.95	0.47
1:B:363:TYR:OH	1:B:368:ARG:HD3	2.14	0.47
2:F:24:ALA:HB3	2:F:76:ASN:HB3	1.96	0.47
1:A:364:SER:O	1:A:367:ASP:HB2	2.15	0.47
1:B:208:HIS:CE1	1:D:387:GLY:HA3	2.49	0.46
1:B:364:SER:O	1:B:367:ASP:HB2	2.15	0.46
1:A:329:ARG:HH22	1:A:353:ASP:CG	2.23	0.46
1:B:23:VAL:O	1:B:93:LEU:HD22	2.16	0.46
1:D:329:ARG:HH22	1:D:353:ASP:CG	2.23	0.46
1:D:394:ALA:HA	1:D:397:MET:HE3	1.97	0.46
1:A:363:TYR:OH	1:A:368:ARG:HD3	2.16	0.46
1:C:37:ALA:O	1:C:41:VAL:HG23	2.16	0.46
1:B:37:ALA:O	1:B:41:VAL:HG23	2.16	0.46
1:C:293:LEU:O	1:C:298:ARG:NH1	2.49	0.46
1:C:363:TYR:OH	1:C:368:ARG:HD3	2.16	0.45
1:B:386:ARG:O	1:D:208:HIS:CE1	2.69	0.45
1:C:423:ALA:HB3	2:K:105:PRO:HA	1.98	0.45
1:A:293:LEU:O	1:A:298:ARG:NH1	2.50	0.45
1:D:64:LEU:C	1:D:64:LEU:HD23	2.41	0.45
1:D:96:ARG:HD2	1:D:122:GLN:HG3	1.99	0.45
1:D:18:SER:O	1:D:22:LYS:N	2.42	0.45
1:D:58:LYS:HE2	1:D:58:LYS:HB3	1.84	0.45
1:D:37:ALA:O	1:D:41:VAL:HG23	2.17	0.45
1:D:433:HIS:HA	1:D:440:VAL:HG21	1.99	0.45
1:D:363:TYR:OH	1:D:368:ARG:HD3	2.17	0.45
1:A:64:LEU:C	1:A:64:LEU:HD23	2.43	0.44
1:D:293:LEU:O	1:D:298:ARG:NH1	2.51	0.44
2:K:24:ALA:HB3	2:K:76:ASN:HB3	1.99	0.44
1:A:253:GLU:HB3	1:A:255:ASP:OD2	2.18	0.44
1:D:57:GLY:C	4:D:502:SO4:O4	2.60	0.44
2:E:18:LEU:HA	2:F:17:SER:O	2.17	0.44
1:B:64:LEU:C	1:B:64:LEU:HD23	2.43	0.44
1:A:118[B]:ARG:NE	5:A:601:HOH:O	2.50	0.44
1:B:293:LEU:O	1:B:298:ARG:NH1	2.51	0.44
1:A:17:ARG:O	1:A:20:LEU:HB3	2.18	0.44
1:B:409:LEU:H	1:B:409:LEU:CD1	2.30	0.44
1:C:18:SER:O	1:C:22:LYS:N	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLN:HE21	1:C:60:LEU:HD23	1.82	0.44
2:G:36:TRP:CD1	2:G:69:ILE:HD13	2.51	0.44
1:A:87:VAL:HG23	1:A:97:VAL:HG22	2.00	0.43
1:C:17:ARG:O	1:C:20:LEU:HB3	2.17	0.43
1:B:402:LEU:O	1:B:405:PHE:HB3	2.18	0.43
1:A:151:LEU:HD21	1:A:183:LEU:HD13	2.01	0.43
1:C:433:HIS:HA	1:C:440:VAL:HG21	2.01	0.43
1:D:17:ARG:O	1:D:20:LEU:HB3	2.19	0.43
1:B:17:ARG:O	1:B:20:LEU:HB3	2.19	0.43
2:K:10:GLY:HA2	2:G:131:PHE:CE1	2.52	0.43
1:C:64:LEU:C	1:C:64:LEU:HD23	2.43	0.43
1:B:433:HIS:HA	1:B:440:VAL:HG21	2.01	0.43
1:A:305:TRP:CZ3	1:A:319:PHE:HZ	2.37	0.43
2:G:69:ILE:HD11	2:G:78:VAL:HG21	2.01	0.43
1:A:37:ALA:O	1:A:41:VAL:HG23	2.18	0.42
2:G:129:LEU:HD12	2:G:129:LEU:HA	1.90	0.42
2:G:69:ILE:HD12	2:G:79:TYR:O	2.19	0.42
1:A:142:LEU:HD23	1:A:179:LEU:HD11	1.97	0.42
1:D:321:MET:HB3	1:D:349:ARG:NE	2.34	0.42
1:A:327:ASN:HA	1:A:353:ASP:OD2	2.20	0.42
1:B:321:MET:HB3	1:B:349:ARG:NE	2.34	0.42
1:D:56:ALA:HA	1:D:58:LYS:HE3	2.01	0.42
1:A:100:LEU:HG	1:A:132:MET:HE2	2.02	0.42
1:D:402:LEU:O	1:D:405:PHE:HB3	2.20	0.42
1:A:340:MET:HE1	1:A:405:PHE:HB2	2.01	0.42
2:G:6:GLU:OE1	2:G:116:GLY:HA3	2.20	0.42
2:K:120:GLN:HB3	2:G:131:PHE:HD2	1.85	0.41
2:E:104:ALA:O	2:E:106:THR:O	2.38	0.41
1:A:59:SER:HA	1:A:62:TYR:CE2	2.56	0.41
1:C:96:ARG:HD2	1:C:122:GLN:HG3	2.02	0.41
2:E:24:ALA:HB3	2:E:76:ASN:HB3	2.02	0.41
1:C:321:MET:HB3	1:C:349:ARG:NE	2.35	0.41
1:C:402:LEU:O	1:C:405:PHE:HB3	2.21	0.41
2:K:129:LEU:HB3	2:K:131:PHE:CZ	2.56	0.41
1:A:69:ALA:O	1:A:70:LYS:HB2	2.21	0.40
1:B:321:MET:HB3	1:B:349:ARG:HE	1.87	0.40
1:C:321:MET:HB3	1:C:349:ARG:HE	1.86	0.40
1:D:151:LEU:HD21	1:D:183:LEU:HD13	2.03	0.40
1:B:51:CYS:HA	1:B:192:THR:O	2.21	0.40
1:B:327:ASN:HA	1:B:353:ASP:OD2	2.21	0.40
1:D:327:ASN:HA	1:D:353:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:O	1:A:22:LYS:N	2.41	0.40
1:A:404:THR:O	1:A:408:GLU:HG2	2.20	0.40
1:C:51:CYS:HA	1:C:192:THR:O	2.21	0.40
1:C:382:LEU:O	1:C:386:ARG:HG2	2.22	0.40
1:D:51:CYS:HA	1:D:192:THR:O	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%)	431 (97%)	12 (3%)	0	100	100
1	B	443/445 (100%)	432 (98%)	11 (2%)	0	100	100
1	C	444/445 (100%)	432 (97%)	12 (3%)	0	100	100
1	D	441/445 (99%)	428 (97%)	13 (3%)	0	100	100
2	E	126/132 (96%)	124 (98%)	2 (2%)	0	100	100
2	F	128/132 (97%)	126 (98%)	2 (2%)	0	100	100
2	G	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
2	K	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
All	All	2283/2308 (99%)	2223 (97%)	60 (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	369/373 (99%)	362 (98%)	7 (2%)	50	81
1	B	365/373 (98%)	355 (97%)	10 (3%)	39	74
1	C	368/373 (99%)	365 (99%)	3 (1%)	73	90
1	D	368/373 (99%)	359 (98%)	9 (2%)	43	77
2	E	98/103 (95%)	93 (95%)	5 (5%)	21	54
2	F	100/103 (97%)	96 (96%)	4 (4%)	28	63
2	G	101/103 (98%)	97 (96%)	4 (4%)	28	63
2	K	101/103 (98%)	95 (94%)	6 (6%)	18	48
All	All	1870/1904 (98%)	1822 (97%)	48 (3%)	40	75

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	98	SER
1	A	236	SER
1	A	248	LYS
1	A	253	GLU
1	A	323	VAL
1	A	409	LEU
1	B	60	LEU
1	B	98	SER
1	B	180	ARG
1	B	236	SER
1	B	248	LYS
1	B	253	GLU
1	B	374	LEU
1	B	409	LEU
1	B	438	THR
1	B	444	LEU
1	C	98	SER
1	C	409	LEU
1	C	438	THR
1	D	79	LEU
1	D	98	SER
1	D	236	SER
1	D	248	LYS

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Mol	Chain	Res	Type
1	D	281	CYS
1	D	374	LEU
1	D	409	LEU
1	D	438	THR
1	D	444	LEU
2	K	7	SER
2	K	56	SER
2	K	102	THR
2	K	106	THR
2	K	122	THR
2	K	129	LEU
2	E	56	SER
2	E	102	THR
2	E	106	THR
2	E	120	GLN
2	E	122	THR
2	F	12	VAL
2	F	56	SER
2	F	120	GLN
2	F	129	LEU
2	G	56	SER
2	G	64	LYS
2	G	106	THR
2	G	120	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	285	ASN
1	A	413	HIS
1	B	86	GLN
1	B	101	ASN
1	B	208	HIS
1	B	285	ASN
1	C	86	GLN
1	C	101	ASN
1	C	208	HIS
1	D	86	GLN
1	D	101	ASN
1	D	208	HIS
1	D	285	ASN

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Mol	Chain	Res	Type
1	D	413	HIS
2	K	3	GLN
2	E	81	GLN
2	E	83	ASN
2	F	3	GLN
2	G	3	GLN
2	G	39	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	C	502	-	4,4,4	0.27	0	6,6,6	0.22	0
4	SO4	D	502	-	4,4,4	0.26	0	6,6,6	0.21	0
4	SO4	A	502	-	4,4,4	0.31	0	6,6,6	0.22	0
4	SO4	B	502	-	4,4,4	0.43	0	6,6,6	0.08	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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	SO4	1	0
4	D	502	SO4	1	0
4	A	502	SO4	2	0
4	B	502	SO4	1	0

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	441/445 (99%)	0.12	11 (2%) 58 48	54, 92, 143, 230	4 (0%)
1	B	441/445 (99%)	0.29	12 (2%) 56 46	65, 109, 177, 212	3 (0%)
1	C	441/445 (99%)	0.11	4 (0%) 81 74	45, 112, 180, 206	3 (0%)
1	D	440/445 (98%)	0.51	22 (5%) 34 26	47, 136, 211, 259	5 (1%)
2	E	128/132 (96%)	-0.01	2 (1%) 70 61	57, 83, 133, 210	0
2	F	130/132 (98%)	0.18	6 (4%) 37 29	55, 82, 131, 243	0
2	G	131/132 (99%)	-0.16	1 (0%) 82 75	55, 78, 157, 169	0
2	K	131/132 (99%)	-0.17	0 100 100	58, 74, 105, 134	0
All	All	2283/2308 (98%)	0.19	58 (2%) 58 48	45, 102, 183, 259	15 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	LEU	5.1
1	B	377	LYS	4.2
1	D	301	VAL	3.9
1	A	12	PRO	3.8
2	F	129	LEU	3.3
1	D	188	CYS	3.2
1	A	123	THR	3.2
1	D	249	ALA	3.2
1	D	305	TRP	3.1
1	D	285	ASN	3.1
1	B	12	PRO	3.1
1	B	138	PHE	3.1
1	B	372	SER	3.1
1	D	154	LEU	3.0
1	A	122	GLN	2.9
2	F	102	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	375	ILE	2.9
1	D	254	ALA	2.8
1	D	284	VAL	2.8
1	B	373	PHE	2.7
1	C	12	PRO	2.7
1	A	452	SER	2.6
1	A	179	LEU	2.6
2	F	47	LEU	2.5
2	F	10	GLY	2.5
1	A	70	LYS	2.5
1	A	96	ARG	2.5
1	B	382	LEU	2.5
1	A	100	LEU	2.5
1	D	125	ILE	2.5
2	E	128	ASN	2.4
1	B	266	CYS	2.4
1	D	312	VAL	2.4
1	C	74	ILE	2.4
1	A	150	LEU	2.4
2	G	129	LEU	2.4
1	D	16	VAL	2.4
1	D	318	SER	2.3
2	E	26	GLY	2.3
1	A	319	PHE	2.3
1	B	183	LEU	2.3
1	D	304	ASP	2.3
1	D	33	LEU	2.3
1	D	425	PRO	2.3
2	F	17	SER	2.3
1	B	116	LEU	2.2
1	D	82	LEU	2.2
1	B	67	LEU	2.2
1	D	167[A]	HIS	2.2
1	C	263	ILE	2.1
1	D	414	ALA	2.1
1	D	194	THR	2.1
1	D	265	TYR	2.1
1	C	262	GLY	2.1
1	D	144	SER	2.0
1	D	310	VAL	2.0
2	F	59	TYR	2.0
1	B	379	VAL	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($\text{\AA}^2$)	Q<0.9
4	SO4	D	502	5/5	0.79	0.09	130,160,175,187	0
4	SO4	C	502	5/5	0.88	0.07	101,123,142,150	0
4	SO4	B	502	5/5	0.94	0.05	93,103,115,124	0
4	SO4	A	502	5/5	0.95	0.05	73,76,115,120	0
3	ZN	A	501	1/1	0.99	0.03	101,101,101,101	0
3	ZN	D	501	1/1	0.99	0.03	146,146,146,146	0
3	ZN	C	501	1/1	1.00	0.01	102,102,102,102	0
3	ZN	B	501	1/1	1.00	0.05	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.