



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:01 PM UTC

PDB ID : 7ZMO / pdb_00007zmo
Title : Crystal structure of human RECQL5 helicase APO form in complex with engineered nanobody (Gluebody) G3-052
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 : 3.75 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

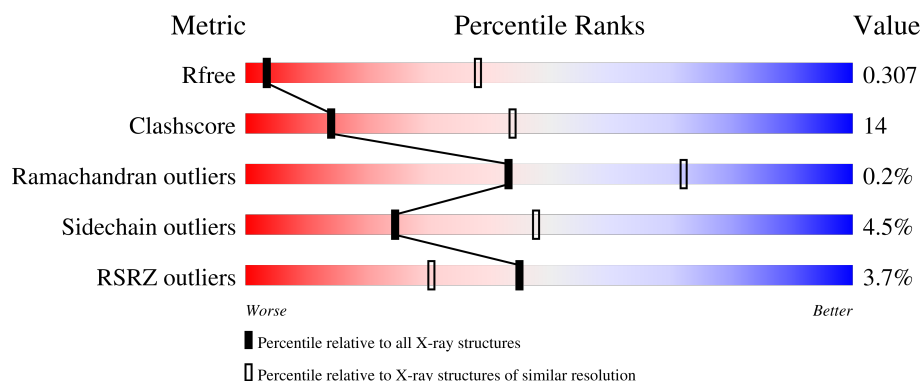
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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	 5% 69% 28% ..
1	B	445	 3% 69% 28% ..
2	C	127	 5% 54% 40% . .
2	K	127	 57% 35% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8605 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	3	0
			3358	2115	594	626	23			
1	B	441	Total	C	N	O	S	0	4	0
			3337	2099	589	626	23			

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 G3-052.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	124	Total	C	N	O	S	0	2	0
			950	592	162	191	5			
2	C	124	Total	C	N	O	S	0	2	0
			944	589	161	189	5			

- 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	B	1	Total	O	S	0	0
			5	4	1		

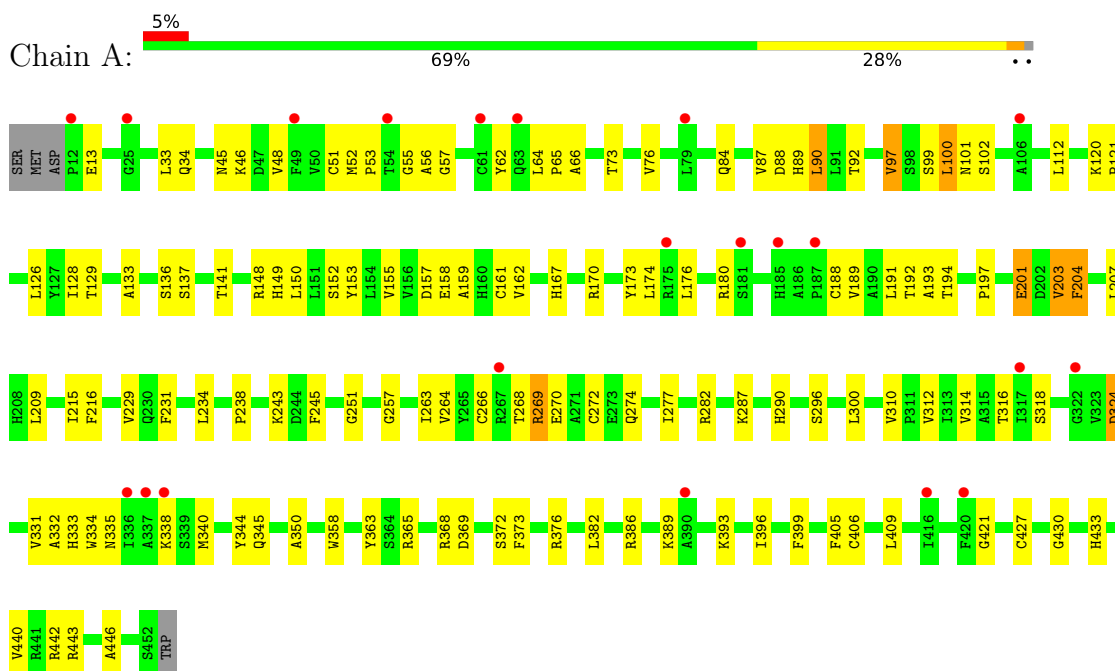
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	K	1	Total	O	0	0
			1	1		

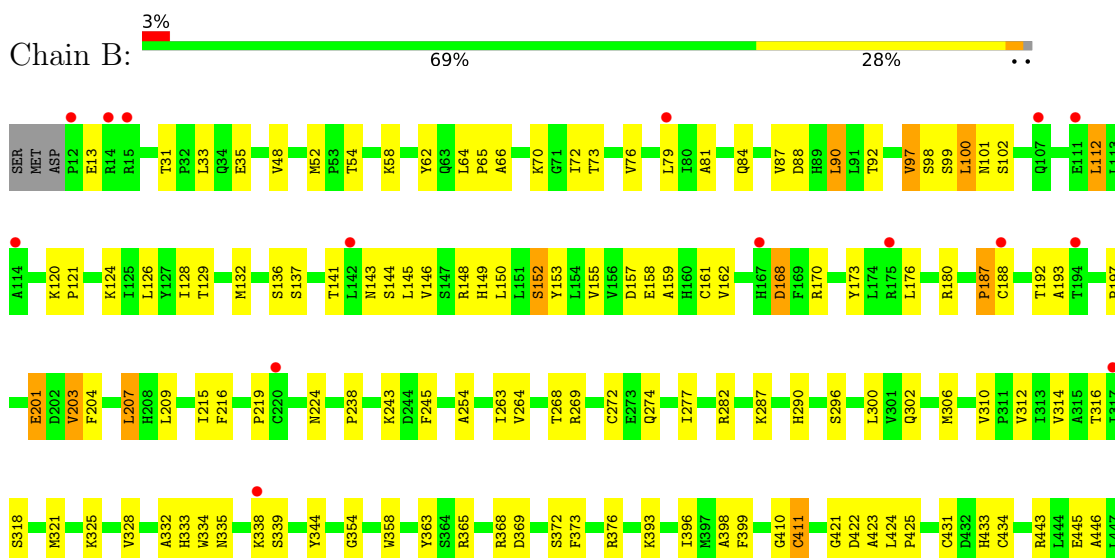
3 Residue-property plots [i](#)

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

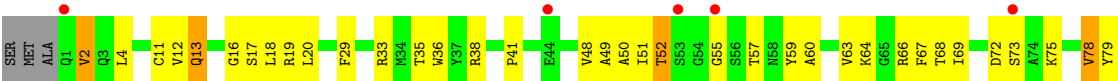




● Molecule 2: Gluebody G3-052



● Molecule 2: Gluebody G3-052



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	89.52Å 150.87Å 269.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.67 – 3.75 100.67 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (100.67-3.75) 99.9 (100.67-3.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.78Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.283 , 0.306 0.285 , 0.307	Depositor DCC
R_{free} test set	1891 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 125.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8605	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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	1.15	1/3440 (0.0%)	1.65	15/4661 (0.3%)
1	B	1.15	0/3423	1.67	17/4646 (0.4%)
2	C	1.18	0/974	1.57	8/1321 (0.6%)
2	K	1.17	0/980	1.64	12/1329 (0.9%)
All	All	1.15	1/8817 (0.0%)	1.65	52/11957 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	HIS	CE1-NE2	8.93	1.41	1.32

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	43	LYS	CA-C-N	7.00	131.05	121.05
2	K	43	LYS	C-N-CA	7.00	131.05	121.05
1	B	168	ASP	CA-CB-CG	6.70	119.30	112.60
2	K	13	GLN	CA-C-N	6.53	130.38	121.05
2	K	13	GLN	C-N-CA	6.53	130.38	121.05
1	A	141	THR	N-CA-CB	6.46	119.37	110.01
1	A	269	ARG	CA-C-N	6.33	129.08	120.54
1	A	269	ARG	C-N-CA	6.33	129.08	120.54
2	C	13	GLN	CA-C-N	6.24	129.98	121.05
2	C	13	GLN	C-N-CA	6.24	129.98	121.05
1	A	112	LEU	CA-C-O	-6.17	114.34	120.70
1	A	344	TYR	N-CA-CB	6.06	118.76	109.91
2	K	41	PRO	CB-CA-C	6.03	119.24	111.46
2	K	44	GLU	CA-C-O	-6.03	114.39	120.96
2	K	10	GLY	CA-C-O	-5.93	116.82	120.91
1	A	55	GLY	CA-C-O	-5.85	116.26	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	73	SER	CA-C-N	5.78	128.28	120.65
2	C	73	SER	C-N-CA	5.78	128.28	120.65
2	K	93	TYR	CB-CA-C	5.78	119.67	110.19
1	B	187	PRO	CA-C-O	-5.75	114.42	121.31
1	B	344	TYR	N-CA-CB	5.75	118.55	109.82
1	A	102	SER	CA-C-N	5.74	128.25	120.38
1	A	102	SER	C-N-CA	5.74	128.25	120.38
2	C	118	GLY	CA-C-O	-5.74	118.49	122.22
1	A	365	ARG	CA-C-N	5.73	128.28	120.54
1	A	365	ARG	C-N-CA	5.73	128.28	120.54
1	B	112	LEU	CA-C-O	-5.69	114.84	120.70
1	B	201	GLU	CB-CG-CD	5.68	122.26	112.60
2	C	93	TYR	CB-CA-C	5.54	119.28	110.19
2	K	73	SER	CA-C-N	5.52	127.93	120.65
2	K	73	SER	C-N-CA	5.52	127.93	120.65
2	C	41	PRO	CB-CA-C	5.48	118.52	111.56
1	B	54	THR	CB-CA-C	5.46	121.28	110.42
1	A	324	ASP	CB-CA-C	5.36	118.59	109.75
1	A	201	GLU	CB-CG-CD	5.34	121.68	112.60
1	B	102	SER	CA-C-N	5.34	127.75	120.54
1	B	102	SER	C-N-CA	5.34	127.75	120.54
1	B	365	ARG	CA-C-N	5.33	127.74	120.54
1	B	365	ARG	C-N-CA	5.33	127.74	120.54
1	B	410	GLY	CA-C-O	-5.27	116.02	120.98
1	B	268	THR	CA-C-N	5.20	127.25	120.28
1	B	268	THR	C-N-CA	5.20	127.25	120.28
1	B	254	ALA	CA-C-N	5.20	127.20	120.44
1	B	254	ALA	C-N-CA	5.20	127.20	120.44
2	K	44	GLU	CB-CA-C	-5.18	102.06	109.84
1	A	204	PHE	CB-CA-C	5.11	118.99	110.81
2	C	66	ARG	N-CA-C	-5.10	107.22	113.50
1	B	136	SER	CA-C-N	5.10	127.36	120.38
1	B	136	SER	C-N-CA	5.10	127.36	120.38
2	K	13	GLN	CA-C-O	-5.07	115.74	121.72
1	A	136	SER	CA-C-N	5.01	127.25	120.38
1	A	136	SER	C-N-CA	5.01	127.25	120.38

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	3358	0	3294	77	0
1	B	3337	0	3203	88	0
2	C	944	0	891	41	0
2	K	950	0	902	40	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
5	A	3	0	0	0	0
5	K	1	0	0	2	0
All	All	8605	0	8290	241	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 14.

All (241) 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:204:PHE:HD1	1:B:209:LEU:HD12	1.18	1.06
1:B:431:CYS:N	1:B:434:CYS:SG	2.32	1.02
1:B:204:PHE:CD1	1:B:209:LEU:HD12	2.05	0.91
1:B:197:PRO:O	1:B:201:GLU:HG2	1.74	0.87
2:K:67:PHE:O	2:K:68:THR:HG23	1.75	0.87
1:A:197:PRO:O	1:A:201:GLU:HG2	1.74	0.86
2:C:67:PHE:O	2:C:68:THR:HG23	1.76	0.85
1:B:274:GLN:O	1:B:277:ILE:HG13	1.79	0.81
1:B:173:TYR:HA	1:B:176:LEU:HD12	1.65	0.79
2:K:104:ALA:HB1	2:K:105:PRO:HD2	1.68	0.75
1:A:173:TYR:HA	1:A:176:LEU:HD12	1.70	0.72
1:A:266:CYS:O	1:A:316:THR:HA	1.90	0.71
1:B:443:ARG:O	1:B:446:ALA:HB3	1.92	0.69
1:A:274:GLN:O	1:A:277:ILE:HG12	1.93	0.69
1:B:203:VAL:O	1:B:207:LEU:HB2	1.94	0.67
1:B:431:CYS:O	1:B:434:CYS:SG	2.52	0.67
2:C:35:THR:O	2:C:95:CYS:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASP:O	1:A:92:THR:HG23	1.96	0.66
1:B:98:SER:HB3	1:B:112:LEU:HD21	1.77	0.66
2:K:90:THR:HG23	2:K:122:THR:HA	1.78	0.66
1:A:203:VAL:O	1:A:207:LEU:HB2	1.96	0.65
2:C:67:PHE:O	2:C:68:THR:CG2	2.44	0.65
1:B:204:PHE:HD1	1:B:209:LEU:CD1	2.02	0.64
1:A:433:HIS:HA	1:A:440:VAL:HG21	1.79	0.64
1:B:58:LYS:HB2	4:B:502:SO4:O1	1.98	0.64
1:B:180:ARG:HD3	1:B:188:CYS:HB2	1.80	0.64
1:A:382:LEU:HD22	1:A:386:ARG:HH11	1.63	0.63
2:K:67:PHE:O	2:K:68:THR:CG2	2.45	0.63
2:C:90:THR:HG23	2:C:122:THR:HA	1.79	0.63
1:A:443:ARG:O	1:A:446:ALA:HB3	1.99	0.63
1:B:100:LEU:HD23	1:B:132:MET:SD	2.40	0.62
1:B:98:SER:CB	1:B:112:LEU:HD21	2.28	0.61
2:K:93:TYR:O	2:K:118:GLY:HA2	2.00	0.61
1:A:66:ALA:HB2	1:A:73:THR:HG21	1.82	0.61
1:B:66:ALA:HB2	1:B:73:THR:HG21	1.82	0.61
1:B:88:ASP:O	1:B:92:THR:HG23	2.00	0.60
1:A:157:ASP:O	1:A:173:TYR:OH	2.20	0.60
2:C:19:ARG:HD3	2:C:81:TYR:CE1	2.36	0.59
1:B:272:CYS:SG	1:B:314:VAL:HG12	2.43	0.59
1:A:158:GLU:O	1:A:161:CYS:SG	2.60	0.59
1:B:79:LEU:HG	1:B:81:ALA:HB3	1.85	0.59
1:A:331:VAL:HG23	1:A:350:ALA:HB2	1.83	0.58
1:B:423:ALA:HB2	2:C:104:ALA:C	2.28	0.58
1:B:321:MET:O	1:B:321:MET:HG3	2.02	0.58
2:K:2:VAL:HB	2:K:114:TYR:CE1	2.39	0.58
2:K:35:THR:O	2:K:95:CYS:HA	2.04	0.58
2:C:2:VAL:HB	2:C:114:TYR:CE1	2.39	0.57
2:K:67:PHE:C	2:K:68:THR:HG23	2.29	0.57
1:A:170:ARG:O	1:A:173:TYR:HB2	2.05	0.56
1:B:62:TYR:HB2	1:B:155:VAL:HG21	1.87	0.56
1:B:159:ALA:O	1:B:162:VAL:HG12	2.04	0.56
2:C:104:ALA:HB1	2:C:105:PRO:HD2	1.88	0.56
2:K:19:ARG:HD3	2:K:81:TYR:CE1	2.40	0.56
1:A:62:TYR:HB2	1:A:155:VAL:HG21	1.88	0.56
1:A:159:ALA:O	1:A:162:VAL:HG12	2.04	0.56
1:A:272:CYS:SG	1:A:314:VAL:HG12	2.46	0.56
1:B:170:ARG:O	1:B:173:TYR:HB2	2.06	0.56
2:C:49:ALA:HB2	2:C:59:TYR:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:ILE:HG23	2:C:51:ILE:O	2.06	0.55
2:C:67:PHE:C	2:C:68:THR:HG23	2.31	0.55
1:A:296:SER:O	1:A:300:LEU:HG	2.07	0.55
1:B:302:GLN:O	1:B:306:MET:HG2	2.06	0.55
1:B:287:LYS:HG2	1:B:310:VAL:HG11	1.89	0.55
1:B:243:LYS:HD3	1:B:282:ARG:HB3	1.89	0.54
2:K:33:ARG:HE	2:K:52:THR:HG22	1.72	0.54
1:B:148:ARG:HB3	1:B:150:LEU:HG	1.89	0.54
2:K:67:PHE:CE2	2:K:82:MET:HE3	2.42	0.54
2:C:29:PHE:HB3	2:C:101:TYR:HD2	1.73	0.54
1:A:148:ARG:O	1:A:149:HIS:C	2.50	0.54
2:K:51:ILE:O	2:K:51:ILE:HG23	2.08	0.54
2:K:11:CYS:SG	2:K:122:THR:OG1	2.66	0.53
1:A:287:LYS:HG2	1:A:310:VAL:HG11	1.91	0.53
1:B:52:MET:O	1:B:193:ALA:HA	2.08	0.53
1:A:148:ARG:HB3	1:A:150:LEU:HG	1.90	0.53
1:B:148:ARG:O	1:B:149:HIS:C	2.52	0.53
1:B:99:SER:OG	1:B:101:ASN:ND2	2.40	0.52
1:B:296:SER:O	1:B:300:LEU:HG	2.08	0.52
2:C:36:TRP:O	2:C:48:VAL:HB	2.09	0.52
1:B:100:LEU:HB2	1:B:126:LEU:HD11	1.91	0.52
2:C:67:PHE:CE2	2:C:82:MET:HE3	2.45	0.52
1:B:269:ARG:HD3	1:B:290:HIS:ND1	2.24	0.52
1:B:431:CYS:CA	1:B:434:CYS:SG	2.99	0.51
1:B:238:PRO:HB2	1:B:334:TRP:CH2	2.46	0.51
2:C:72:ASP:HB3	2:C:75:LYS:HB2	1.92	0.51
1:A:13:GLU:O	1:A:13:GLU:HG2	2.10	0.50
1:B:180:ARG:HD3	1:B:188:CYS:CB	2.41	0.50
2:K:72:ASP:HB3	2:K:75:LYS:HB2	1.93	0.50
1:B:70:LYS:HA	1:B:124:LYS:HZ1	1.77	0.50
1:A:45:ASN:OD1	1:A:45:ASN:N	2.44	0.50
1:A:238:PRO:HB2	1:A:334:TRP:CH2	2.46	0.50
1:A:90:LEU:HB3	1:A:97:VAL:HG11	1.94	0.49
2:C:112:ASP:HB3	2:C:114:TYR:CE2	2.46	0.49
1:A:243:LYS:HD3	1:A:282:ARG:HB3	1.93	0.49
2:K:20:LEU:CD1	2:K:82:MET:SD	3.00	0.49
1:A:84:GLN:HA	1:A:87:VAL:HG12	1.94	0.49
1:B:224:ASN:HD22	1:B:354:GLY:HA2	1.77	0.49
1:B:264:VAL:HA	1:B:332:ALA:O	2.13	0.49
2:C:20:LEU:CD1	2:C:82:MET:SD	3.01	0.49
1:A:51:CYS:HA	1:A:192:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:CYS:SG	1:B:434:CYS:SG	3.11	0.48
2:K:78:VAL:HG23	2:K:79:TYR:N	2.27	0.48
1:A:204:PHE:HD1	1:A:209:LEU:HD22	1.79	0.48
1:B:173:TYR:O	1:B:176:LEU:HB2	2.13	0.48
2:K:112:ASP:HB3	2:K:114:TYR:CE2	2.49	0.48
1:B:204:PHE:CD1	1:B:209:LEU:CD1	2.85	0.48
1:B:423:ALA:HB2	2:C:104:ALA:O	2.14	0.48
1:A:33:LEU:HG	1:A:52:MET:HE2	1.96	0.48
1:A:128:ILE:HG12	1:A:129:THR:O	2.13	0.48
1:B:411:CYS:HA	1:B:433:HIS:HB3	1.96	0.48
2:C:55:GLY:O	2:C:57:THR:HG23	2.13	0.48
2:C:64:LYS:O	2:C:64:LYS:HG3	2.12	0.48
1:B:90:LEU:HB3	1:B:97:VAL:HG11	1.96	0.47
1:A:173:TYR:O	1:A:176:LEU:HB2	2.14	0.47
2:K:11:CYS:O	2:K:12:VAL:HG23	2.14	0.47
2:K:12:VAL:HG12	2:K:13:GLN:N	2.29	0.47
1:A:238:PRO:HB2	1:A:334:TRP:HH2	1.79	0.47
1:A:245:PHE:CZ	1:A:358:TRP:HB3	2.49	0.47
1:A:251:GLY:HA2	1:A:257:GLY:O	2.14	0.47
2:C:78:VAL:HG23	2:C:79:TYR:N	2.28	0.47
1:A:269:ARG:HH11	1:A:290:HIS:HB2	1.79	0.47
1:B:152:SER:O	1:B:187:PRO:HD2	2.14	0.47
1:A:99:SER:OG	1:A:101:ASN:ND2	2.44	0.47
1:A:229:VAL:HG11	1:A:406:CYS:HB3	1.96	0.47
1:B:100:LEU:HD23	1:B:132:MET:CE	2.45	0.47
1:A:197:PRO:HG3	1:A:421:GLY:HA3	1.95	0.47
1:B:238:PRO:HB2	1:B:334:TRP:HH2	1.80	0.46
1:A:427:CYS:SG	1:A:430:GLY:N	2.88	0.46
2:C:35:THR:HG23	2:C:50:ALA:HB2	1.97	0.46
1:A:34:GLN:NE2	1:A:57:GLY:HA2	2.30	0.46
2:K:33:ARG:HD2	2:K:50:ALA:HB1	1.98	0.46
1:A:393:LYS:HA	1:A:396:ILE:HD12	1.97	0.46
2:K:60:ALA:HB3	2:K:63:VAL:HG22	1.98	0.46
1:B:84:GLN:HA	1:B:87:VAL:HG12	1.98	0.46
1:B:128:ILE:HG12	1:B:129:THR:O	2.16	0.46
1:B:197:PRO:HG3	1:B:421:GLY:HA3	1.98	0.46
1:A:338:LYS:O	1:A:399:PHE:HB2	2.16	0.46
1:B:70:LYS:CA	1:B:124:LYS:HZ1	2.29	0.46
1:B:373:PHE:HA	1:B:376:ARG:HB2	1.98	0.46
2:K:16:GLY:C	2:K:17:SER:HG	2.24	0.46
1:A:180:ARG:HD3	1:A:188:CYS:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:TYR:OH	1:A:368:ARG:HD3	2.15	0.45
1:B:64:LEU:N	1:B:65:PRO:CD	2.79	0.45
2:C:4:LEU:HD21	2:C:95:CYS:HB2	1.98	0.45
1:A:73:THR:HG23	1:A:153:TYR:HB2	1.97	0.45
1:B:393:LYS:HA	1:B:396:ILE:HD12	1.97	0.45
1:A:52:MET:O	1:A:193:ALA:HA	2.17	0.45
1:A:369:ASP:HA	1:A:372:SER:HB3	1.97	0.45
1:A:51:CYS:SG	1:A:194:THR:HA	2.57	0.45
1:B:269:ARG:O	1:B:272:CYS:HB3	2.17	0.45
2:C:20:LEU:O	2:C:79:TYR:HA	2.17	0.45
2:C:20:LEU:HD12	2:C:82:MET:SD	2.56	0.45
1:A:316:THR:HG23	1:A:318:SER:OG	2.17	0.45
2:K:36:TRP:O	2:K:48:VAL:HB	2.16	0.45
1:B:339:SER:HB2	1:B:398:ALA:HB1	1.98	0.45
2:K:104:ALA:HB1	2:K:105:PRO:CD	2.44	0.45
2:C:16:GLY:C	2:C:17:SER:HG	2.25	0.45
1:A:245:PHE:HZ	1:A:358:TRP:HB3	1.82	0.45
2:K:20:LEU:HD12	2:K:82:MET:SD	2.57	0.45
2:K:86:LYS:HB3	2:K:88:GLU:OE1	2.16	0.45
1:A:87:VAL:HG23	1:A:97:VAL:HG22	1.99	0.44
1:B:363:TYR:OH	1:B:368:ARG:HD3	2.18	0.44
1:B:153:TYR:CE1	1:B:187:PRO:HG2	2.52	0.44
1:B:203:VAL:HG12	1:B:204:PHE:N	2.31	0.44
1:B:33:LEU:HD11	1:B:216:PHE:HB3	1.98	0.44
1:B:76:VAL:HG22	1:B:128:ILE:HG23	1.98	0.44
1:A:120:LYS:N	1:A:121:PRO:HD3	2.33	0.44
1:B:98:SER:HB2	1:B:112:LEU:HD21	1.98	0.44
1:B:333:HIS:HB3	1:B:335:ASN:O	2.17	0.44
2:K:33:ARG:CZ	5:K:201:HOH:O	2.66	0.44
2:K:35:THR:HG23	2:K:50:ALA:HB2	1.99	0.44
1:A:333:HIS:HB3	1:A:335:ASN:O	2.17	0.44
1:B:73:THR:HG23	1:B:153:TYR:HB2	1.98	0.44
2:C:60:ALA:HB3	2:C:63:VAL:HG22	1.99	0.44
2:K:11:CYS:C	2:K:12:VAL:HG23	2.42	0.44
1:A:189:VAL:HG12	1:A:191:LEU:HD11	1.99	0.44
2:K:40:ALA:HB3	2:K:43:LYS:HB2	1.99	0.44
2:K:67:PHE:HA	2:K:81:TYR:O	2.17	0.44
1:A:64:LEU:N	1:A:65:PRO:CD	2.80	0.44
1:B:87:VAL:HG23	1:B:97:VAL:HG22	2.00	0.44
1:B:245:PHE:CZ	1:B:358:TRP:HB3	2.52	0.44
2:C:38:ARG:NH1	2:C:89:ASP:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:H	1:A:270:GLU:CD	2.25	0.44
1:A:310:VAL:HG12	1:A:312:VAL:O	2.17	0.44
1:B:310:VAL:HG12	1:B:312:VAL:O	2.18	0.44
1:B:338:LYS:O	1:B:399:PHE:HB2	2.17	0.43
2:C:12:VAL:HG12	2:C:13:GLN:N	2.33	0.43
1:A:264:VAL:HA	1:A:332:ALA:O	2.18	0.43
1:A:373:PHE:HA	1:A:376:ARG:HB2	2.00	0.43
1:A:33:LEU:HD11	1:A:216:PHE:HB3	2.01	0.43
2:C:18:LEU:HD12	2:C:85:LEU:CD1	2.48	0.43
2:C:33:ARG:NH2	2:C:52:THR:HG22	2.32	0.43
1:A:204:PHE:CD1	1:A:209:LEU:HD22	2.53	0.43
1:A:263:ILE:HG22	1:A:264:VAL:N	2.33	0.43
1:A:64:LEU:HB3	1:A:65:PRO:HD3	2.00	0.43
1:B:157:ASP:O	1:B:158:GLU:C	2.61	0.43
1:B:423:ALA:HB3	2:C:105:PRO:HA	2.01	0.43
1:B:245:PHE:HZ	1:B:358:TRP:HB3	1.84	0.43
1:A:89:HIS:O	1:A:92:THR:OG1	2.32	0.43
1:A:100:LEU:HB2	1:A:126:LEU:HD11	2.00	0.43
2:K:20:LEU:O	2:K:79:TYR:HA	2.19	0.43
1:A:76:VAL:HG22	1:A:128:ILE:HG23	2.01	0.43
1:A:340:MET:HE1	1:A:405:PHE:HB2	2.01	0.43
1:A:203:VAL:HG12	1:A:204:PHE:N	2.34	0.42
1:A:269:ARG:O	1:A:272:CYS:HB3	2.19	0.42
1:B:70:LYS:HA	1:B:124:LYS:NZ	2.34	0.42
1:A:268:THR:HB	1:A:270:GLU:OE1	2.19	0.42
1:B:219:PRO:HA	1:B:422:ASP:CG	2.44	0.42
1:B:316:THR:C	1:B:318:SER:H	2.26	0.42
2:C:50:ALA:C	2:C:69:ILE:HD11	2.45	0.42
1:B:263:ILE:HG22	1:B:264:VAL:N	2.34	0.42
2:K:18:LEU:HA	2:C:17:SER:O	2.19	0.42
2:C:11:CYS:C	2:C:12:VAL:HG23	2.45	0.42
2:C:97:ALA:O	2:C:100:THR:OG1	2.35	0.42
2:K:19:ARG:HB3	2:C:17:SER:HB2	2.02	0.42
1:B:124:LYS:HD2	1:B:124:LYS:HA	1.91	0.42
1:B:161:CYS:O	1:B:170:ARG:N	2.48	0.42
2:K:50:ALA:C	2:K:69:ILE:HD11	2.45	0.42
1:B:316:THR:HG23	1:B:318:SER:H	1.85	0.41
1:A:56:ALA:HA	4:A:502:SO4:O3	2.20	0.41
1:B:143:ASN:O	1:B:146:VAL:HB	2.21	0.41
2:C:33:ARG:HH21	2:C:52:THR:CG2	2.32	0.41
1:A:197:PRO:HG3	1:A:421:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLN:O	1:A:277:ILE:CG1	2.65	0.41
1:B:369:ASP:HA	1:B:372:SER:HB3	2.02	0.41
1:A:316:THR:CG2	1:A:318:SER:OG	2.69	0.41
1:B:13:GLU:OE2	1:B:35:GLU:OE1	2.39	0.41
2:K:67:PHE:HB3	2:K:80:LEU:HD11	2.03	0.41
1:B:120:LYS:N	1:B:121:PRO:HD3	2.35	0.41
1:B:325:LYS:O	1:B:328:VAL:HG23	2.21	0.41
2:K:59:TYR:CZ	2:K:68:THR:HA	2.56	0.41
2:K:100:THR:O	2:K:102:THR:HG23	2.21	0.41
2:C:103:LEU:HA	2:C:109:GLY:HA2	2.03	0.41
1:A:231:PHE:HB2	1:A:234:LEU:HD12	2.03	0.40
1:B:445:GLU:HA	1:B:448:GLU:CG	2.50	0.40
2:C:18:LEU:HD12	2:C:85:LEU:HD11	2.02	0.40
2:C:67:PHE:HA	2:C:81:TYR:O	2.20	0.40
1:A:128:ILE:HD11	1:A:133:ALA:N	2.36	0.40
1:B:144:SER:CB	1:B:148:ARG:HH21	2.34	0.40
1:B:424:LEU:HA	1:B:425:PRO:HD3	1.91	0.40
2:K:33:ARG:HG2	5:K:201:HOH:O	2.20	0.40
2:K:66:ARG:C	2:K:67:PHE:HD1	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	442/445 (99%)	419 (95%)	22 (5%)	1 (0%)	43	72
1	B	443/445 (100%)	413 (93%)	29 (6%)	1 (0%)	43	72
2	C	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
2	K	124/127 (98%)	116 (94%)	8 (6%)	0	100	100
All	All	1133/1144 (99%)	1066 (94%)	65 (6%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	ASP
1	A	53	PRO

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	352/373 (94%)	337 (96%)	15 (4%)	26	49
1	B	344/373 (92%)	329 (96%)	15 (4%)	25	48
2	C	97/99 (98%)	93 (96%)	4 (4%)	27	51
2	K	99/99 (100%)	93 (94%)	6 (6%)	17	42
All	All	892/944 (94%)	852 (96%)	40 (4%)	24	48

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	48	VAL
1	A	90	LEU
1	A	97	VAL
1	A	100	LEU
1	A	137	SER
1	A	152	SER
1	A	174	LEU
1	A	203	VAL
1	A	215	ILE
1	A	324	ASP
1	A	345	GLN
1	A	389	LYS
1	A	409	LEU
1	A	442	ARG
1	B	31	THR
1	B	48	VAL
1	B	72	ILE

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Mol	Chain	Res	Type
1	B	90	LEU
1	B	97	VAL
1	B	100	LEU
1	B	137	SER
1	B	141	THR
1	B	145	LEU
1	B	152	SER
1	B	192	THR
1	B	203	VAL
1	B	207	LEU
1	B	215	ILE
1	B	411	CYS
2	K	2	VAL
2	K	13	GLN
2	K	18	LEU
2	K	78	VAL
2	K	119	THR
2	K	121	VAL
2	C	2	VAL
2	C	52	THR
2	C	78	VAL
2	C	80	LEU

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	139	GLN
1	A	200	GLN
1	A	285	ASN
1	A	345	GLN
1	A	370	GLN
1	B	107	GLN
1	B	122	GLN
1	B	139	GLN
1	B	185	HIS
1	B	224	ASN
1	B	241	ASN
2	K	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	502	-	4,4,4	0.33	0	6,6,6	0.18	0
4	SO4	A	502	-	4,4,4	0.31	0	6,6,6	0.12	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	SO4	1	0
4	A	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%)	0.34	21 (4%) 35 26	75, 140, 215, 258	2 (0%)
1	B	441/445 (99%)	0.27	15 (3%) 48 32	68, 140, 212, 279	3 (0%)
2	C	124/127 (97%)	0.42	6 (4%) 35 26	72, 113, 172, 198	2 (1%)
2	K	124/127 (97%)	0.26	0 100 100	64, 109, 163, 186	2 (1%)
All	All	1130/1144 (98%)	0.31	42 (3%) 45 30	64, 134, 205, 279	9 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167[A]	HIS	6.9
1	B	12	PRO	5.9
1	A	338	LYS	5.3
1	A	61	CYS	4.2
1	A	12	PRO	3.9
1	B	338	LYS	3.7
1	A	337	ALA	3.7
1	A	317	ILE	3.6
1	B	317	ILE	3.6
1	A	79	LEU	3.5
1	B	188	CYS	3.3
1	A	390	ALA	3.2
1	A	322	GLY	3.1
1	B	175[A]	ARG	3.0
1	B	194	THR	3.0
1	A	175[A]	ARG	2.9
1	A	49	PHE	2.8
1	B	14	ARG	2.8
1	B	107	GLN	2.8
1	A	185	HIS	2.7
1	B	79	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	53	SER	2.7
1	A	267	ARG	2.7
1	A	416	ILE	2.6
1	A	420	PHE	2.6
2	C	120	GLN	2.5
1	B	142	LEU	2.5
1	A	187	PRO	2.4
1	A	54	THR	2.4
2	C	73	SER	2.4
2	C	44	GLU	2.4
2	C	1	GLN	2.3
1	A	106	ALA	2.3
1	A	336	ILE	2.2
1	A	63	GLN	2.2
1	B	114	ALA	2.2
1	B	15	ARG	2.2
1	A	25	GLY	2.1
1	B	111	GLU	2.1
1	B	220	CYS	2.1
2	C	55	GLY	2.1
1	A	181	SER	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	B	502	5/5	0.89	0.09	141,150,157,163	0
4	SO4	A	502	5/5	0.93	0.09	154,172,174,195	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	501	1/1	0.98	0.04	141,141,141,141	0
3	ZN	B	501	1/1	0.98	0.03	98,98,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.