



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:32 PM UTC

PDB ID : 7ZMM / pdb_00007zmm
Title : Crystal structure of human RECQL5 helicase APO form in complex with engineered nanobody (Gluebody) G2-001
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 : 2.50 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
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

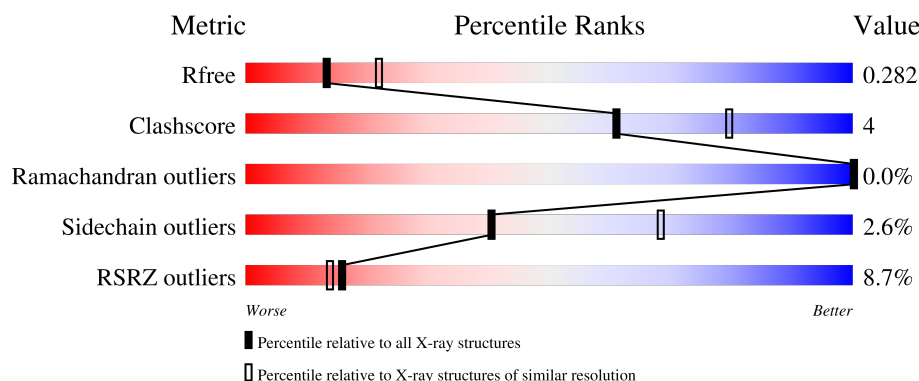
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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% 85% 11% 5%
2	G	132	5% 83% 13%
2	K	132	3% 87% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17749 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	B	441	Total	C	N	O	S	0	5	0
			3455	2181	623	628	23			
1	A	440	Total	C	N	O	S	0	5	0
			3448	2178	620	627	23			
1	C	441	Total	C	N	O	S	0	5	0
			3437	2170	616	628	23			
1	D	441	Total	C	N	O	S	0	4	0
			3424	2163	610	628	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	SER	-	expression tag	UNP O94762
B	10	MET	-	expression tag	UNP O94762
A	9	SER	-	expression tag	UNP O94762
A	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 G2-001.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	131	Total	C	N	O	S	0	0	0
			996	621	170	200	5			
2	E	130	Total	C	N	O	S	0	0	0
			985	612	169	199	5			
2	F	126	Total	C	N	O	S	0	0	0
			948	588	164	191	5			
2	G	127	Total	C	N	O	S	0	0	0
			957	593	165	194	5			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

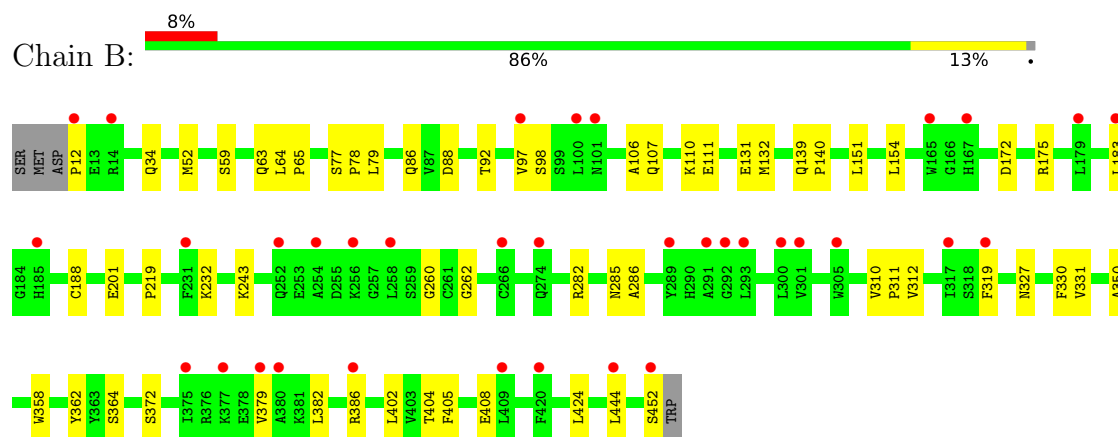
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	24	Total 24	O 24	0	0
4	A	21	Total 21	O 21	0	0
4	C	14	Total 14	O 14	0	0
4	D	2	Total 2	O 2	0	0
4	K	11	Total 11	O 11	0	0
4	E	12	Total 12	O 12	0	0
4	F	6	Total 6	O 6	0	0
4	G	5	Total 5	O 5	0	0

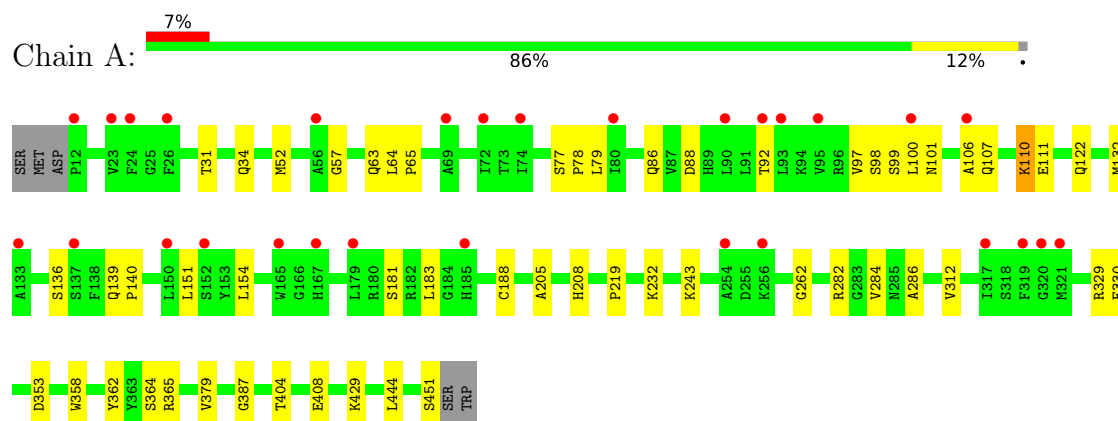
3 Residue-property plots

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.

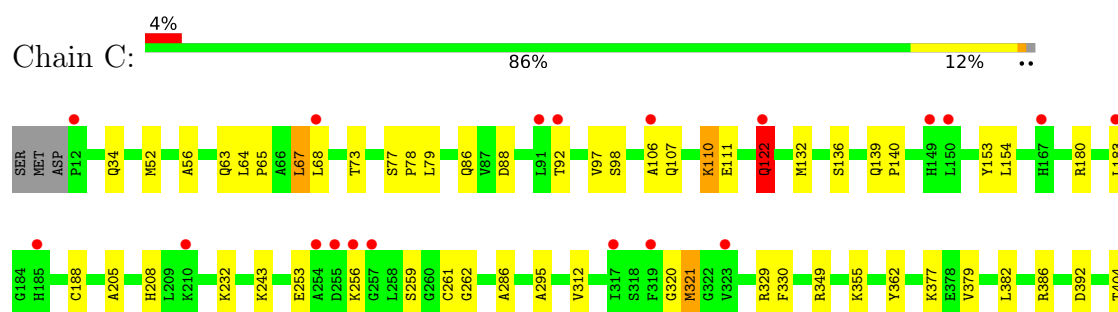
• Molecule 1: ATP-dependent DNA helicase Q5

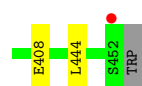


• Molecule 1: ATP-dependent DNA helicase Q5

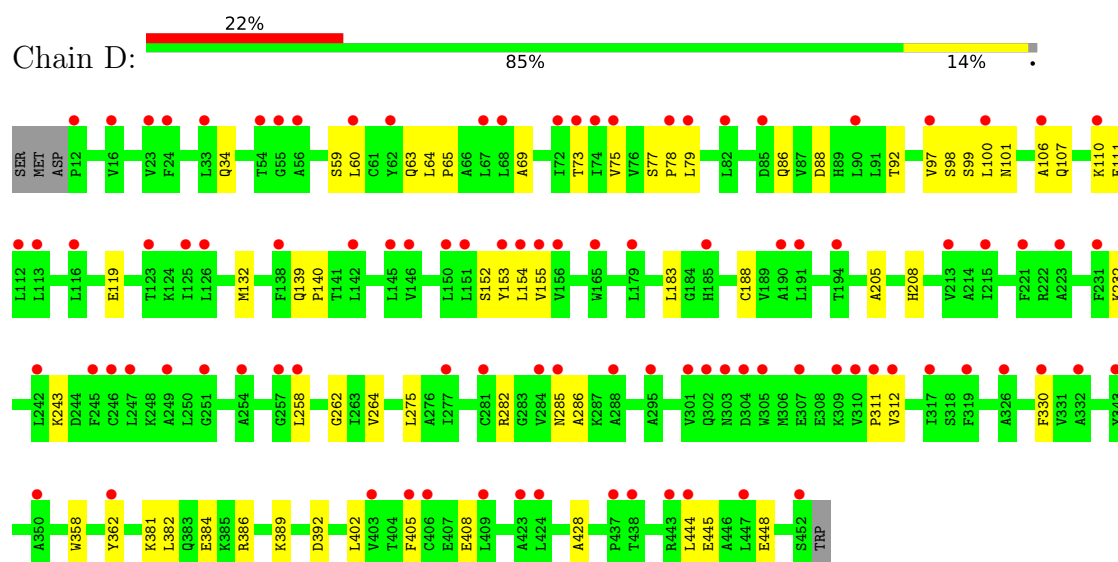


• Molecule 1: ATP-dependent DNA helicase Q5

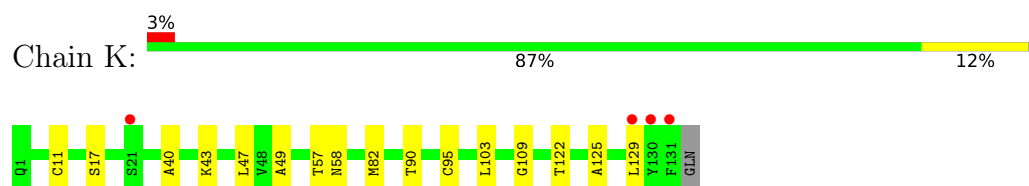




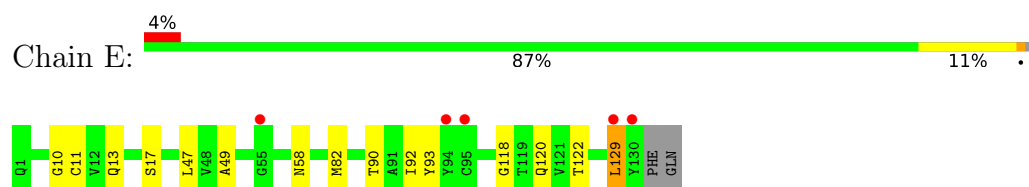
• Molecule 1: ATP-dependent DNA helicase Q5



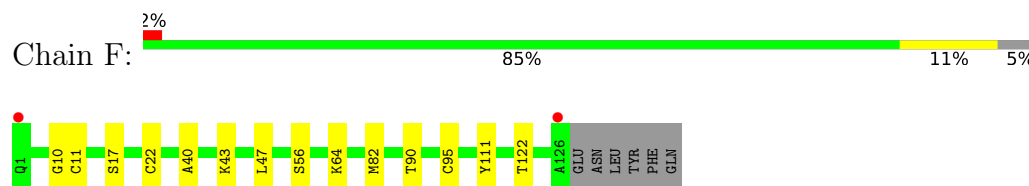
• Molecule 2: Gluebody G2-001



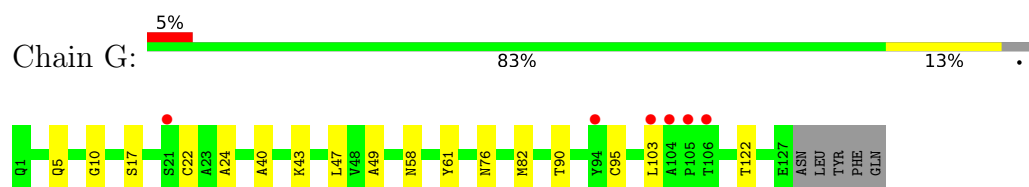
• Molecule 2: Gluebody G2-001



• Molecule 2: Gluebody G2-001



• Molecule 2: Gluebody G2-001



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.61Å 183.97Å 100.95Å 90.00° 108.12° 90.00°	Depositor
Resolution (Å)	95.94 – 2.50 95.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (95.94-2.50) 99.4 (95.94-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.236 , 0.281 0.239 , 0.282	Depositor DCC
R_{free} test set	4407 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17749	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: 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	1.04	1/3531 (0.0%)	1.47	2/4770 (0.0%)
1	B	1.04	1/3537 (0.0%)	1.47	5/4778 (0.1%)
1	C	1.04	0/3533	1.47	2/4774 (0.0%)
1	D	1.03	0/3514	1.47	0/4750
2	E	1.01	0/1004	1.25	0/1361
2	F	0.98	0/966	1.24	0/1309
2	G	1.02	0/975	1.23	0/1321
2	K	1.00	0/1016	1.26	2/1377 (0.1%)
All	All	1.03	2/18076 (0.0%)	1.42	11/24440 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	THR	N-CA	5.13	1.50	1.45
1	B	310	VAL	N-CA	5.06	1.50	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	GLN	CB-CG-CD	-6.67	101.25	112.60
1	C	67	LEU	N-CA-C	-5.52	102.31	110.48
1	A	219	PRO	CA-C-N	5.50	127.66	120.28
1	A	219	PRO	C-N-CA	5.50	127.66	120.28
1	B	319	PHE	CA-C-N	5.42	125.12	119.92
1	B	319	PHE	C-N-CA	5.42	125.12	119.92
1	B	12	PRO	CA-N-CD	-5.12	104.83	112.00
2	K	125	ALA	CA-C-N	5.00	128.31	120.75
2	K	125	ALA	C-N-CA	5.00	128.31	120.75
1	B	219	PRO	CA-C-N	5.00	126.98	120.28
1	B	219	PRO	C-N-CA	5.00	126.98	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	3448	0	3468	30	0
1	B	3455	0	3479	28	0
1	C	3437	0	3432	30	0
1	D	3424	0	3429	33	0
2	E	985	0	933	9	0
2	F	948	0	901	8	0
2	G	957	0	907	10	0
2	K	996	0	940	7	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	21	0	0	3	0
4	B	24	0	0	1	0
4	C	14	0	0	2	0
4	D	2	0	0	1	0
4	E	12	0	0	0	0
4	F	6	0	0	0	0
4	G	5	0	0	0	0
4	K	11	0	0	1	0
All	All	17749	0	17489	148	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 4.

All (148) 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:A:181:SER:HB2	4:A:614:HOH:O	1.44	1.17
1:D:382:LEU:HB3	1:D:386:ARG:HH22	1.16	1.04
1:D:382:LEU:HB3	1:D:386:ARG:NH2	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LYS:CB	4:A:620:HOH:O	2.21	0.89
2:G:22:CYS:HG	2:G:95:CYS:HG	1.23	0.85
1:C:122:GLN:NE2	1:C:122:GLN:HA	2.03	0.73
1:D:386:ARG:HE	1:D:389:LYS:HD2	1.54	0.71
1:D:428:ALA:HB3	4:D:602:HOH:O	1.92	0.70
1:C:64:LEU:HB3	1:C:65:PRO:HD3	1.75	0.69
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.74	0.68
1:D:64:LEU:HB3	1:D:65:PRO:HD3	1.76	0.68
1:B:64:LEU:HB3	1:B:65:PRO:HD3	1.76	0.66
1:D:243:LYS:HD3	1:D:282:ARG:HB3	1.80	0.64
2:E:13:GLN:HG3	2:E:129:LEU:HD21	1.80	0.63
1:D:386:ARG:NE	1:D:389:LYS:HD2	2.15	0.62
1:C:56:ALA:HB1	4:C:603:HOH:O	2.02	0.60
1:C:154:LEU:HD22	1:C:183:LEU:HD12	1.84	0.59
1:C:256:LYS:HB3	1:C:259:SER:HB3	1.85	0.59
1:B:404:THR:HG23	1:B:408:GLU:HG3	1.83	0.59
1:A:243:LYS:HG3	1:A:284:VAL:HG23	1.85	0.59
1:D:382:LEU:CB	1:D:386:ARG:HH22	2.04	0.57
1:C:106:ALA:O	1:C:110:LYS:HD3	2.04	0.57
1:B:243:LYS:HD3	1:B:282:ARG:HB3	1.87	0.57
1:A:232:LYS:HD2	1:A:362:TYR:HB3	1.87	0.57
1:A:106:ALA:O	1:A:110:LYS:HD3	2.05	0.56
1:A:404:THR:HG23	1:A:408:GLU:HG3	1.87	0.56
2:K:103:LEU:HD12	2:K:109:GLY:HA3	1.87	0.56
1:D:386:ARG:NH1	1:D:392:ASP:OD1	2.38	0.56
1:D:106:ALA:O	1:D:110:LYS:HD3	2.06	0.56
1:B:106:ALA:O	1:B:110:LYS:HD3	2.06	0.55
1:D:99:SER:OG	1:D:101:ASN:ND2	2.40	0.54
1:D:232:LYS:HD2	1:D:362:TYR:HB3	1.88	0.54
1:C:404:THR:HG23	1:C:408:GLU:HG3	1.90	0.54
1:C:232:LYS:HD2	1:C:362:TYR:HB3	1.90	0.53
1:B:154:LEU:HD22	1:B:183:LEU:HD12	1.91	0.52
1:A:154:LEU:HD22	1:A:183:LEU:HD12	1.91	0.52
1:A:243:LYS:HD3	1:A:282:ARG:HB3	1.91	0.52
1:D:139:GLN:N	1:D:140:PRO:HD2	2.25	0.52
1:C:67:LEU:O	1:C:68:LEU:HB2	2.09	0.51
1:D:285:ASN:HB3	1:D:311:PRO:HD2	1.92	0.51
1:A:387:GLY:HA3	1:C:208:HIS:CE1	2.45	0.51
1:D:100:LEU:HG	1:D:132:MET:HE2	1.93	0.51
1:A:139:GLN:N	1:A:140:PRO:HD2	2.26	0.51
1:C:139:GLN:N	1:C:140:PRO:HD2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:SER:HA	4:B:604:HOH:O	2.11	0.50
1:B:139:GLN:N	1:B:140:PRO:HD2	2.26	0.50
1:A:99:SER:OG	1:A:101:ASN:ND2	2.44	0.50
1:D:77:SER:OG	1:D:78:PRO:HD2	2.11	0.50
1:C:386:ARG:NH1	1:C:392:ASP:OD1	2.43	0.50
1:B:77:SER:OG	1:B:78:PRO:HD2	2.12	0.50
1:B:232:LYS:HD2	1:B:362:TYR:HB3	1.94	0.49
1:A:262:GLY:HA3	1:A:330:PHE:CE2	2.47	0.49
1:A:286:ALA:HA	1:A:312:VAL:O	2.12	0.49
1:A:77:SER:OG	1:A:78:PRO:HD2	2.12	0.49
1:C:382:LEU:O	1:C:386:ARG:HG2	2.13	0.49
1:B:331:VAL:HG23	1:B:350:ALA:HB2	1.95	0.49
1:D:73:THR:HG23	1:D:153:TYR:HB2	1.93	0.49
1:D:154:LEU:HD22	1:D:183:LEU:HD12	1.94	0.49
1:C:77:SER:OG	1:C:78:PRO:HD2	2.12	0.49
1:A:107:GLN:NE2	1:A:111:GLU:OE2	2.46	0.49
1:D:286:ALA:HA	1:D:312:VAL:O	2.13	0.49
1:C:73:THR:HG23	1:C:153:TYR:HB2	1.95	0.48
1:D:107:GLN:NE2	1:D:111:GLU:OE2	2.47	0.48
2:F:22:CYS:SG	2:F:95:CYS:SG	3.07	0.48
1:B:107:GLN:NE2	1:B:111:GLU:OE2	2.47	0.48
1:C:63:GLN:NE2	1:C:86:GLN:OE1	2.47	0.48
2:E:13:GLN:HG3	2:E:129:LEU:CD2	2.42	0.48
2:E:92:ILE:HG12	2:E:120:GLN:HE21	1.79	0.48
1:C:107:GLN:NE2	1:C:111:GLU:OE2	2.47	0.48
1:A:329:ARG:NH2	1:A:353:ASP:OD2	2.27	0.47
1:A:387:GLY:HA3	1:C:208:HIS:ND1	2.30	0.47
1:C:286:ALA:HA	1:C:312:VAL:O	2.14	0.47
1:B:63:GLN:NE2	1:B:86:GLN:OE1	2.48	0.47
1:A:63:GLN:NE2	1:A:86:GLN:OE1	2.48	0.47
1:A:181:SER:CB	4:A:614:HOH:O	2.26	0.47
1:D:34:GLN:NE2	1:D:60:LEU:HD23	2.30	0.47
1:D:262:GLY:HA3	1:D:330:PHE:CE2	2.49	0.47
1:B:262:GLY:HA3	1:B:330:PHE:CE2	2.50	0.46
1:A:330:PHE:HA	1:A:358:TRP:O	2.15	0.46
1:C:329:ARG:HH22	1:C:355:LYS:HB2	1.80	0.46
1:D:63:GLN:NE2	1:D:86:GLN:OE1	2.48	0.46
1:B:382:LEU:O	1:B:386:ARG:HG2	2.15	0.46
1:B:34:GLN:HA	1:B:52:MET:HE1	1.97	0.46
1:B:286:ALA:HA	1:B:312:VAL:O	2.15	0.46
1:D:330:PHE:HA	1:D:358:TRP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HG	1:A:132:MET:HE2	1.98	0.45
2:K:17:SER:HA	2:K:82:MET:O	2.16	0.45
1:B:330:PHE:HA	1:B:358:TRP:O	2.16	0.45
2:F:90:THR:HG23	2:F:122:THR:HA	1.99	0.45
1:C:205:ALA:O	1:C:208:HIS:HD2	2.00	0.45
1:C:321:MET:HE2	1:C:349:ARG:HE	1.82	0.45
2:E:90:THR:HG23	2:E:122:THR:HA	1.98	0.45
2:G:24:ALA:HB3	2:G:76:ASN:HB3	1.98	0.45
1:A:34:GLN:HA	1:A:52:MET:HE1	1.99	0.45
1:C:295:ALA:N	4:C:602:HOH:O	2.39	0.45
2:F:17:SER:HA	2:F:82:MET:O	2.17	0.44
1:C:34:GLN:HA	1:C:52:MET:HE1	1.99	0.44
1:B:201:GLU:OE1	2:F:111:TYR:OH	2.29	0.44
2:E:17:SER:HA	2:E:82:MET:O	2.17	0.44
2:E:10:GLY:HA3	2:F:11:CYS:O	2.18	0.44
1:B:172:ASP:OD1	1:B:175[B]:ARG:NH2	2.50	0.44
2:K:40:ALA:HB3	2:K:43:LYS:HE3	2.00	0.44
1:C:262:GLY:HA3	1:C:330:PHE:CE2	2.53	0.43
1:B:88:ASP:O	1:B:92:THR:HG23	2.18	0.43
1:B:285:ASN:HB3	1:B:311:PRO:HD2	2.01	0.43
1:A:88:ASP:O	1:A:92:THR:HG23	2.18	0.43
1:A:154:LEU:O	1:A:188:CYS:HA	2.18	0.43
1:D:154:LEU:O	1:D:188:CYS:HA	2.19	0.43
1:C:88:ASP:O	1:C:92:THR:HG23	2.18	0.42
2:G:22:CYS:CB	2:G:95:CYS:HG	2.28	0.42
1:A:205:ALA:O	1:A:208:HIS:HD2	2.02	0.42
1:C:154:LEU:O	1:C:188:CYS:HA	2.19	0.42
1:D:381:LYS:O	1:D:384:GLU:HG2	2.19	0.42
2:K:90:THR:HG23	2:K:122:THR:HA	2.01	0.42
1:B:262:GLY:HA3	1:B:330:PHE:CZ	2.54	0.42
1:C:253:GLU:HB2	1:C:259:SER:OG	2.18	0.42
1:B:372:SER:OG	2:G:61:TYR:HD2	2.03	0.42
2:E:49:ALA:HA	2:E:58:ASN:O	2.20	0.42
2:F:40:ALA:HB3	2:F:43:LYS:HE3	2.02	0.42
1:D:445:GLU:O	1:D:448:GLU:HB2	2.19	0.42
1:A:151:LEU:HD21	1:A:183:LEU:HD13	2.02	0.42
1:B:154:LEU:O	1:B:188:CYS:HA	2.20	0.41
2:G:5:GLN:O	2:G:22:CYS:HA	2.20	0.41
1:A:262:GLY:HA3	1:A:330:PHE:CZ	2.55	0.41
1:D:88:ASP:O	1:D:92:THR:HG23	2.19	0.41
2:E:11:CYS:O	2:F:10:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:17:SER:HA	2:G:82:MET:O	2.20	0.41
2:G:90:THR:HG23	2:G:122:THR:HA	2.03	0.41
2:F:22:CYS:CB	2:F:95:CYS:HG	2.33	0.41
1:D:205:ALA:O	1:D:208:HIS:HD2	2.03	0.41
1:B:260:GLY:HA2	1:B:327:ASN:HD22	1.85	0.41
1:B:402:LEU:O	1:B:405:PHE:HB3	2.20	0.41
1:D:69:ALA:HB1	1:D:152:SER:HB3	2.02	0.41
2:G:49:ALA:HA	2:G:58:ASN:O	2.20	0.41
1:B:132:MET:HE3	1:B:132:MET:HB3	1.99	0.41
1:A:34:GLN:CD	1:A:57:GLY:HA3	2.46	0.41
1:C:261:CYS:O	1:C:329:ARG:N	2.52	0.41
2:K:11:CYS:O	2:G:10:GLY:HA3	2.21	0.40
2:G:40:ALA:HB3	2:G:43:LYS:HE3	2.03	0.40
1:D:264:VAL:HG11	1:D:275:LEU:HD23	2.03	0.40
2:K:57:THR:HG21	4:K:202:HOH:O	2.21	0.40
1:A:365:ARG:HH11	1:A:451:SER:HB3	1.86	0.40
1:D:75:VAL:HG22	1:D:155:VAL:HB	2.04	0.40
1:B:151:LEU:HD21	1:B:183:LEU:HD13	2.03	0.40
1:C:320:GLY:O	1:C:321:MET:C	2.63	0.40
1:D:402:LEU:O	1:D:405:PHE:HB3	2.21	0.40
2:K:49:ALA:HA	2:K:58:ASN:O	2.22	0.40
2:E:93:TYR:O	2:E:118:GLY:HA2	2.22	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%)	433 (98%)	10 (2%)	0	100	100
1	B	444/445 (100%)	433 (98%)	11 (2%)	0	100	100
1	C	444/445 (100%)	434 (98%)	9 (2%)	1 (0%)	43	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	443/445 (100%)	435 (98%)	8 (2%)	0	100	100
2	E	128/132 (97%)	126 (98%)	2 (2%)	0	100	100
2	F	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	G	125/132 (95%)	123 (98%)	2 (2%)	0	100	100
2	K	129/132 (98%)	127 (98%)	2 (2%)	0	100	100
All	All	2280/2308 (99%)	2232 (98%)	47 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	321	MET

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%)	360 (98%)	9 (2%)	43	70
1	B	370/373 (99%)	361 (98%)	9 (2%)	43	70
1	C	369/373 (99%)	357 (97%)	12 (3%)	33	61
1	D	367/373 (98%)	359 (98%)	8 (2%)	45	73
2	E	100/103 (97%)	98 (98%)	2 (2%)	48	75
2	F	96/103 (93%)	93 (97%)	3 (3%)	35	62
2	G	97/103 (94%)	95 (98%)	2 (2%)	47	74
2	K	101/103 (98%)	98 (97%)	3 (3%)	36	64
All	All	1869/1904 (98%)	1821 (97%)	48 (3%)	40	68

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

Mol	Chain	Res	Type
1	B	59	SER
1	B	79	LEU

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Mol	Chain	Res	Type
1	B	97	VAL
1	B	98	SER
1	B	131	GLU
1	B	364	SER
1	B	379	VAL
1	B	424	LEU
1	B	444	LEU
1	A	79	LEU
1	A	97	VAL
1	A	98	SER
1	A	110	LYS
1	A	122	GLN
1	A	136	SER
1	A	364	SER
1	A	379	VAL
1	A	444	LEU
1	C	79	LEU
1	C	97	VAL
1	C	98	SER
1	C	110	LYS
1	C	122	GLN
1	C	132	MET
1	C	136	SER
1	C	180	ARG
1	C	243	LYS
1	C	377	LYS
1	C	379	VAL
1	C	444	LEU
1	D	59	SER
1	D	79	LEU
1	D	97	VAL
1	D	98	SER
1	D	119	GLU
1	D	258	LEU
1	D	408	GLU
1	D	444	LEU
2	K	47	LEU
2	K	95	CYS
2	K	129	LEU
2	E	47	LEU
2	E	129	LEU
2	F	47	LEU

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Mol	Chain	Res	Type
2	F	56	SER
2	F	64	LYS
2	G	47	LEU
2	G	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	107	GLN
1	B	208	HIS
1	A	101	ASN
1	A	139	GLN
1	A	208	HIS
1	A	241	ASN
1	C	107	GLN
1	C	208	HIS
1	C	241	ASN
1	C	285	ASN
1	C	388	ASN
1	D	101	ASN
1	D	107	GLN
1	D	139	GLN
1	D	208	HIS
1	D	285	ASN
2	K	3	GLN
2	K	7	ASN
2	K	44	GLN
2	K	81	GLN
2	K	83	ASN
2	E	3	GLN
2	E	81	GLN
2	E	83	ASN
2	F	3	GLN
2	F	81	GLN
2	F	83	ASN
2	G	3	GLN

5.3.3 RNA ⓘ

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, 4 are monoatomic - leaving 0 for Mogul analysis.

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%)	0.62	29 (6%)	24 21	30, 75, 142, 180	4 (0%)
1	B	441/445 (99%)	0.60	35 (7%)	18 16	37, 74, 140, 180	5 (1%)
1	C	441/445 (99%)	0.52	20 (4%)	38 33	37, 72, 120, 173	3 (0%)
1	D	441/445 (99%)	1.33	97 (21%)	2 2	34, 123, 173, 215	2 (0%)
2	E	130/132 (98%)	0.12	5 (3%)	44 39	41, 56, 90, 208	0
2	F	126/132 (95%)	-0.01	2 (1%)	70 67	43, 58, 92, 140	0
2	G	127/132 (96%)	0.35	6 (4%)	36 32	43, 65, 118, 157	0
2	K	131/132 (99%)	0.17	4 (3%)	51 47	43, 55, 86, 145	0
All	All	2277/2308 (98%)	0.63	198 (8%)	16 14	30, 75, 152, 215	14 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	12	PRO	6.4
1	D	12	PRO	4.8
1	B	183	LEU	4.3
1	C	183	LEU	4.2
1	D	310	VAL	4.1
1	A	23	VAL	4.0
1	D	155	VAL	3.9
1	C	317	ILE	3.9
1	C	150	LEU	3.9
1	D	247	LEU	3.9
1	A	69	ALA	3.8
1	A	90	LEU	3.8
1	B	100	LEU	3.7
1	B	375	ILE	3.7
2	K	131	PHE	3.7
1	B	12	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	305	TRP	3.6
1	D	125	ILE	3.5
2	K	130	TYR	3.5
1	D	154	LEU	3.5
2	K	129	LEU	3.5
1	C	167[A]	HIS	3.5
2	E	129	LEU	3.5
1	B	305	TRP	3.5
1	D	215	ILE	3.4
1	D	301	VAL	3.4
1	D	249	ALA	3.4
2	G	105	PRO	3.3
1	C	319	PHE	3.3
1	D	145	LEU	3.3
1	D	138	PHE	3.3
1	D	319	PHE	3.3
1	D	153	TYR	3.3
1	A	12	PRO	3.3
1	D	100	LEU	3.3
1	D	317	ILE	3.2
1	D	332	ALA	3.2
1	D	116	LEU	3.2
1	A	95	VAL	3.2
1	D	72	ILE	3.2
1	A	254	ALA	3.1
2	K	21	SER	3.1
1	C	68	LEU	3.1
1	D	281	CYS	3.1
1	D	55	GLY	3.1
1	A	92	THR	3.1
1	D	423	ALA	3.0
2	E	94	TYR	3.0
1	D	424	LEU	3.0
1	D	54	THR	3.0
1	D	67	LEU	3.0
1	D	16	VAL	3.0
1	D	23	VAL	3.0
1	D	437	PRO	2.9
1	C	452	SER	2.9
1	C	122	GLN	2.9
1	B	317	ILE	2.9
1	A	320	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	285	ASN	2.8
1	D	288	ALA	2.8
1	D	126	LEU	2.8
2	G	94	TYR	2.8
1	B	301	VAL	2.8
1	A	100	LEU	2.8
1	D	303	ASN	2.8
1	D	258	LEU	2.8
1	D	82	LEU	2.8
1	D	150	LEU	2.7
1	D	245	PHE	2.7
1	D	78	PRO	2.7
1	A	133	ALA	2.7
1	D	190	ALA	2.7
1	D	330	PHE	2.7
1	D	75	VAL	2.7
1	D	304	ASP	2.7
1	B	292	GLY	2.7
1	B	231	PHE	2.7
1	D	277	ILE	2.7
1	D	151	LEU	2.7
1	D	343	TYR	2.7
2	G	106	THR	2.7
1	D	326	ALA	2.6
2	F	126	ALA	2.6
1	A	167[A]	HIS	2.6
1	D	221	PHE	2.6
1	B	14	ARG	2.6
1	D	438	THR	2.6
1	A	24	PHE	2.6
1	D	73	THR	2.6
1	B	319	PHE	2.6
1	D	246	CYS	2.6
1	D	223	ALA	2.6
1	D	90	LEU	2.5
1	B	185	HIS	2.5
1	C	185	HIS	2.5
1	B	380	ALA	2.5
2	E	95	CYS	2.5
1	C	256	LYS	2.5
1	D	106	ALA	2.5
1	D	452	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	101	ASN	2.5
1	D	312	VAL	2.5
1	A	80	ILE	2.5
1	B	409	LEU	2.5
1	D	113	LEU	2.5
1	D	242	LEU	2.5
1	B	420	PHE	2.5
1	A	185	HIS	2.5
1	D	146	VAL	2.5
1	D	307	GLU	2.4
1	C	149	HIS	2.4
1	D	165	TRP	2.4
1	B	97	VAL	2.4
1	B	254	ALA	2.4
1	A	74	ILE	2.4
1	A	317	ILE	2.4
1	D	405	PHE	2.4
1	D	194	THR	2.4
1	B	452	SER	2.4
1	D	74	ILE	2.4
1	D	179	LEU	2.4
2	F	1	GLN	2.4
2	G	103	LEU	2.4
1	C	210	LYS	2.4
1	B	179	LEU	2.4
1	B	274	GLN	2.4
1	D	409	LEU	2.4
1	D	444	LEU	2.4
1	D	231	PHE	2.4
1	C	323	VAL	2.4
1	D	257	GLY	2.3
2	E	55	GLY	2.3
1	D	24	PHE	2.3
1	D	284	VAL	2.3
1	D	403	VAL	2.3
1	D	350	ALA	2.3
1	D	60	LEU	2.3
1	C	254	ALA	2.3
1	B	167[A]	HIS	2.3
1	B	444	LEU	2.3
1	A	93	LEU	2.3
1	D	110	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	291	ALA	2.3
1	B	252	GLN	2.3
1	B	165	TRP	2.3
1	D	156	VAL	2.3
1	C	257	GLY	2.2
1	D	185	HIS	2.2
1	B	293	LEU	2.2
1	A	152	SER	2.2
1	D	79	LEU	2.2
1	D	112	LEU	2.2
1	A	179	LEU	2.2
1	A	106	ALA	2.2
1	C	106	ALA	2.2
1	D	302	GLN	2.2
1	D	309	LYS	2.2
1	D	362	TYR	2.2
1	B	300	LEU	2.2
1	D	191	LEU	2.2
1	A	137	SER	2.2
2	G	104	ALA	2.2
1	C	92	THR	2.2
1	D	97	VAL	2.1
1	D	142	LEU	2.1
1	B	289	TYR	2.1
1	A	72	ILE	2.1
2	E	130	TYR	2.1
1	B	266	CYS	2.1
1	A	321	MET	2.1
1	D	295	ALA	2.1
1	D	443	ARG	2.1
2	G	21	SER	2.1
1	B	256	LYS	2.1
1	B	377	LYS	2.1
1	B	379	VAL	2.1
1	A	56	ALA	2.1
1	D	251	GLY	2.1
1	B	386	ARG	2.1
1	D	254	ALA	2.1
1	B	258	LEU	2.1
1	A	150	LEU	2.1
1	C	91	LEU	2.1
1	D	33	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	68	LEU	2.1
1	D	447	LEU	2.1
1	D	123	THR	2.1
1	A	319	PHE	2.0
1	D	213	VAL	2.0
1	A	165	TRP	2.0
1	A	256	LYS	2.0
1	D	85	ASP	2.0
1	D	311	PRO	2.0
1	D	406	CYS	2.0
1	A	26	PHE	2.0
1	D	56	ALA	2.0
1	C	255	ASP	2.0
1	D	62	TYR	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
3	ZN	D	501	1/1	0.96	0.05	166,166,166,166	0
3	ZN	C	501	1/1	0.99	0.03	69,69,69,69	0
3	ZN	B	501	1/1	0.99	0.02	63,63,63,63	0
3	ZN	A	501	1/1	1.00	0.02	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.