



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:56 AM UTC

PDB ID : 5N96 / pdb_00005n96
Title : Crystal Structure of Drosophila DHX36 helicase in complex with AGGGTTTTTT
Authors : Chen, W.-F.; Rety, S.; Guo, H.-L.; Wu, W.-Q.; Liu, N.-N.; Liu, Q.-W.; Dai, Y.-X.; Xi, X.-G.
Deposited on : 2017-02-24
Resolution : 2.72 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

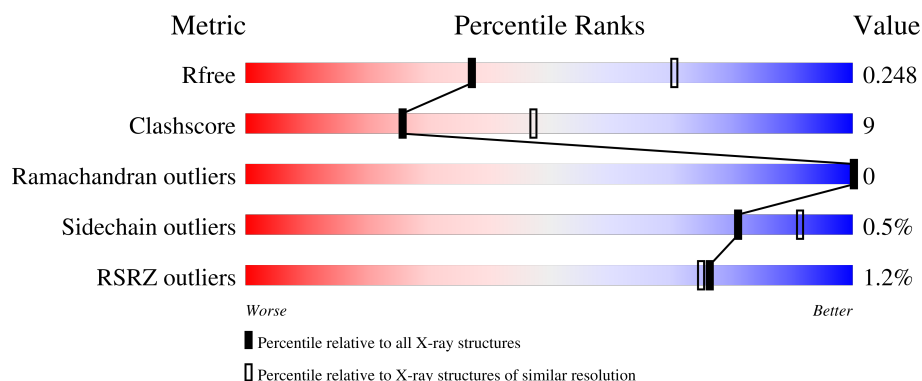
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	944	10% 71% 18% 10%
1	B	944	70% 19% 10%
2	C	10	10% 90% 10%
2	D	10	10% 90% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14156 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 CG9323, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	849	Total	C	N	O	S	0	0	0
			6814	4304	1200	1265	45			
1	B	851	Total	C	N	O	S	0	0	0
			6829	4312	1202	1270	45			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	943	VAL	-	expression tag	UNP Q8SWT2
A	944	ASP	-	expression tag	UNP Q8SWT2
B	943	VAL	-	expression tag	UNP Q8SWT2
B	944	ASP	-	expression tag	UNP Q8SWT2

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*GP*GP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			191	90	30	61	10			
2	D	10	Total	C	N	O	P	0	0	0
			191	90	30	61	10			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

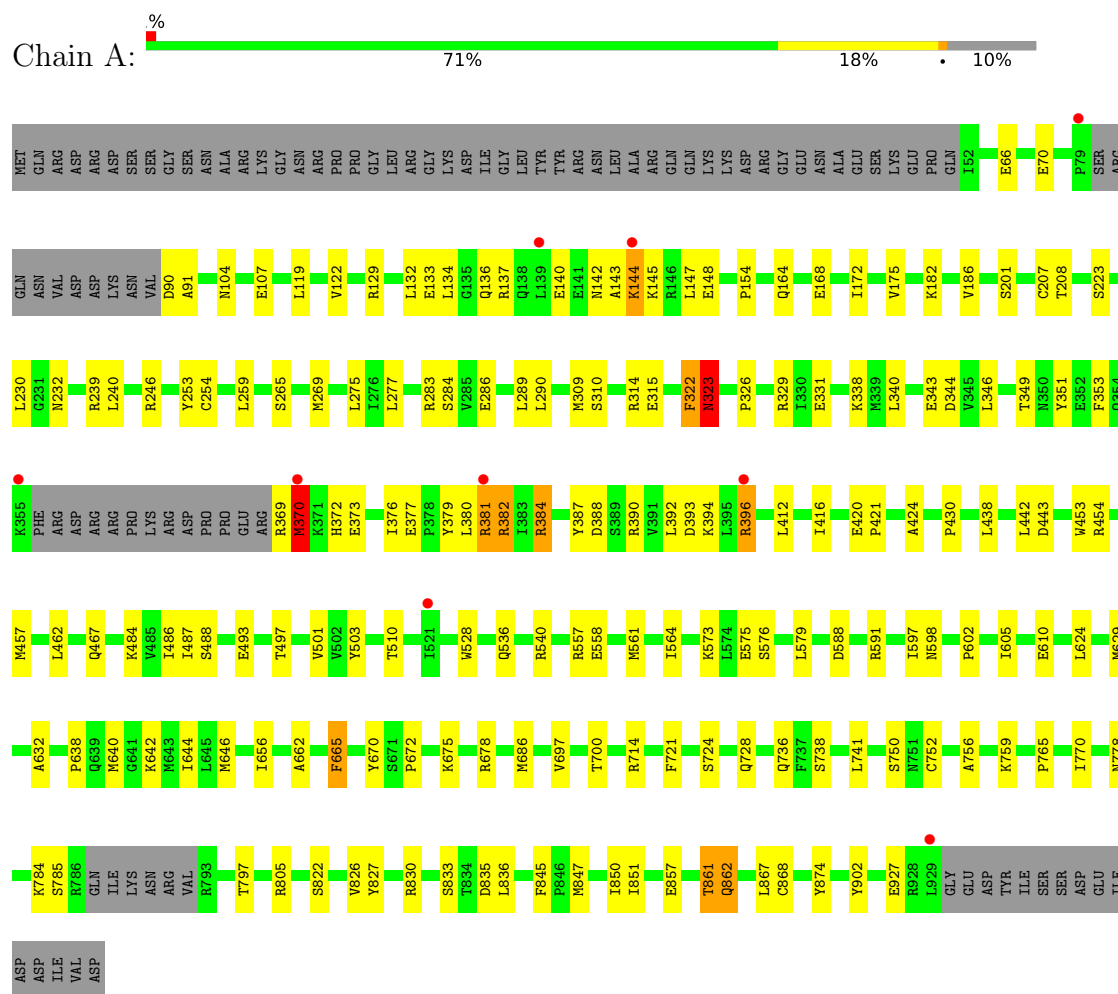
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total 57	O 57	0	0
4	B	67	Total 67	O 67	0	0
4	C	3	Total 3	O 3	0	0
4	D	2	Total 2	O 2	0	0

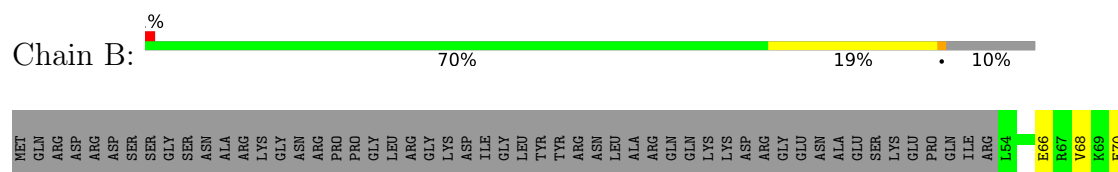
3 Residue-property plots

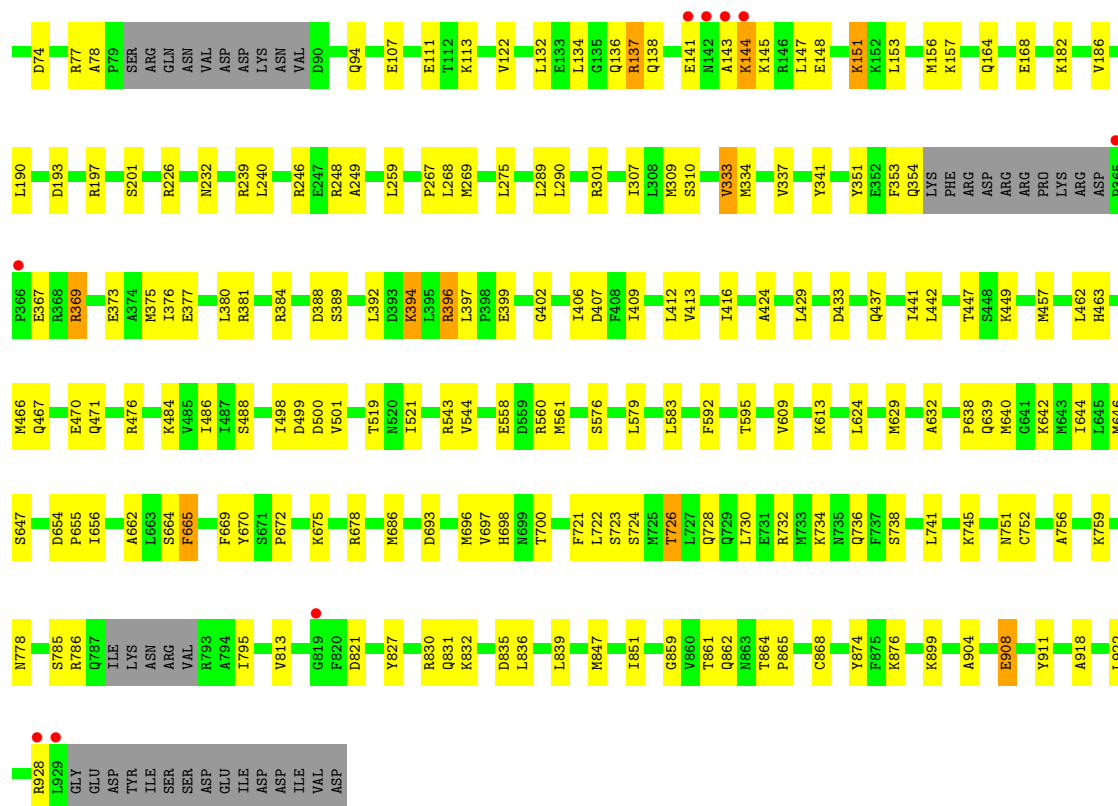
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CG9323, isoform A

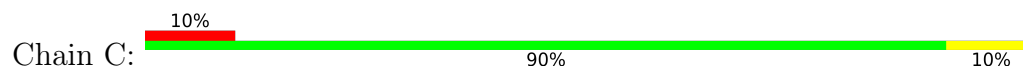


• Molecule 1: CG9323, isoform A

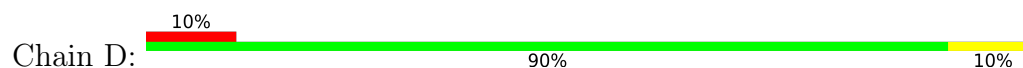




- Molecule 2: DNA (5'-D(P*AP*GP*GP*GP*TP*TP*TP*TP*TP*T)-3')



- Molecule 2: DNA (5'-D(P*AP*GP*GP*GP*TP*TP*TP*TP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	303.39Å 51.32Å 164.60Å 90.00° 114.57° 90.00°	Depositor
Resolution (Å)	56.65 – 2.72 56.65 – 2.72	Depositor EDS
% Data completeness (in resolution range)	97.6 (56.65-2.72) 97.6 (56.65-2.72)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.73Å)	Xtriage
Refinement program	PHENIX (dev_2427: ???)	Depositor
R, R_{free}	0.180 , 0.248 0.184 , 0.248	Depositor DCC
R_{free} test set	3131 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14156	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: MG

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	0.48	2/6933 (0.0%)	0.84	20/9353 (0.2%)
1	B	0.49	5/6950 (0.1%)	0.81	14/9378 (0.1%)
2	C	0.51	0/212	0.63	0/327
2	D	0.57	0/212	0.64	0/327
All	All	0.49	7/14307 (0.0%)	0.82	34/19385 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	ARG	NE-CZ	12.86	1.47	1.33
1	B	369	ARG	NE-CZ	8.00	1.41	1.33
1	B	396	ARG	NE-CZ	7.79	1.41	1.33
1	B	369	ARG	CD-NE	6.92	1.55	1.46
1	A	396	ARG	CG-CD	-6.33	1.33	1.52
1	B	151	LYS	CG-CD	5.30	1.68	1.52
1	B	137	ARG	CB-CG	-5.11	1.37	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ARG	CA-CB-CG	-10.77	92.56	114.10
1	A	396	ARG	NE-CZ-NH2	10.33	128.50	119.20
1	A	323	ASN	CA-C-N	9.21	139.31	122.54
1	A	323	ASN	C-N-CA	9.21	139.31	122.54
1	A	861	THR	CA-C-N	-8.72	105.85	121.81
1	A	861	THR	C-N-CA	-8.72	105.85	121.81
1	A	322	PHE	CA-C-N	8.36	137.50	121.54
1	A	322	PHE	C-N-CA	8.36	137.50	121.54
1	B	137	ARG	CG-CD-NE	-7.99	94.43	112.00
1	A	396	ARG	NE-CZ-NH1	-7.93	113.57	121.50
1	A	382	ARG	CD-NE-CZ	7.88	135.43	124.40
1	B	908	GLU	CA-CB-CG	-7.69	98.71	114.10
1	B	113	LYS	CA-CB-CG	7.40	128.90	114.10
1	B	369	ARG	CG-CD-NE	-7.38	95.76	112.00
1	A	323	ASN	N-CA-C	7.20	126.13	110.80
1	A	370	MET	CA-C-N	7.09	134.47	121.70
1	A	370	MET	C-N-CA	7.09	134.47	121.70
1	B	151	LYS	CB-CA-C	6.90	123.23	110.11
1	A	396	ARG	CB-CG-CD	-6.48	96.40	111.30
1	B	151	LYS	CG-CD-CE	6.10	125.33	111.30
1	A	323	ASN	O-C-N	-5.82	114.84	122.59
1	B	664	SER	CA-C-N	-5.62	113.70	122.42
1	B	664	SER	C-N-CA	-5.62	113.70	122.42
1	A	382	ARG	CA-CB-CG	5.56	125.23	114.10
1	A	144	LYS	CA-CB-CG	5.55	125.20	114.10
1	B	333	VAL	CA-C-N	5.50	131.80	122.12
1	B	333	VAL	C-N-CA	5.50	131.80	122.12
1	B	665	PHE	N-CA-CB	-5.41	100.59	110.27
1	B	144	LYS	CA-C-N	5.40	131.96	122.79
1	B	144	LYS	C-N-CA	5.40	131.96	122.79
1	A	833	SER	N-CA-C	5.38	119.33	112.12
1	A	665	PHE	N-CA-C	5.21	119.30	111.96
1	A	420	GLU	N-CA-C	5.05	120.98	109.81
1	B	369	ARG	CA-CB-CG	-5.03	104.05	114.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	322	PHE	Peptide
1	A	323	ASN	Peptide
1	A	353	PHE	Peptide
1	A	370	MET	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	862	GLN	Peptide
1	B	665	PHE	Mainchain
1	B	861	THR	Peptide

5.2 Too-close contacts [i](#)

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	6814	0	6911	127	3
1	B	6829	0	6918	139	2
2	C	191	0	104	2	0
2	D	191	0	104	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	57	0	0	1	0
4	B	67	0	0	6	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
All	All	14156	0	14037	266	3

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 9.

All (266) 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:380:LEU:HD13	1:B:396:ARG:NH1	1.91	0.85
1:A:784:LYS:HB3	1:A:797:THR:H	1.43	0.83
1:A:380:LEU:HD13	1:A:396:ARG:NH1	1.93	0.82
1:B:141:GLU:HB2	1:B:144:LYS:HZ3	1.44	0.81
1:B:442:LEU:HD22	1:B:457:MET:HE1	1.63	0.81
1:B:380:LEU:HD22	1:B:392:LEU:HB3	1.64	0.80
1:B:756:ALA:HA	1:B:759:LYS:HE2	1.65	0.79
1:B:406:ILE:HD13	1:B:441:ILE:HD12	1.65	0.79
1:A:90:ASP:N	4:A:1101:HOH:O	2.16	0.78
1:A:558:GLU:HA	1:A:561:MET:HG3	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HD22	1:A:392:LEU:HB3	1.66	0.77
1:B:380:LEU:HD13	1:B:396:ARG:HH11	1.46	0.77
1:B:353:PHE:O	4:B:1101:HOH:O	2.05	0.74
1:A:686:MET:HE2	1:A:700:THR:HA	1.70	0.74
1:A:421:PRO:O	1:A:503:TYR:OH	2.05	0.73
1:B:745:LYS:NZ	4:B:1104:HOH:O	2.21	0.72
1:A:805:ARG:NH2	1:A:835:ASP:OD2	2.22	0.71
1:A:323:ASN:O	1:A:323:ASN:ND2	2.24	0.70
1:B:193:ASP:O	1:B:197:ARG:HG3	1.92	0.69
1:A:847:MET:O	1:A:851:ILE:HG13	1.93	0.69
1:B:381:ARG:HG3	1:B:384:ARG:HH11	1.58	0.69
1:A:373:GLU:HA	1:A:376:ILE:HG22	1.74	0.68
1:A:412:LEU:O	1:A:416:ILE:HG13	1.94	0.68
1:A:644:ILE:HG22	1:A:741:LEU:HD11	1.76	0.68
1:B:137:ARG:NH2	1:B:226:ARG:O	2.25	0.68
1:B:484:LYS:HD3	1:B:486:ILE:HD11	1.76	0.68
1:A:443:ASP:OD1	1:A:454:ARG:NH2	2.28	0.67
1:B:730:LEU:O	1:B:734:LYS:HG3	1.94	0.67
1:B:375:MET:HG3	1:B:560:ARG:HD3	1.76	0.67
1:A:66:GLU:O	1:A:70:GLU:HG3	1.94	0.67
1:A:624:LEU:HD21	1:A:629:MET:HB2	1.75	0.67
1:B:141:GLU:HB2	1:B:144:LYS:NZ	2.08	0.66
1:B:558:GLU:HA	1:B:561:MET:HG3	1.76	0.66
1:B:786:ARG:HB3	1:B:795:ILE:HG22	1.78	0.66
1:B:394:LYS:HA	1:B:397:LEU:HD12	1.78	0.66
1:B:259:LEU:HD23	1:B:290:LEU:HD11	1.79	0.64
1:A:381:ARG:HG2	1:A:384:ARG:HG2	1.79	0.64
1:A:493:GLU:HG2	1:A:536:GLN:HG2	1.77	0.64
1:B:143:ALA:C	1:B:145:LYS:H	2.05	0.64
1:A:140:GLU:CD	1:A:142:ASN:H	2.06	0.63
1:B:654:ASP:OD1	1:B:734:LYS:NZ	2.27	0.63
1:B:141:GLU:HA	1:B:144:LYS:HG2	1.81	0.62
1:B:137:ARG:HH22	1:B:226:ARG:C	2.08	0.62
1:B:724:SER:O	1:B:728:GLN:HG3	2.01	0.61
1:B:558:GLU:HG3	1:B:561:MET:HE2	1.82	0.61
1:B:399:GLU:N	1:B:399:GLU:OE1	2.34	0.61
1:A:164:GLN:HE21	1:A:168:GLU:CD	2.08	0.61
1:A:283:ARG:NH2	1:A:598:ASN:OD1	2.25	0.61
1:B:153:LEU:O	1:B:157:LYS:NZ	2.33	0.61
1:B:579:LEU:HG	1:B:632:ALA:HB2	1.82	0.61
1:A:379:TYR:HD1	1:A:382:ARG:NH2	1.99	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:O	1:B:70:GLU:HG3	2.02	0.60
1:B:376:ILE:HG23	1:B:380:LEU:HD12	1.84	0.60
1:B:462:LEU:HB3	1:B:488:SER:HB2	1.83	0.60
1:B:132:LEU:O	1:B:136:GLN:HG3	2.01	0.60
1:B:644:ILE:HG22	1:B:741:LEU:HD21	1.82	0.60
1:A:380:LEU:CD2	1:A:392:LEU:HB3	2.33	0.59
1:A:579:LEU:HG	1:A:632:ALA:HB2	1.84	0.58
1:B:592:PHE:O	1:B:595:THR:HB	2.03	0.58
1:A:381:ARG:HG2	1:A:384:ARG:CG	2.32	0.58
1:B:232:ASN:O	1:B:246:ARG:HG2	2.02	0.58
1:B:723:SER:OG	1:B:726:THR:HG23	2.05	0.57
1:A:528:TRP:CZ2	1:A:557:ARG:HD3	2.40	0.57
1:B:78:ALA:HB2	1:B:911:TYR:CG	2.40	0.57
1:A:756:ALA:HA	1:A:759:LYS:HE2	1.87	0.56
1:A:380:LEU:CD1	1:A:396:ARG:NH1	2.67	0.56
1:A:784:LYS:HG3	1:A:785:SER:H	1.71	0.56
1:A:239:ARG:HG3	2:C:10:DT:OP1	2.06	0.56
1:B:447:THR:HG22	1:B:449:LYS:H	1.70	0.56
1:A:462:LEU:HB3	1:A:488:SER:HB2	1.87	0.55
1:A:373:GLU:HG3	1:A:377:GLU:HG3	1.88	0.55
1:B:470:GLU:OE1	1:B:670:TYR:OH	2.23	0.55
1:B:409:ILE:O	1:B:413:VAL:HG23	2.06	0.55
1:B:141:GLU:CB	1:B:144:LYS:HZ3	2.17	0.55
1:A:381:ARG:O	1:A:384:ARG:HG3	2.05	0.55
1:A:91:ALA:HB2	1:A:902:TYR:HD1	1.71	0.55
1:A:277:LEU:HD21	1:A:290:LEU:HD13	1.89	0.55
1:A:784:LYS:HG3	1:A:785:SER:N	2.22	0.55
1:A:573:LYS:HG3	1:A:575:GLU:OE1	2.07	0.55
1:B:373:GLU:HG2	1:B:377:GLU:HG3	1.89	0.55
1:A:738:SER:HB3	1:A:750:SER:O	2.05	0.54
1:A:154:PRO:HB3	1:A:331:GLU:HG2	1.88	0.54
1:B:821:ASP:OD2	1:B:928:ARG:NH1	2.40	0.54
1:B:333:VAL:HG12	1:B:334:MET:N	2.21	0.54
1:A:442:LEU:HD22	1:A:457:MET:HE1	1.88	0.54
1:A:140:GLU:OE2	1:A:142:ASN:N	2.40	0.54
1:A:259:LEU:HD23	1:A:290:LEU:HD11	1.88	0.54
1:B:148:GLU:HA	1:B:151:LYS:HB3	1.88	0.54
1:A:338:LYS:HG2	1:A:340:LEU:CD1	2.38	0.54
1:B:576:SER:HB2	1:B:638:PRO:HD3	1.89	0.54
1:B:908:GLU:CG	1:B:908:GLU:O	2.55	0.54
1:A:387:TYR:HB2	1:A:392:LEU:HD21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:THR:HG23	1:A:351:TYR:H	1.72	0.53
1:B:406:ILE:HD12	1:B:407:ASP:N	2.24	0.53
1:A:672:PRO:HG2	1:A:675:LYS:HB2	1.89	0.53
1:B:182:LYS:NZ	1:B:310:SER:O	2.41	0.53
1:A:370:MET:HA	1:A:372:HIS:H	1.73	0.53
1:B:134:LEU:O	1:B:138:GLN:HG3	2.09	0.53
1:A:724:SER:O	1:A:728:GLN:HG3	2.08	0.53
1:B:678:ARG:HG2	1:B:721:PHE:HE2	1.74	0.52
1:A:424:ALA:HB3	1:A:501:VAL:HA	1.92	0.52
1:A:642:LYS:O	1:A:646:MET:HG2	2.10	0.52
1:A:240:LEU:HD21	1:A:736:GLN:HB2	1.92	0.52
1:A:172:ILE:HG22	1:A:326:PRO:HG2	1.92	0.52
1:A:850:ILE:HD13	1:A:867:LEU:HD23	1.92	0.52
1:B:686:MET:HE2	1:B:700:THR:HA	1.92	0.52
1:B:186:VAL:HB	1:B:309:MET:HE1	1.91	0.52
1:B:424:ALA:HB3	1:B:501:VAL:HA	1.90	0.52
1:A:861:THR:HG23	1:A:862:GLN:HG2	1.91	0.51
1:B:583:LEU:HD21	1:B:629:MET:HG3	1.92	0.51
1:B:269:MET:O	1:B:301:ARG:NH1	2.43	0.51
1:A:738:SER:OG	1:A:752:CYS:HB3	2.10	0.51
1:B:156:MET:HB2	1:B:157:LYS:NZ	2.26	0.51
1:B:373:GLU:CG	1:B:377:GLU:HG3	2.41	0.51
1:B:519:THR:OG1	1:B:521:ILE:HG12	2.10	0.51
1:A:868:CYS:HB3	1:A:874:TYR:CD2	2.46	0.50
1:B:141:GLU:HA	1:B:143:ALA:O	2.11	0.50
1:B:864:THR:HG21	1:B:876:LYS:HG2	1.93	0.50
1:B:137:ARG:HH22	1:B:226:ARG:CA	2.25	0.50
1:A:137:ARG:NH2	1:A:142:ASN:HD21	2.09	0.50
1:A:182:LYS:NZ	1:A:310:SER:O	2.45	0.50
1:B:388:ASP:OD1	1:B:389:SER:N	2.45	0.50
1:B:639:GLN:HG2	4:B:1148:HOH:O	2.12	0.49
1:B:908:GLU:O	1:B:908:GLU:HG3	2.12	0.49
1:B:830:ARG:HD2	1:B:836:LEU:HD21	1.93	0.49
1:B:240:LEU:HD21	1:B:736:GLN:HB2	1.93	0.49
1:A:314:ARG:HD3	1:A:564:ILE:HD13	1.95	0.49
1:A:430:PRO:HA	1:A:510:THR:HA	1.94	0.49
1:A:857:GLU:HG2	1:A:868:CYS:SG	2.53	0.49
1:B:662:ALA:HB2	1:B:697:VAL:HG11	1.94	0.49
1:B:137:ARG:NH1	1:B:226:ARG:O	2.44	0.49
1:A:122:VAL:HG13	1:A:201:SER:OG	2.12	0.49
1:B:373:GLU:HG2	1:B:373:GLU:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLU:OE2	1:A:379:TYR:OH	2.30	0.48
1:B:670:TYR:CZ	1:B:723:SER:HB2	2.48	0.48
1:B:433:ASP:O	1:B:437:GLN:HG3	2.13	0.48
1:A:370:MET:HA	1:A:372:HIS:N	2.29	0.48
1:A:576:SER:HB2	1:A:638:PRO:HD3	1.96	0.48
1:A:338:LYS:HG2	1:A:340:LEU:HD11	1.94	0.48
1:B:246:ARG:NH1	1:B:249:ALA:O	2.46	0.48
1:B:239:ARG:HG3	2:D:10:DT:OP1	2.13	0.48
1:B:267:PRO:C	1:B:268:LEU:HD12	2.39	0.48
1:B:333:VAL:HG12	1:B:334:MET:O	2.13	0.48
1:A:765:PRO:HG2	1:A:927:GLU:CG	2.44	0.48
1:B:672:PRO:HG2	1:B:675:LYS:HB2	1.95	0.48
1:A:381:ARG:CG	1:A:384:ARG:HG2	2.42	0.47
1:B:899:LYS:HE3	1:B:904:ALA:O	2.14	0.47
1:A:588:ASP:HB3	1:A:591:ARG:HG2	1.96	0.47
1:B:476:ARG:O	1:B:484:LYS:NZ	2.39	0.47
1:A:830:ARG:HD3	1:A:836:LEU:HD21	1.95	0.47
1:B:107:GLU:O	1:B:111:GLU:HG3	2.14	0.47
1:A:91:ALA:HB2	1:A:902:TYR:CD1	2.48	0.47
1:A:453:TRP:O	1:A:457:MET:HG3	2.15	0.47
1:A:351:TYR:O	1:A:394:LYS:HE3	2.15	0.47
1:B:122:VAL:HB	1:B:201:SER:OG	2.15	0.47
1:A:656:ILE:HG12	1:A:770:ILE:HG21	1.95	0.47
1:A:662:ALA:HB2	1:A:697:VAL:HG11	1.95	0.47
1:B:333:VAL:CG1	1:B:334:MET:N	2.77	0.47
1:B:269:MET:HE1	1:B:275:LEU:HD22	1.95	0.47
1:B:147:LEU:CD1	1:B:151:LYS:HE3	2.45	0.47
1:A:346:LEU:HA	1:A:349:THR:HG22	1.96	0.46
1:B:402:GLY:O	4:B:1102:HOH:O	2.20	0.46
1:A:286:GLU:OE1	1:A:286:GLU:N	2.45	0.46
1:B:412:LEU:O	1:B:416:ILE:HG13	2.15	0.46
1:A:175:VAL:HG11	1:A:315:GLU:HG2	1.97	0.46
1:A:830:ARG:HD2	1:A:836:LEU:HD11	1.97	0.46
1:A:132:LEU:O	1:A:136:GLN:HG3	2.16	0.46
1:A:323:ASN:O	1:A:323:ASN:CG	2.57	0.46
1:B:190:LEU:HD11	1:B:307:ILE:CD1	2.45	0.46
1:A:575:GLU:HG2	1:A:576:SER:N	2.31	0.46
1:B:447:THR:HG22	1:B:449:LYS:N	2.31	0.46
1:B:486:ILE:HD13	1:B:498:ILE:HD13	1.96	0.46
1:B:751:ASN:O	4:B:1103:HOH:O	2.20	0.46
1:A:388:ASP:O	1:A:392:LEU:HG	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:MET:CE	1:A:700:THR:HA	2.42	0.46
1:A:380:LEU:HD13	1:A:396:ARG:HH12	1.76	0.46
1:B:723:SER:CB	1:B:726:THR:HG23	2.46	0.46
1:A:778:ASN:O	1:A:826:VAL:HA	2.16	0.45
1:B:862:GLN:H	1:B:862:GLN:CD	2.25	0.45
1:B:647:SER:HB3	1:B:656:ILE:HG21	1.98	0.45
1:A:340:LEU:HB3	1:A:344:ASP:HB2	1.98	0.45
1:A:315:GLU:OE2	1:A:329:ARG:NH2	2.49	0.45
1:B:669:PHE:CE2	1:B:722:LEU:HD21	2.52	0.45
1:A:380:LEU:HA	1:A:380:LEU:HD23	1.61	0.45
1:B:728:GLN:O	1:B:732:ARG:HG3	2.17	0.45
1:B:899:LYS:HA	1:B:899:LYS:HD2	1.61	0.45
1:A:467:GLN:HG3	1:A:670:TYR:CZ	2.52	0.45
1:B:734:LYS:HB3	1:B:734:LYS:HE2	1.59	0.45
1:A:646:MET:HE3	1:A:646:MET:HB3	1.87	0.45
1:A:778:ASN:HB3	1:A:827:TYR:CZ	2.52	0.45
1:B:409:ILE:HD13	1:B:429:LEU:HD21	1.98	0.45
1:B:341:TYR:OH	1:B:558:GLU:OE2	2.32	0.45
1:A:129:ARG:O	1:A:133:GLU:HG3	2.17	0.44
1:A:822:SER:HB2	1:A:845:PHE:CE1	2.53	0.44
1:B:376:ILE:HG23	1:B:380:LEU:CD1	2.47	0.44
1:A:393:ASP:HA	1:A:396:ARG:NE	2.32	0.44
1:B:500:ASP:OD1	1:B:500:ASP:N	2.50	0.44
1:B:738:SER:OG	1:B:752:CYS:HB3	2.17	0.44
1:B:778:ASN:HB3	1:B:827:TYR:CZ	2.52	0.44
1:A:269:MET:HE1	1:A:275:LEU:HD22	2.00	0.44
1:A:765:PRO:HG2	1:A:927:GLU:HG3	1.99	0.44
1:B:333:VAL:CG1	1:B:334:MET:H	2.30	0.44
1:B:354:GLN:HB3	4:B:1101:HOH:O	2.17	0.44
1:A:588:ASP:CG	1:A:591:ARG:HG2	2.43	0.44
1:B:859:GLY:O	1:B:865:PRO:HA	2.17	0.44
1:A:232:ASN:O	1:A:246:ARG:HG2	2.18	0.44
1:B:696:MET:HE2	1:B:813:VAL:CG1	2.48	0.44
1:B:246:ARG:HD2	1:B:248:ARG:O	2.17	0.44
1:A:283:ARG:NH2	1:A:597:ILE:HG23	2.32	0.44
1:A:830:ARG:CD	1:A:836:LEU:HD11	2.47	0.43
1:A:104:ASN:OD1	1:A:107:GLU:HG2	2.18	0.43
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.77	0.43
1:A:778:ASN:HB3	1:A:827:TYR:CE2	2.54	0.43
1:A:784:LYS:CB	1:A:797:THR:H	2.24	0.43
1:B:646:MET:HE3	1:B:646:MET:HB3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:THR:HA	1:A:254:CYS:O	2.19	0.43
1:B:381:ARG:HG3	1:B:384:ARG:NH1	2.29	0.43
1:B:847:MET:O	1:B:851:ILE:HG13	2.18	0.43
1:B:186:VAL:CB	1:B:309:MET:HE1	2.48	0.43
1:A:147:LEU:HD23	1:A:147:LEU:O	2.19	0.43
1:B:164:GLN:O	1:B:168:GLU:HG3	2.19	0.43
1:B:609:VAL:O	1:B:613:LYS:HG3	2.17	0.43
1:B:693:ASP:OD1	1:B:813:VAL:HG13	2.19	0.43
1:B:868:CYS:HB3	1:B:874:TYR:CD2	2.53	0.43
1:B:642:LYS:O	1:B:646:MET:HG2	2.19	0.43
1:B:655:PRO:HB3	1:B:698:HIS:CD2	2.54	0.43
1:B:74:ASP:O	1:B:77:ARG:HG2	2.19	0.43
1:A:678:ARG:HG2	1:A:721:PHE:HE2	1.83	0.43
1:B:156:MET:HB2	1:B:157:LYS:HZ2	1.81	0.42
1:B:640:MET:HE3	1:B:640:MET:HB2	1.82	0.42
1:B:832:LYS:HA	1:B:835:ASP:O	2.19	0.42
1:A:134:LEU:HD23	1:A:134:LEU:C	2.43	0.42
1:B:137:ARG:HH22	1:B:226:ARG:HB3	1.84	0.42
1:A:265:SER:HB3	2:C:10:DT:H3	1.85	0.42
1:B:94:GLN:HE21	1:B:94:GLN:HB3	1.60	0.42
1:A:338:LYS:HE2	1:A:340:LEU:HD11	2.00	0.42
1:A:602:PRO:HA	1:A:605:ILE:HD12	2.00	0.42
1:B:467:GLN:HG3	1:B:471:GLN:OE1	2.20	0.42
1:B:922:LEU:HD23	1:B:922:LEU:HA	1.79	0.42
1:A:145:LYS:NZ	1:A:148:GLU:OE1	2.41	0.42
1:B:624:LEU:HD21	1:B:629:MET:HB2	2.00	0.42
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.83	0.42
1:A:207:CYS:O	1:A:253:TYR:HA	2.18	0.42
1:B:68:VAL:HG13	1:B:918:ALA:HB1	2.02	0.42
1:A:369:ARG:NE	1:A:369:ARG:HA	2.35	0.41
1:B:499:ASP:O	1:B:544:VAL:HG13	2.21	0.41
1:B:351:TYR:O	1:B:394:LYS:NZ	2.53	0.41
1:A:137:ARG:O	1:A:137:ARG:HG2	2.20	0.41
1:B:686:MET:CE	1:B:700:THR:HA	2.51	0.41
1:A:497:THR:HG23	1:A:540:ARG:NH1	2.35	0.41
1:A:143:ALA:O	1:A:144:LYS:HB3	2.21	0.41
1:A:186:VAL:HB	1:A:309:MET:HE1	2.03	0.41
1:B:137:ARG:CZ	1:B:226:ARG:O	2.69	0.41
1:B:147:LEU:HD13	1:B:151:LYS:HE3	2.03	0.41
1:B:839:LEU:HD23	1:B:839:LEU:HA	1.76	0.41
1:A:438:LEU:HG	1:A:487:ILE:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:O	1:B:147:LEU:HD22	2.21	0.41
1:A:850:ILE:HG21	1:A:867:LEU:HD21	2.03	0.40
1:A:289:LEU:HA	1:A:289:LEU:HD12	1.82	0.40
1:B:499:ASP:OD2	1:B:543:ARG:NH1	2.55	0.40
1:A:484:LYS:HD3	1:A:486:ILE:HD11	2.03	0.40
1:A:665:PHE:CD1	1:A:665:PHE:C	2.97	0.40
1:B:289:LEU:HD12	1:B:289:LEU:HA	1.84	0.40
1:B:463:HIS:CB	1:B:466:MET:HE3	2.51	0.40
1:A:145:LYS:HA	1:A:145:LYS:HD2	1.82	0.40
1:A:640:MET:HB2	1:A:640:MET:HE3	1.89	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:GLU:OE2	1:A:714:ARG:NH2[1_565]	2.04	0.16
1:A:390:ARG:NH2	1:B:367:GLU:OE2[3_555]	2.08	0.12
1:A:396:ARG:NE	1:B:369:ARG:NH1[3_555]	2.15	0.05

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	841/944 (89%)	825 (98%)	16 (2%)	0	100	100
1	B	843/944 (89%)	832 (99%)	11 (1%)	0	100	100
All	All	1684/1888 (89%)	1657 (98%)	27 (2%)	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	757/842 (90%)	754 (100%)	3 (0%)	84	92
1	B	759/842 (90%)	754 (99%)	5 (1%)	76	89
All	All	1516/1684 (90%)	1508 (100%)	8 (0%)	81	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	SER
1	A	284	SER
1	A	384	ARG
1	B	337	VAL
1	B	394	LYS
1	B	726	THR
1	B	785	SER
1	B	831	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	164	GLN
1	A	169	ASN
1	A	232	ASN
1	A	323	ASN
1	A	324	ASN
1	B	95	GLN
1	B	169	ASN
1	B	232	ASN
1	B	237	GLN
1	B	271	ASN
1	B	324	ASN
1	B	437	GLN
1	B	451	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	535	GLN
1	B	807	ASN
1	B	829	GLN
1	B	891	ASN

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 2 ligands modelled in this entry, 2 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	849/944 (89%)	-0.13	9 (1%) 78 76	30, 54, 95, 123	0
1	B	851/944 (90%)	-0.20	9 (1%) 78 76	30, 52, 91, 161	0
2	C	10/10 (100%)	-0.12	1 (10%) 12 11	42, 67, 95, 104	0
2	D	10/10 (100%)	-0.15	1 (10%) 12 11	41, 58, 96, 115	0
All	All	1720/1908 (90%)	-0.17	20 (1%) 76 75	30, 53, 93, 161	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	929	LEU	4.0
2	D	11	DT	3.5
1	A	79	PRO	3.5
1	B	929	LEU	3.4
1	B	928	ARG	2.8
1	A	355	LYS	2.8
1	B	142	ASN	2.7
1	A	370	MET	2.7
1	B	143	ALA	2.6
1	A	396	ARG	2.5
1	B	141	GLU	2.4
1	B	365	PRO	2.4
1	A	144	LYS	2.4
1	B	366	PRO	2.4
1	B	819	GLY	2.4
1	A	381	ARG	2.3
2	C	11	DT	2.2
1	A	139	LEU	2.2
1	B	144	LYS	2.1
1	A	521	ILE	2.1

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
3	MG	B	1001	1/1	0.89	0.31	76,76,76,76	0
3	MG	A	1001	1/1	0.94	0.12	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.