



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:31 PM UTC

PDB ID : 7ZJS / pdb_00007zjs
Title : Structural basis of centromeric cohesion protection by SGO1
Authors : Patel, A.; Panne, D.
Deposited on : 2022-04-11
Resolution : 3.24 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

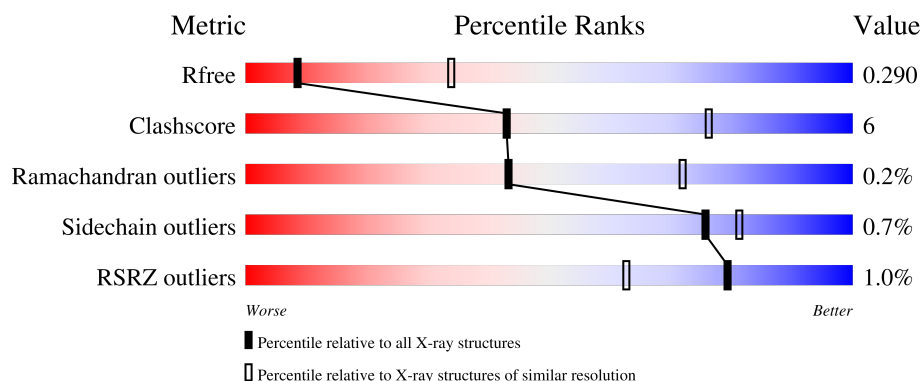
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	1231	65% 10% 25%
1	C	1231	% 59% 13% 28%
2	B	631	10% 88%
2	D	631	11% 88%
3	E	11	100%

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Mol	Chain	Length	Quality of chain
3	F	11	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32423 atoms, of which 16202 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 Cohesin subunit SA-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	929	Total	C	H	N	O	S	0	0	0
			15102	4813	7544	1261	1429	55			
1	C	891	Total	C	H	N	O	S	0	0	0
			14480	4615	7236	1206	1372	51			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	545	ARG	LYS	conflict	UNP Q8N3U4
A	546	LYS	ARG	conflict	UNP Q8N3U4
C	545	ARG	LYS	conflict	UNP Q8N3U4
C	546	LYS	ARG	conflict	UNP Q8N3U4

- Molecule 2 is a protein called Double-strand-break repair protein rad21 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	74	Total	C	H	N	O	S	0	0	0
			1235	385	639	101	107	3			
2	D	74	Total	C	H	N	O	S	0	0	0
			1235	385	639	101	107	3			

- Molecule 3 is a protein called Shugoshin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	11	Total	C	H	N	O	0	0	0
			164	56	72	14	22			
3	F	11	Total	C	H	N	O	0	0	0
			164	56	72	14	22			

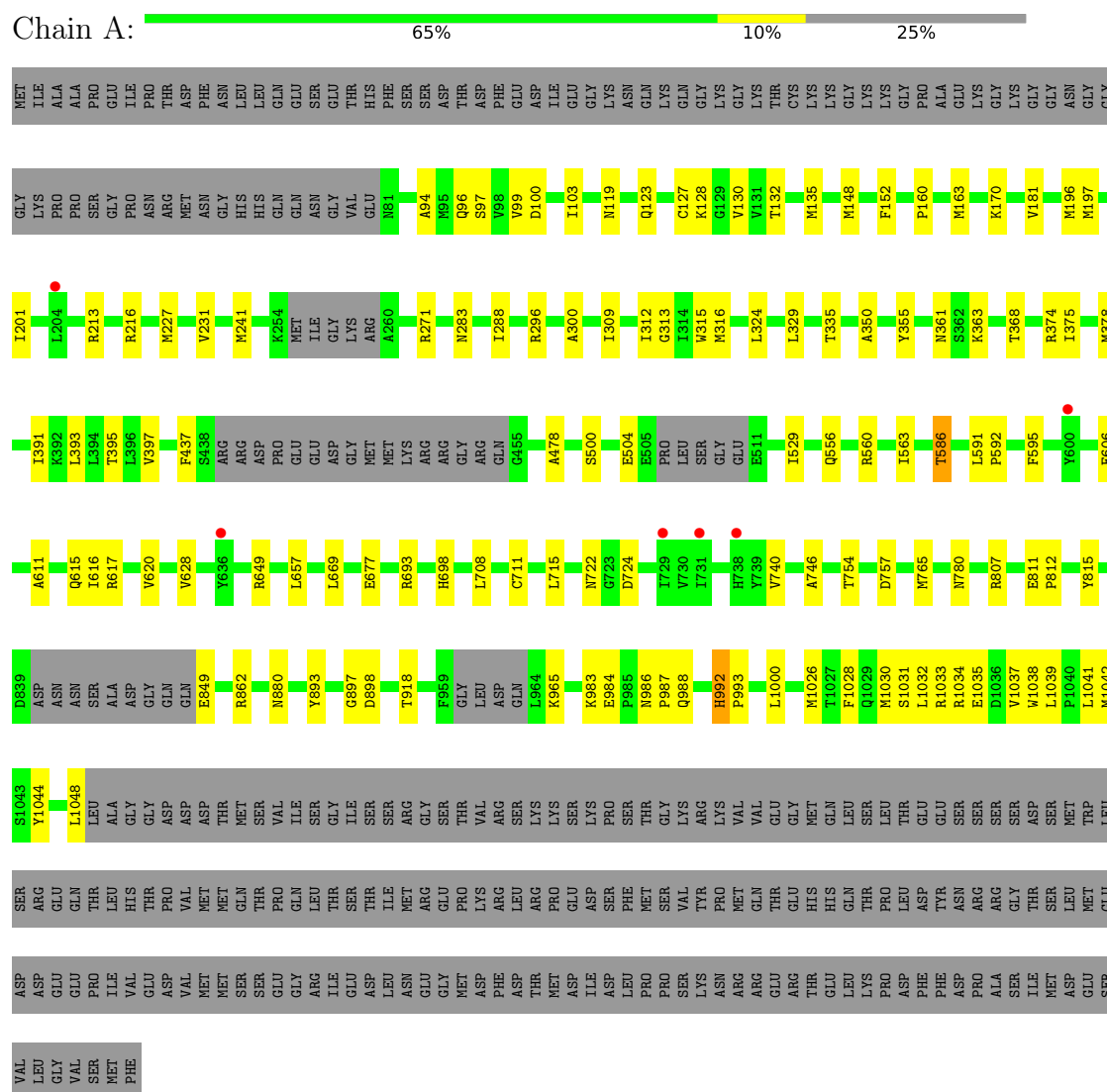
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	1	Total 1	O 1	0	0
4	C	32	Total 32	O 32	0	0
4	D	3	Total 3	O 3	0	0

3 Residue-property plots

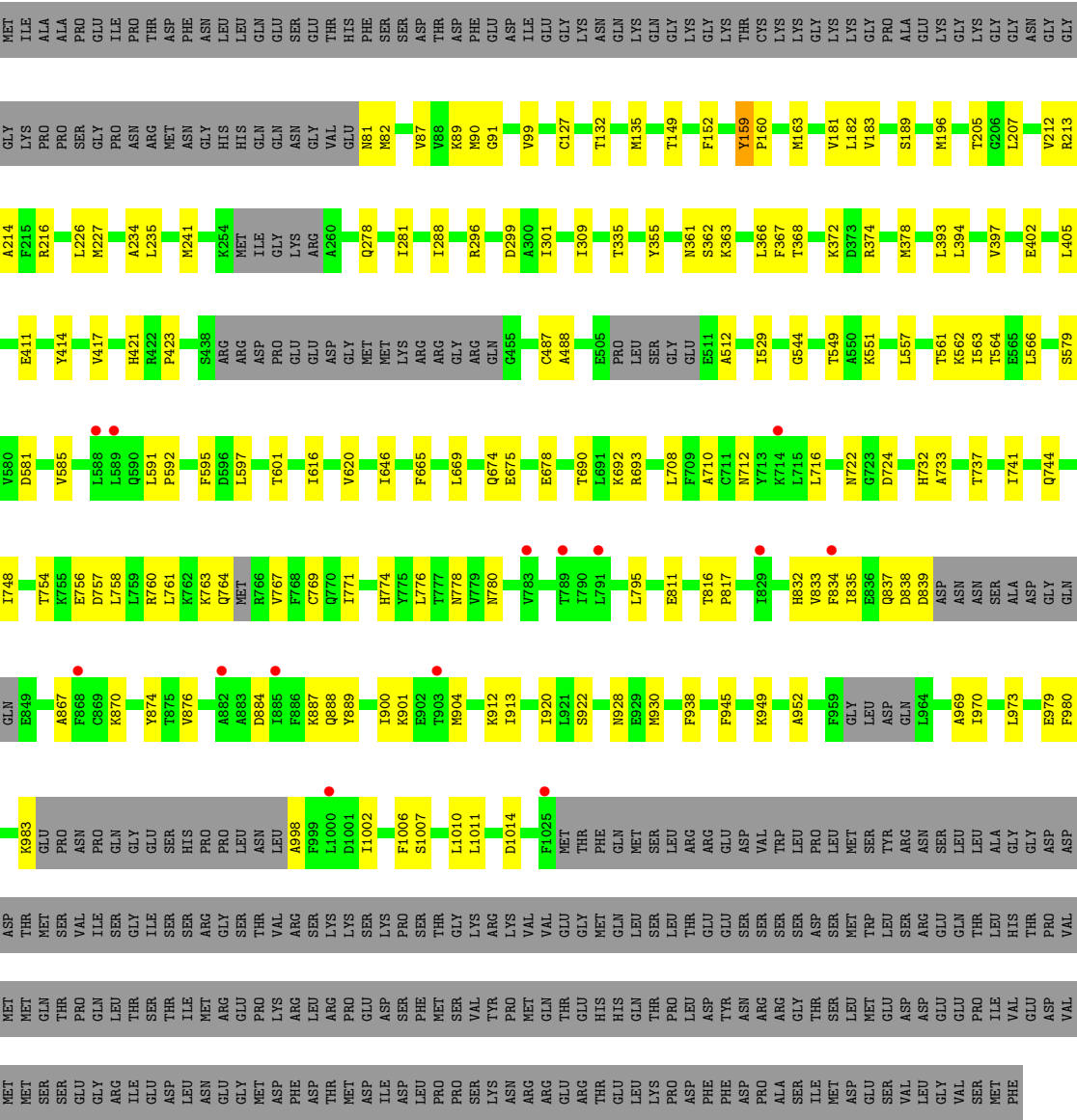
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cohesin subunit SA-2

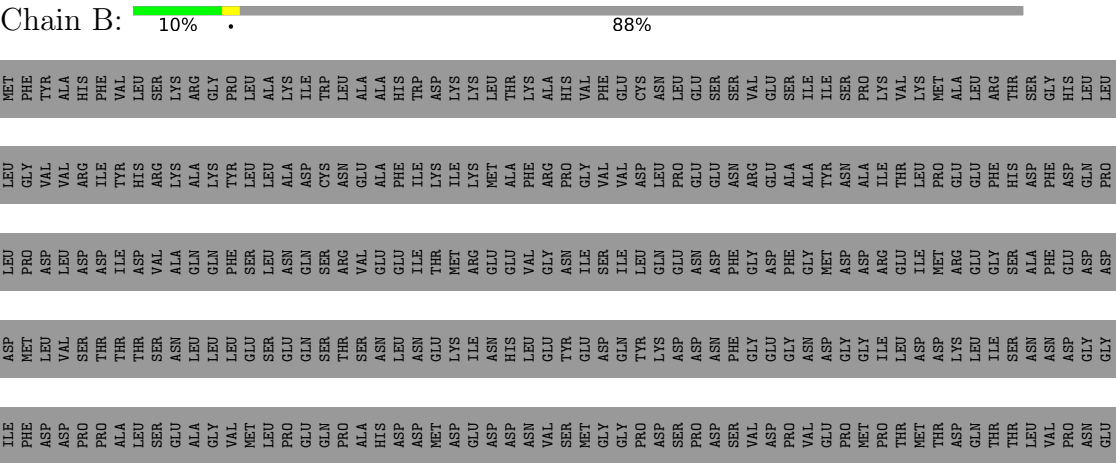


• Molecule 1: Cohesin subunit SA-2





● Molecule 2: Double-strand-break repair protein rad21 homolog



Chain F:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.81Å 181.10Å 111.37Å 90.00° 94.25° 90.00°	Depositor
Resolution (Å)	47.87 – 3.24 47.87 – 3.24	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.87-3.24) 97.8 (47.87-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.269 , 0.289 0.269 , 0.290	Depositor DCC
R_{free} test set	2422 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	108.4	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32423	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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

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	0.34	1/7690 (0.0%)	0.54	8/10366 (0.1%)
1	C	0.46	2/7364 (0.0%)	0.66	8/9919 (0.1%)
2	B	0.57	1/606 (0.2%)	0.83	1/818 (0.1%)
2	D	0.27	0/606	0.46	0/818
3	E	0.12	0/93	0.30	0/125
3	F	1.23	0/93	1.43	0/125
All	All	0.42	4/16452 (0.0%)	0.61	17/22171 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	ARG	C-O	-8.13	1.14	1.23
1	C	159	TYR	C-O	-6.43	1.17	1.24
1	C	216	ARG	C-O	-6.31	1.16	1.24
2	B	355	PRO	C-O	-5.34	1.18	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	LEU	N-CA-C	-6.45	103.76	111.69
1	A	628	VAL	N-CA-C	-5.91	104.75	110.42
1	C	832	HIS	CA-C-O	-5.76	115.84	121.02
1	C	544	GLY	CA-C-O	-5.72	117.06	122.39
1	A	231	VAL	N-CA-C	-5.56	104.94	111.00
1	C	769	CYS	N-CA-C	-5.54	105.32	111.36
1	A	300	ALA	N-CA-C	-5.40	106.86	113.50
1	A	288	ILE	N-CA-C	-5.36	105.51	113.39
1	C	771	ILE	N-CA-C	-5.33	105.19	110.62
1	C	288	ILE	N-CA-C	-5.28	105.29	113.16
1	C	207	LEU	N-CA-C	-5.28	105.70	111.82
1	A	586	THR	N-CA-C	-5.24	105.57	111.28
1	A	201	ILE	N-CA-C	-5.21	105.42	110.42
1	C	205	THR	N-CA-C	-5.20	106.44	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	ASN	N-CA-C	-5.17	105.53	111.07
1	A	227	MET	N-CA-C	-5.13	105.58	111.07
2	B	360	LEU	N-CA-C	-5.12	105.78	111.36

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	7558	7544	7544	86	1
1	C	7244	7236	7236	101	1
2	B	596	639	639	9	0
2	D	596	639	639	11	0
3	E	92	72	72	0	0
3	F	92	72	72	0	0
4	A	7	0	0	1	0
4	B	1	0	0	0	0
4	C	32	0	0	11	0
4	D	3	0	0	0	0
All	All	16221	16202	16202	200	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (200) 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:C:213:ARG:NE	4:C:1301:HOH:O	1.64	1.24
4:C:1301:HOH:O	2:D:325:ILE:CG2	2.08	1.01
4:C:1301:HOH:O	2:D:325:ILE:HG22	1.66	0.94
1:C:748:ILE:HD13	1:C:761:LEU:HD22	1.56	0.87
1:A:1039:LEU:HA	1:A:1042:MET:HE2	1.66	0.78
1:C:394:LEU:HD22	1:C:405:LEU:HD21	1.67	0.77
1:C:213:ARG:HB2	4:C:1301:HOH:O	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ARG:CB	4:C:1301:HOH:O	2.35	0.74
4:C:1301:HOH:O	2:D:325:ILE:HG21	1.79	0.73
2:B:387:LYS:O	2:B:391:ARG:HG3	1.90	0.70
1:C:952:ALA:HB1	1:C:1002:ILE:HD11	1.75	0.68
1:A:746:ALA:HB2	2:B:388:LEU:HD11	1.76	0.68
1:A:807:ARG:HD3	2:B:391:ARG:NH1	2.08	0.68
1:C:355:TYR:OH	1:C:368:THR:HG21	1.92	0.68
1:A:993:PRO:HG3	1:A:1037:VAL:HG11	1.76	0.68
1:C:888:GLN:N	1:C:888:GLN:OE1	2.27	0.67
1:C:744:GLN:C	1:C:748:ILE:HD12	2.19	0.67
1:A:119:ASN:HB3	1:A:123:GLN:NE2	2.09	0.67
1:A:355:TYR:OH	1:A:368:THR:HG21	1.94	0.67
1:A:374:ARG:HG3	1:A:378:MET:HE2	1.76	0.66
1:C:213:ARG:CD	4:C:1301:HOH:O	2.23	0.66
1:C:361:ASN:OD1	1:C:363:LYS:N	2.30	0.65
1:C:674:GLN:OE1	1:C:675:GLU:OE1	2.13	0.65
1:C:887:LYS:C	1:C:888:GLN:OE1	2.39	0.65
1:A:620:VAL:O	1:A:693:ARG:NE	2.30	0.64
1:C:744:GLN:O	1:C:748:ILE:HD12	1.98	0.64
1:A:119:ASN:HB3	1:A:123:GLN:HE22	1.63	0.64
1:C:296:ARG:NH1	1:C:299:ASP:OD2	2.31	0.63
1:C:970:ILE:HD12	1:C:1006:PHE:CD2	2.33	0.63
1:A:361:ASN:OD1	1:A:363:LYS:N	2.33	0.61
1:C:620:VAL:O	1:C:693:ARG:NE	2.34	0.61
1:C:708:LEU:O	1:C:712:ASN:ND2	2.33	0.60
1:A:617:ARG:HD2	1:A:657:LEU:HD13	1.84	0.60
1:C:402:GLU:OE1	1:C:402:GLU:N	2.35	0.60
1:C:887:LYS:HG2	1:C:888:GLN:OE1	2.02	0.59
2:D:333:ASP:N	2:D:333:ASP:OD1	2.35	0.59
1:A:862:ARG:NH2	1:A:898:ASP:OD2	2.36	0.59
1:C:597:LEU:HB3	1:C:646:ILE:HD11	1.85	0.59
1:C:737:THR:O	1:C:741:ILE:HD13	2.02	0.59
1:C:1007:SER:HA	1:C:1010:LEU:HB2	1.85	0.59
1:C:309:ILE:HG13	1:C:335:THR:HG21	1.85	0.58
1:C:374:ARG:HG3	1:C:378:MET:HE2	1.84	0.58
1:C:710:ALA:N	4:C:1302:HOH:O	2.37	0.58
1:C:1011:LEU:HB2	1:C:1014:ASP:OD1	2.04	0.57
1:C:87:VAL:O	1:C:91:GLY:N	2.38	0.56
1:A:1039:LEU:HA	1:A:1042:MET:CE	2.32	0.56
2:B:354:ALA:O	2:B:355:PRO:C	2.46	0.56
1:A:807:ARG:HD3	2:B:391:ARG:HH12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ILE:HG13	1:A:335:THR:HG21	1.88	0.56
1:C:913:ILE:HG22	1:C:969:ALA:HA	1.87	0.55
1:A:393:LEU:O	1:A:397:VAL:HG23	2.07	0.55
1:C:579:SER:N	4:C:1303:HOH:O	2.39	0.55
1:A:316:MET:HE1	1:A:329:LEU:HD23	1.88	0.55
1:A:592:PRO:HA	1:A:595:PHE:CD2	2.42	0.55
1:A:992:HIS:CG	1:A:993:PRO:HD2	2.41	0.54
1:C:920:ILE:CG1	1:C:973:LEU:HG	2.37	0.54
2:D:337:ILE:H	2:D:337:ILE:HD12	1.73	0.54
1:C:1006:PHE:O	1:C:1010:LEU:N	2.39	0.53
1:A:395:THR:HG21	4:A:1303:HOH:O	2.09	0.53
1:A:160:PRO:HA	1:A:163:MET:HE2	1.91	0.53
1:A:669:LEU:CD2	1:A:715:LEU:HD11	2.39	0.52
1:C:592:PRO:HA	1:C:595:PHE:CD2	2.44	0.52
1:A:983:LYS:HG3	1:A:984:GLU:OE2	2.10	0.51
1:C:901:LYS:O	1:C:904:MET:HG2	2.10	0.51
1:A:1026:MET:HA	1:A:1030:MET:HE2	1.93	0.51
1:C:678:GLU:O	1:C:678:GLU:HG2	2.09	0.51
1:C:867:ALA:HA	1:C:870:LYS:HE2	1.93	0.51
1:C:920:ILE:HD11	1:C:973:LEU:HD21	1.93	0.50
1:A:754:THR:HG23	1:A:757:ASP:CB	2.42	0.50
1:A:170:LYS:O	1:A:170:LYS:HD3	2.12	0.50
1:C:690:THR:HG22	4:C:1326:HOH:O	2.12	0.50
1:C:887:LYS:CG	1:C:888:GLN:OE1	2.59	0.50
1:A:1031:SER:O	1:A:1034:ARG:NH1	2.45	0.50
1:A:1000:LEU:HD22	1:A:1044:TYR:CD2	2.48	0.49
1:C:748:ILE:O	1:C:748:ILE:HG22	2.12	0.49
1:C:887:LYS:HB3	1:C:922:SER:HB3	1.95	0.49
2:D:333:ASP:OD1	2:D:336:THR:HG23	2.13	0.49
1:A:99:VAL:HG21	1:A:181:VAL:HG12	1.92	0.49
1:A:500:SER:HA	1:A:504:GLU:OE1	2.12	0.49
1:A:606:GLU:OE1	1:A:606:GLU:N	2.45	0.49
1:A:754:THR:HG23	1:A:757:ASP:HB2	1.94	0.49
1:A:529:ILE:HG23	1:A:563:ILE:HD13	1.93	0.49
1:C:838:ASP:O	1:C:839:ASP:C	2.57	0.48
1:C:81:ASN:O	1:C:82:MET:HG3	2.13	0.48
1:C:149:THR:HG23	1:C:212:VAL:HG21	1.95	0.48
1:A:1038:TRP:HE3	1:A:1041:LEU:HD12	1.78	0.47
1:C:616:ILE:O	1:C:620:VAL:HG23	2.14	0.47
1:C:748:ILE:HG23	1:C:758:LEU:HD11	1.94	0.47
1:C:874:TYR:CE1	2:D:393:LEU:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:HIS:NE2	1:A:740:VAL:HG22	2.29	0.47
1:A:780:ASN:OD1	1:A:780:ASN:C	2.58	0.47
1:C:692:LYS:HG2	1:C:732:HIS:NE2	2.29	0.47
2:D:333:ASP:O	2:D:337:ILE:HD12	2.14	0.47
1:A:127:CYS:O	1:A:128:LYS:HB2	2.13	0.47
1:A:1033:ARG:NH1	1:A:1035:GLU:OE2	2.47	0.47
1:C:756:GLU:HG3	1:C:757:ASP:N	2.29	0.47
1:C:564:THR:HA	1:C:595:PHE:CD1	2.50	0.47
1:A:94:ALA:O	1:A:97:SER:N	2.41	0.47
1:C:393:LEU:O	1:C:397:VAL:HG23	2.15	0.46
1:C:562:LYS:O	1:C:566:LEU:HD13	2.16	0.46
1:C:884:ASP:O	1:C:888:GLN:OE1	2.33	0.46
1:A:616:ILE:O	1:A:620:VAL:HG23	2.16	0.46
1:C:760:ARG:O	1:C:764:GLN:N	2.49	0.46
1:A:983:LYS:O	1:A:983:LYS:HD2	2.16	0.45
1:A:606:GLU:HG2	1:A:649:ARG:NH2	2.31	0.45
1:A:708:LEU:HD23	1:A:711:CYS:SG	2.56	0.45
1:C:89:LYS:HE2	1:C:90:MET:CE	2.46	0.45
1:C:581:ASP:O	1:C:585:VAL:HG22	2.16	0.45
1:C:716:LEU:HD21	1:C:733:ALA:HB3	1.98	0.45
1:A:965:LYS:O	1:A:965:LYS:HG3	2.17	0.45
1:C:362:SER:O	1:C:366:LEU:HD23	2.17	0.45
1:A:677:GLU:O	1:A:677:GLU:HG3	2.16	0.45
1:A:992:HIS:ND1	1:A:993:PRO:HD2	2.32	0.45
1:C:811:GLU:HG3	4:C:1317:HOH:O	2.16	0.44
1:C:1010:LEU:CD2	1:C:1014:ASP:OD2	2.65	0.44
2:D:346:ASP:OD1	2:D:346:ASP:N	2.46	0.44
1:A:241:MET:HE3	1:A:271:ARG:HG3	1.99	0.44
1:A:722:ASN:HB2	1:A:724:ASP:OD1	2.17	0.44
1:C:234:ALA:HB2	1:C:281:ILE:HG21	2.00	0.44
1:C:368:THR:O	1:C:372:LYS:HB2	2.16	0.44
1:A:375:ILE:HA	1:A:378:MET:HE3	1.99	0.44
1:A:669:LEU:HD21	1:A:715:LEU:HD11	1.99	0.44
1:A:1032:LEU:C	1:A:1034:ARG:NH1	2.75	0.44
1:C:665:PHE:O	1:C:669:LEU:HG	2.17	0.44
1:A:119:ASN:C	1:A:123:GLN:NE2	2.76	0.44
1:A:986:ASN:HB2	1:A:993:PRO:O	2.17	0.44
1:C:299:ASP:OD1	1:C:301:ILE:N	2.51	0.44
1:C:1010:LEU:HD22	1:C:1014:ASP:OD2	2.17	0.44
1:A:324:LEU:HD23	1:A:324:LEU:C	2.43	0.44
1:C:414:TYR:O	1:C:417:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:928:ASN:OD1	1:C:980:PHE:HZ	2.01	0.44
1:C:421:HIS:CE1	1:C:423:PRO:HG2	2.53	0.43
1:C:795:LEU:HD22	1:C:817:PRO:HG3	1.99	0.43
1:C:876:VAL:HG12	1:C:876:VAL:O	2.18	0.43
2:D:334:SER:HA	2:D:337:ILE:HD13	1.99	0.43
1:A:316:MET:CE	1:A:329:LEU:HD23	2.47	0.43
1:A:391:ILE:O	1:A:395:THR:HG23	2.18	0.43
1:C:778:ASN:ND2	1:C:780:ASN:HB3	2.33	0.43
1:A:127:CYS:O	1:A:152:PHE:HA	2.17	0.43
1:A:130:VAL:N	1:A:148:MET:HE1	2.33	0.43
1:A:811:GLU:N	1:A:812:PRO:HD2	2.33	0.43
1:A:880:ASN:HA	1:A:918:THR:HG22	1.99	0.43
1:A:1032:LEU:HA	1:A:1034:ARG:HH12	1.83	0.43
1:C:132:THR:OG1	1:C:135:MET:HG3	2.18	0.43
1:C:557:LEU:O	1:C:561:THR:HG23	2.19	0.43
1:C:591:LEU:N	1:C:592:PRO:CD	2.82	0.43
1:A:96:GLN:NE2	1:A:100:ASP:OD2	2.52	0.43
1:A:754:THR:CG2	1:A:757:ASP:HB2	2.49	0.43
1:A:987:PRO:HB2	1:A:988:GLN:OE1	2.19	0.43
2:D:333:ASP:OD1	2:D:336:THR:CG2	2.66	0.43
1:A:119:ASN:O	1:A:123:GLN:NE2	2.52	0.42
1:C:99:VAL:HG21	1:C:181:VAL:HG12	1.99	0.42
1:C:487:CYS:SG	1:C:488:ALA:N	2.92	0.42
1:C:912:LYS:O	1:C:912:LYS:HD2	2.19	0.42
1:C:601:THR:CG2	1:C:646:ILE:HG23	2.49	0.42
1:A:765:MET:HE1	1:A:815:TYR:HB2	2.02	0.42
1:C:930:MET:HE3	1:C:930:MET:HB3	1.97	0.42
1:A:478:ALA:HB3	2:B:361:MET:HE1	2.02	0.42
1:C:182:LEU:HD11	1:C:196:MET:HE1	2.01	0.42
1:C:754:THR:O	1:C:758:LEU:HD13	2.19	0.42
1:A:335:THR:HG22	1:A:335:THR:O	2.20	0.42
1:A:132:THR:OG1	1:A:135:MET:HG3	2.19	0.42
1:A:1044:TYR:O	1:A:1048:LEU:HD12	2.20	0.42
1:C:127:CYS:O	1:C:152:PHE:HA	2.18	0.42
1:C:763:LYS:O	1:C:763:LYS:HD2	2.20	0.42
1:C:159:TYR:O	1:C:163:MET:SD	2.77	0.42
1:C:741:ILE:HD12	1:C:741:ILE:N	2.35	0.42
1:C:183:VAL:HG21	1:C:226:LEU:CD1	2.49	0.42
1:C:241:MET:CE	1:C:278:GLN:OE1	2.68	0.42
1:A:591:LEU:N	1:A:592:PRO:CD	2.82	0.42
1:A:893:TYR:O	1:A:897:GLY:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:PHE:CD1	1:C:367:PHE:C	2.98	0.42
1:C:529:ILE:HG23	1:C:563:ILE:HD13	2.02	0.41
1:A:669:LEU:HD22	1:A:715:LEU:HD11	2.00	0.41
1:C:1014:ASP:OD1	1:C:1014:ASP:N	2.42	0.41
1:A:437:PHE:N	1:A:437:PHE:CD1	2.88	0.41
2:B:322:ARG:NH2	2:B:324:LEU:HD22	2.35	0.41
1:C:737:THR:HG22	1:C:741:ILE:CD1	2.49	0.41
1:A:324:LEU:HD22	1:A:361:ASN:ND2	2.35	0.41
1:C:722:ASN:HB2	1:C:724:ASP:OD1	2.20	0.41
1:C:949:LYS:HG2	1:C:998:ALA:HB2	2.02	0.41
1:C:979:GLU:O	1:C:983:LYS:HB2	2.21	0.41
1:C:889:TYR:HB2	1:C:900:ILE:HG21	2.01	0.41
1:A:213:ARG:NH2	2:B:327:ASP:OD1	2.47	0.41
1:C:549:THR:HG22	1:C:551:LYS:H	1.86	0.41
1:A:196:MET:HE2	1:A:197:MET:HE3	2.02	0.41
1:A:312:ILE:HA	1:A:315:TRP:CE3	2.56	0.41
1:A:313:GLY:HA3	1:A:350:ALA:HB1	2.01	0.41
1:A:849:GLU:OE2	1:C:512:ALA:HB3	2.20	0.41
1:C:411:GLU:HA	1:C:414:TYR:CD2	2.56	0.41
1:C:213:ARG:O	1:C:214:ALA:C	2.64	0.41
1:A:99:VAL:O	1:A:103:ILE:HG13	2.21	0.40
1:A:1032:LEU:C	1:A:1034:ARG:HH12	2.28	0.40
1:A:1032:LEU:CA	1:A:1034:ARG:HH12	2.34	0.40
2:B:346:ASP:OD1	2:B:346:ASP:N	2.51	0.40
1:C:938:PHE:CZ	1:C:945:PHE:CZ	3.09	0.40
1:A:724:ASP:OD1	1:A:724:ASP:O	2.39	0.40
1:A:556:GLN:O	1:A:560:ARG:HG3	2.22	0.40
1:A:611:ALA:O	1:A:615:GLN:HG2	2.21	0.40
1:C:763:LYS:HD2	1:C:767:VAL:CG2	2.51	0.40

All (1) 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:1028:PHE:CE1	1:C:774:HIS:NE2[2_455]	2.12	0.08

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	917/1231 (74%)	887 (97%)	30 (3%)	0	100	100
1	C	875/1231 (71%)	847 (97%)	25 (3%)	3 (0%)	36	66
2	B	72/631 (11%)	69 (96%)	3 (4%)	0	100	100
2	D	72/631 (11%)	72 (100%)	0	0	100	100
3	E	9/11 (82%)	7 (78%)	2 (22%)	0	100	100
3	F	9/11 (82%)	7 (78%)	2 (22%)	0	100	100
All	All	1954/3746 (52%)	1889 (97%)	62 (3%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	833	VAL
1	C	189	SER
1	C	835	ILE

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	840/1106 (76%)	837 (100%)	3 (0%)	84	85
1	C	803/1106 (73%)	797 (99%)	6 (1%)	76	81
2	B	69/566 (12%)	66 (96%)	3 (4%)	26	56
2	D	69/566 (12%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	10/10 (100%)	10 (100%)	0	100	100
3	F	10/10 (100%)	10 (100%)	0	100	100
All	All	1801/3364 (54%)	1789 (99%)	12 (1%)	76	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	ARG
1	A	586	THR
1	A	992	HIS
2	B	334	SER
2	B	355	PRO
2	B	363	TRP
1	C	160	PRO
1	C	227	MET
1	C	776	LEU
1	C	816	THR
1	C	834	PHE
1	C	837	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	185	GLN
1	A	357	ASN
1	A	573	GLN
1	A	656	GLN
1	A	674	GLN
1	A	837	GLN
1	A	859	HIS
1	A	863	ASN
1	A	937	ASN
1	A	1046	ASN
2	B	340	GLN
1	C	138	HIS
1	C	421	HIS
1	C	770	GLN
1	C	786	GLN
1	C	800	HIS

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](#)

There are no ligands in this entry.

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	929/1231 (75%)	-0.10	6 (0%) 85 73	73, 149, 203, 234	0
1	C	891/1231 (72%)	0.02	14 (1%) 70 51	75, 139, 236, 379	0
2	B	74/631 (11%)	-0.15	0 100 100	74, 123, 181, 194	0
2	D	74/631 (11%)	-0.16	0 100 100	81, 116, 151, 182	0
3	E	11/11 (100%)	0.46	0 100 100	101, 128, 169, 172	0
3	F	11/11 (100%)	0.45	0 100 100	119, 130, 149, 159	0
All	All	1990/3746 (53%)	-0.04	20 (1%) 79 63	73, 141, 216, 379	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	885	ILE	5.8
1	C	882	ALA	4.8
1	A	600	TYR	3.3
1	C	868	PHE	3.0
1	C	834	PHE	2.9
1	C	789	THR	2.7
1	A	738	HIS	2.6
1	C	1025	PHE	2.5
1	C	714	LYS	2.4
1	C	588	LEU	2.3
1	A	636	TYR	2.3
1	A	731	ILE	2.2
1	C	903	THR	2.2
1	A	729	ILE	2.2
1	C	589	LEU	2.2
1	C	783	VAL	2.1
1	C	791	LEU	2.1
1	A	204	LEU	2.1
1	C	829	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	1000	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.