



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:06 AM UTC

PDB ID : 6H8Q / pdb_00006h8q
Title : Structural basis for Scc3-dependent cohesin recruitment to chromatin
Authors : Li, Y.; Muir, K.; Panne, D.
Deposited on : 2018-08-03
Resolution : 3.63 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:

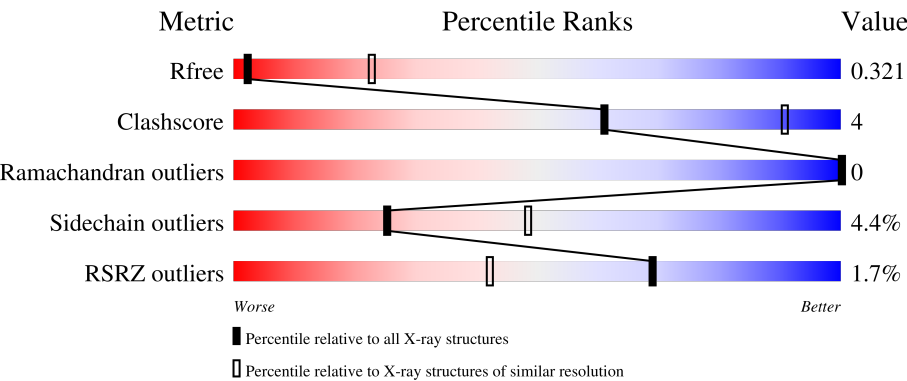
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.63 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	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)

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	1150	% 65%11%24%
1	B	1150	2% 65%10%24%
2	G	100	% 26%70%
2	H	100	% 21%6%73%
3	E	19	63%37%

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Mol	Chain	Length	Quality of chain
4	F	19	 89%11%
5	C	19	 42%58%
6	D	19	 79%21%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16363 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 Cohesin subunit SCC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	879	Total	C	N	O	S	0	0	0
			7182	4657	1161	1340	24			
1	B	873	Total	C	N	O	S	0	0	0
			7149	4639	1156	1330	24			

- Molecule 2 is a protein called Sister chromatid cohesion protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	30	Total	C	N	O	S	0	0	0
			248	162	38	47	1			
2	H	27	Total	C	N	O	S	0	0	0
			226	149	34	42	1			

- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*TP*TP*TP*CP*GP*TP*TP*TP*CP*CP*TP*TP*GP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	19	Total	C	N	O	P	0	0	0
			393	187	77	110	19			

- Molecule 4 is a DNA chain called DNA (5'-D(P*CP*TP*TP*TP*TP*CP*GP*TP*TP*TP*CP*CP*TP*TP*GP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	19	Total	C	N	O	P	0	0	0
			386	186	63	118	19			

- Molecule 5 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*CP*AP*AP*GP*GP*AP*AP*AP*CP*GP*AP*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	19	Total	C	N	O	P	0	0	0
			394	188	76	111	19			

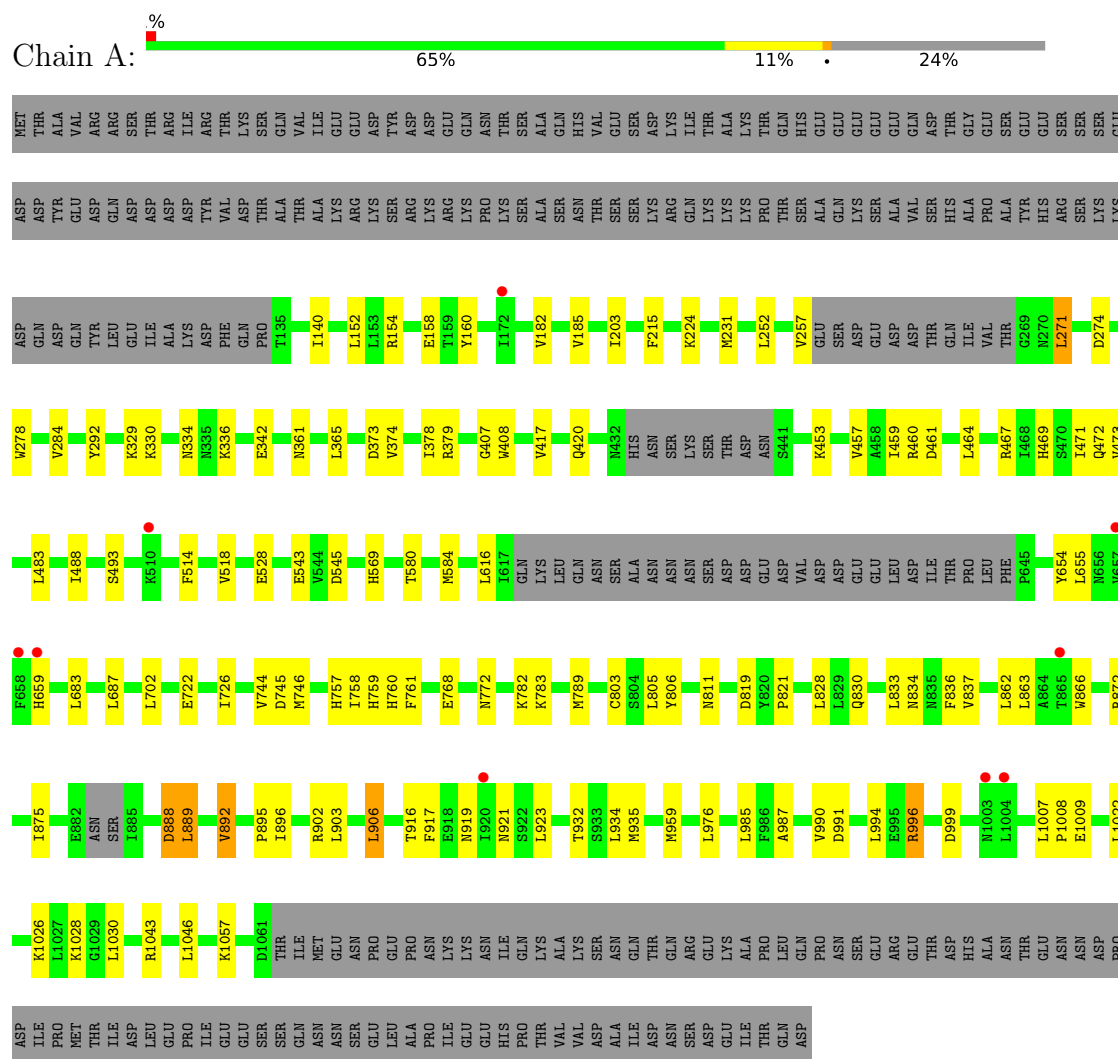
- Molecule 6 is a DNA chain called DNA (5'-D(P*CP*TP*TP*TP*CP*GP*TP*TP*TP*CP*CP*TP*TP*GP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	19	Total	C	N	O	P	0	0	0
			385	186	63	117	19			

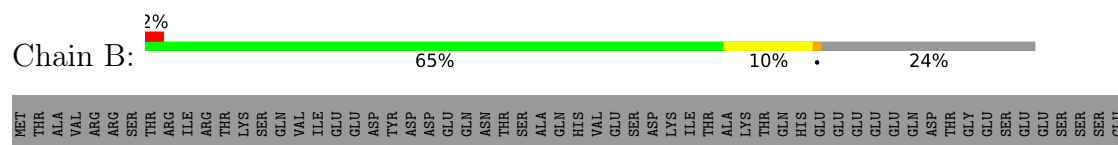
3 Residue-property plots

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 SCC3



• Molecule 1: Cohesin subunit SCC3





Chain E:  63% 37%



- Molecule 4: DNA (5'-D(P*CP*TP*TP*TP*CP*GP*TP*TP*TP*CP*CP*TP*TP*GP*AP*A P*AP*AP*A)-3')

Chain F:  89% 11%



- Molecule 5: DNA (5'-D(P*TP*TP*TP*TP*TP*CP*AP*AP*GP*GP*AP*AP*AP*CP*GP*A P*AP*AP*G)-3')

Chain C:  42% 58%



- Molecule 6: DNA (5'-D(P*CP*TP*TP*TP*CP*GP*TP*TP*TP*CP*CP*TP*TP*GP*AP*A P*AP*AP*A)-3')

Chain D:  79% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	296.24Å 110.02Å 115.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.63 50.00 – 3.63	Depositor EDS
% Data completeness (in resolution range)	48.3 (50.00-3.63) 48.3 (50.00-3.63)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.283 , 0.319 0.291 , 0.321	Depositor DCC
R_{free} test set	1094 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	173.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 164.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16363	wwPDB-VP
Average B, all atoms (Å ²)	214.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.81% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.10	0/7316	0.26	0/9882
1	B	0.10	0/7283	0.25	0/9835
2	G	0.10	0/255	0.25	0/346
2	H	0.09	0/232	0.24	0/314
3	E	0.16	0/442	0.37	0/680
4	F	0.18	0/430	0.40	0/661
5	C	0.16	0/443	0.36	0/682
6	D	0.18	0/429	0.38	0/659
All	All	0.11	0/16830	0.27	0/23059

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	7182	0	7295	54	0
1	B	7149	0	7288	59	0
2	G	248	0	248	1	0
2	H	226	0	227	4	0
3	E	393	0	214	5	0
4	F	386	0	218	1	0
5	C	394	0	215	10	0
6	D	385	0	218	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16363	0	15923	133	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 (133) 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:834:ASN:OD1	1:A:902:ARG:NH2	2.22	0.71
1:B:806:TYR:HE1	1:B:858:LYS:HZ3	1.43	0.65
1:A:493:SER:HB2	1:A:569:HIS:HB2	1.80	0.62
1:B:768:GLU:O	1:B:772:ASN:ND2	2.30	0.61
1:B:756:HIS:NE2	2:H:378:ASP:OD2	2.30	0.61
1:B:865:THR:HB	2:H:380:ILE:HG21	1.83	0.59
1:B:856:ASN:O	1:B:858:LYS:NZ	2.33	0.59
1:B:782:LYS:HB2	1:B:828:LEU:HD12	1.84	0.58
6:D:17:DA:H2''	6:D:18:DA:C8	2.37	0.58
1:B:834:ASN:OD1	1:B:902:ARG:NH2	2.24	0.58
1:B:493:SER:HB2	1:B:569:HIS:HB2	1.86	0.57
1:B:543:GLU:OE1	1:B:544:VAL:N	2.34	0.57
1:A:782:LYS:HB2	1:A:828:LEU:HD12	1.87	0.56
1:A:461:ASP:O	1:A:467:ARG:NH2	2.40	0.55
1:A:833:LEU:HB3	1:A:902:ARG:HG2	1.88	0.55
1:A:379:ARG:HD2	1:A:417:VAL:HG21	1.88	0.55
1:B:292:TYR:HD1	1:B:378:ILE:HG12	1.72	0.55
1:B:987:ALA:HA	1:B:990:VAL:HG22	1.90	0.54
1:A:888:ASP:O	1:A:892:VAL:N	2.39	0.53
1:B:916:THR:OG1	1:B:919:ASN:OD1	2.26	0.53
1:A:373:ASP:OD1	1:A:374:VAL:N	2.41	0.53
1:A:916:THR:OG1	1:A:919:ASN:OD1	2.25	0.53
1:A:987:ALA:HA	1:A:990:VAL:HG22	1.90	0.53
1:B:379:ARG:HD2	1:B:417:VAL:HG21	1.90	0.52
3:E:9:DG:H2''	3:E:10:DA:C8	2.45	0.52
1:A:935:MET:HG2	1:A:1030:LEU:HD11	1.93	0.51
1:B:373:ASP:OD1	1:B:374:VAL:N	2.43	0.51
5:C:16:DA:H2''	5:C:17:DA:C8	2.45	0.51
1:A:459:ILE:HG22	1:A:460:ARG:HG3	1.93	0.51
1:B:833:LEU:HB3	1:B:902:ARG:HG2	1.93	0.51
1:B:373:ASP:O	1:B:379:ARG:NH2	2.43	0.51
6:D:18:DA:H2''	6:D:19:DA:C8	2.46	0.51
1:A:224:LYS:HG3	1:A:231:MET:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:LEU:HD22	1:A:889:LEU:H	1.76	0.51
1:A:457:VAL:O	1:A:461:ASP:HB2	2.11	0.50
5:C:7:DA:H2"	5:C:8:DA:C8	2.47	0.50
1:A:292:TYR:HD1	1:A:378:ILE:HG12	1.75	0.50
1:A:921:ASN:ND2	1:A:1009:GLU:O	2.44	0.50
1:B:461:ASP:O	1:B:467:ARG:NH2	2.45	0.49
1:B:1043:ARG:HD2	1:B:1046:LEU:HD12	1.94	0.49
1:B:903:LEU:HB3	1:B:934:LEU:HG	1.94	0.49
1:B:459:ILE:HG22	1:B:460:ARG:HG3	1.94	0.49
1:A:154:ARG:HG3	1:A:252:LEU:HD11	1.95	0.49
1:A:806:TYR:O	1:A:811:ASN:ND2	2.35	0.49
5:C:12:DA:H2"	5:C:13:DA:C8	2.46	0.49
1:A:768:GLU:O	1:A:772:ASN:ND2	2.26	0.48
3:E:6:DA:H2"	3:E:7:DA:C8	2.48	0.48
3:E:15:DA:H2"	3:E:16:DA:C8	2.49	0.48
1:A:830:GLN:O	1:A:834:ASN:HB2	2.14	0.48
1:A:329:LYS:HA	1:A:330:LYS:HA	1.65	0.47
1:B:759:HIS:CG	1:B:819:ASP:HB3	2.49	0.47
1:B:997:VAL:HG13	1:B:1000:GLU:HB2	1.96	0.47
3:E:5:DC:H2"	3:E:6:DA:C8	2.48	0.47
1:A:407:GLY:O	1:A:453:LYS:NZ	2.41	0.47
1:B:830:GLN:O	1:B:834:ASN:HB2	2.15	0.47
1:A:759:HIS:CG	1:A:819:ASP:HB3	2.50	0.47
1:A:514:PHE:O	1:A:518:VAL:HG23	2.15	0.47
1:B:802:THR:HG21	1:B:855:ILE:HD11	1.97	0.47
1:B:862:LEU:HD22	2:H:377:PRO:HD3	1.96	0.47
3:E:5:DC:H2"	3:E:6:DA:H8	1.80	0.46
1:A:999:ASP:OD1	1:A:999:ASP:N	2.48	0.46
1:A:745:ASP:OD1	1:A:746:MET:N	2.47	0.46
5:C:10:DG:H2"	5:C:11:DA:C8	2.50	0.46
1:B:514:PHE:O	1:B:518:VAL:HG23	2.16	0.46
1:B:457:VAL:O	1:B:461:ASP:HB2	2.16	0.46
1:B:914:ASN:N	1:B:914:ASN:OD1	2.47	0.46
1:B:285:CYS:O	1:B:291:ARG:NH1	2.49	0.46
1:B:483:LEU:HD23	1:B:488:ILE:HG12	1.98	0.45
1:B:745:ASP:OD1	1:B:746:MET:N	2.50	0.45
5:C:6:DC:H2"	5:C:7:DA:H8	1.80	0.45
5:C:6:DC:H2"	5:C:7:DA:C8	2.51	0.45
1:B:667:ASN:HB2	1:B:668:PRO:HD3	1.97	0.45
1:A:917:PHE:CE1	1:A:1008:PRO:HB3	2.52	0.45
1:A:1043:ARG:HD2	1:A:1046:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LYS:HA	1:B:330:LYS:HA	1.62	0.45
1:A:545:ASP:N	1:A:545:ASP:OD1	2.49	0.45
1:A:655:LEU:O	1:A:659:HIS:ND1	2.29	0.45
1:A:821:PRO:HA	1:A:866:TRP:CE2	2.52	0.45
1:B:994:LEU:O	1:B:996:ARG:NH2	2.50	0.45
1:A:994:LEU:O	1:A:996:ARG:NH2	2.50	0.45
1:B:580:THR:O	1:B:584:MET:HG2	2.17	0.45
1:B:616:LEU:HD23	1:B:617:ILE:H	1.81	0.45
1:B:334:ASN:O	1:B:336:LYS:N	2.45	0.44
1:A:903:LEU:HB3	1:A:934:LEU:HG	1.98	0.44
1:B:659:HIS:NE2	1:B:702:LEU:HD23	2.32	0.44
1:A:580:THR:O	1:A:584:MET:HG2	2.18	0.44
1:A:837:VAL:HG13	1:A:906:LEU:HD13	1.99	0.44
1:A:932:THR:HG23	1:A:1026:LYS:HE3	2.00	0.44
1:A:334:ASN:O	1:A:336:LYS:N	2.43	0.44
1:A:659:HIS:NE2	1:A:702:LEU:HD23	2.33	0.44
1:B:1031:MET:HG3	1:B:1036:LEU:HD12	2.00	0.43
1:A:722:GLU:O	1:A:726:ILE:HG12	2.18	0.43
1:A:987:ALA:O	1:A:991:ASP:N	2.52	0.43
1:B:678:GLU:HA	1:B:717:ILE:HD12	2.00	0.43
1:B:888:ASP:OD1	1:B:888:ASP:N	2.50	0.43
1:A:483:LEU:HD23	1:A:488:ILE:HG12	1.99	0.43
1:A:895:PRO:HG2	1:A:896:ILE:HD12	2.01	0.43
1:B:1057:LYS:HE2	1:B:1057:LYS:HB2	1.87	0.43
1:B:432:ASN:HD21	1:B:443:ILE:HD13	1.83	0.43
5:C:5:DT:H2"	5:C:6:DC:C6	2.54	0.43
1:A:789:MET:HE2	1:A:836:PHE:HD2	1.83	0.42
1:B:907:VAL:HG21	1:B:934:LEU:HD12	2.01	0.42
1:B:559:ILE:HG12	1:B:654:TYR:CE2	2.55	0.42
1:A:469:HIS:O	1:A:473:VAL:HG23	2.20	0.42
1:B:683:LEU:O	1:B:687:LEU:HG	2.20	0.42
1:A:160:TYR:CZ	1:A:271:LEU:HD23	2.55	0.42
2:H:371:GLU:O	2:H:374:SER:OG	2.31	0.42
1:A:758:ILE:O	1:A:761:PHE:HB2	2.20	0.42
1:B:806:TYR:O	1:B:811:ASN:ND2	2.35	0.42
1:A:683:LEU:O	1:A:687:LEU:HG	2.20	0.42
1:B:361:ASN:O	1:B:365:LEU:HG	2.20	0.42
1:A:464:LEU:HG	1:A:467:ARG:HH12	1.83	0.42
1:B:723:LEU:HD21	1:B:766:LEU:HD11	2.02	0.42
1:A:1007:LEU:HD23	1:A:1007:LEU:HA	1.85	0.41
1:B:814:THR:HG23	1:B:862:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:HIS:HA	1:B:472:GLN:HB2	2.03	0.41
4:F:15:DG:H2''	4:F:16:DA:C8	2.56	0.41
1:B:832:PHE:HE2	1:B:860:LEU:HD21	1.86	0.41
5:C:11:DA:H2''	5:C:12:DA:C8	2.56	0.41
1:A:361:ASN:O	1:A:365:LEU:HG	2.21	0.41
1:A:469:HIS:HA	1:A:472:GLN:HB2	2.02	0.41
1:B:722:GLU:O	1:B:726:ILE:HG12	2.21	0.41
1:B:821:PRO:HA	1:B:866:TRP:CE2	2.56	0.41
5:C:7:DA:H2''	5:C:8:DA:H8	1.86	0.41
1:A:471:ILE:HD13	1:A:518:VAL:HG22	2.02	0.41
1:A:274:ASP:O	1:A:278:TRP:HD1	2.04	0.40
1:B:469:HIS:O	1:B:473:VAL:HG23	2.21	0.40
1:B:858:LYS:HD2	1:B:859:MET:H	1.85	0.40
1:B:839:ARG:HG3	1:B:842:ILE:HD11	2.03	0.40
2:G:376:LEU:HB2	2:G:379:PRO:HD2	2.04	0.40
1:B:160:TYR:CZ	1:B:271:LEU:HD23	2.56	0.40
1:B:1018:THR:O	1:B:1022:LEU:HG	2.21	0.40
5:C:15:DG:C2	6:D:6:DG:C2	3.09	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	869/1150 (76%)	816 (94%)	53 (6%)	0	100	100
1	B	863/1150 (75%)	809 (94%)	54 (6%)	0	100	100
2	G	28/100 (28%)	26 (93%)	2 (7%)	0	100	100
2	H	25/100 (25%)	23 (92%)	2 (8%)	0	100	100
All	All	1785/2500 (71%)	1674 (94%)	111 (6%)	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	815/1075 (76%)	776 (95%)	39 (5%)	23	46
1	B	814/1075 (76%)	783 (96%)	31 (4%)	29	51
2	G	30/96 (31%)	27 (90%)	3 (10%)	7	28
2	H	27/96 (28%)	26 (96%)	1 (4%)	30	52
All	All	1686/2342 (72%)	1612 (96%)	74 (4%)	25	48

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ILE
1	A	152	LEU
1	A	158	GLU
1	A	182	VAL
1	A	185	VAL
1	A	203	ILE
1	A	215	PHE
1	A	257	VAL
1	A	271	LEU
1	A	284	VAL
1	A	342	GLU
1	A	408	TRP
1	A	420	GLN
1	A	528	GLU
1	A	543	GLU
1	A	616	LEU
1	A	654	TYR
1	A	744	VAL
1	A	757	HIS
1	A	760	HIS
1	A	783	LYS
1	A	803	CYS
1	A	805	LEU
1	A	862	LEU

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Mol	Chain	Res	Type
1	A	863	LEU
1	A	872	ARG
1	A	875	ILE
1	A	888	ASP
1	A	889	LEU
1	A	892	VAL
1	A	906	LEU
1	A	923	LEU
1	A	959	MET
1	A	976	LEU
1	A	985	LEU
1	A	996	ARG
1	A	1022	LEU
1	A	1028	LYS
1	A	1057	LYS
1	B	152	LEU
1	B	170	GLU
1	B	182	VAL
1	B	185	VAL
1	B	203	ILE
1	B	215	PHE
1	B	257	VAL
1	B	271	LEU
1	B	284	VAL
1	B	342	GLU
1	B	420	GLN
1	B	504	LYS
1	B	528	GLU
1	B	543	GLU
1	B	583	ARG
1	B	616	LEU
1	B	654	TYR
1	B	705	SER
1	B	743	LYS
1	B	744	VAL
1	B	803	CYS
1	B	805	LEU
1	B	856	ASN
1	B	858	LYS
1	B	906	LEU
1	B	914	ASN
1	B	920	ILE

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Mol	Chain	Res	Type
1	B	923	LEU
1	B	985	LEU
1	B	996	ARG
1	B	1026	LYS
2	G	371	GLU
2	G	375	TYR
2	G	376	LEU
2	H	382	LYS

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	177	ASN
1	A	193	ASN
1	A	197	ASN
1	A	385	HIS
1	A	569	HIS
1	A	767	GLN
1	B	177	ASN
1	B	204	GLN
1	B	385	HIS
1	B	537	HIS
1	B	569	HIS
1	B	767	GLN
1	B	773	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	879/1150 (76%)	-0.13	9 (1%) 79 54	78, 196, 281, 329	0
1	B	873/1150 (75%)	0.01	21 (2%) 59 35	104, 216, 293, 335	0
2	G	30/100 (30%)	0.32	1 (3%) 49 29	147, 188, 245, 255	0
2	H	27/100 (27%)	0.35	1 (3%) 45 27	175, 198, 242, 259	0
3	E	19/19 (100%)	-0.22	0 100 100	227, 251, 287, 291	0
4	F	19/19 (100%)	-0.11	0 100 100	232, 247, 279, 291	0
5	C	19/19 (100%)	-0.14	0 100 100	259, 273, 298, 300	0
6	D	19/19 (100%)	-0.02	0 100 100	253, 266, 282, 290	0
All	All	1885/2576 (73%)	-0.05	32 (1%) 69 42	78, 209, 288, 335	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1027	LEU	4.4
1	B	245	LEU	4.4
1	B	431	GLN	4.2
1	B	428	LEU	4.1
1	B	274	ASP	3.7
1	A	865	THR	3.4
1	A	172	ILE	2.9
1	B	172	ILE	2.9
1	B	659	HIS	2.9
1	B	587	GLN	2.9
1	A	659	HIS	2.8
1	A	658	PHE	2.7
1	A	510	LYS	2.7
1	A	657	VAL	2.6
1	A	1003	ASN	2.6
1	B	972	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	938	ILE	2.5
1	B	931	CYS	2.5
1	B	1040	PHE	2.4
1	B	517	THR	2.4
1	A	1004	LEU	2.4
1	B	658	PHE	2.3
1	B	857	PHE	2.3
2	G	365	LEU	2.3
2	H	365	LEU	2.2
1	B	234	LEU	2.2
1	B	278	TRP	2.2
1	B	672	THR	2.2
1	B	982	LEU	2.1
1	B	603	ILE	2.1
1	B	934	LEU	2.0
1	A	920	ILE	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.