



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:59 PM UTC

PDB ID : 5FRP / pdb_00005frp
Title : Structure of the Pds5-Scc1 complex and implications for cohesin function
Authors : Muir, K.W.; Kschonsak, M.; Li, Y.; Metz, J.; Haering, C.H.; Panne, D.
Deposited on : 2015-12-21
Resolution : 2.90 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

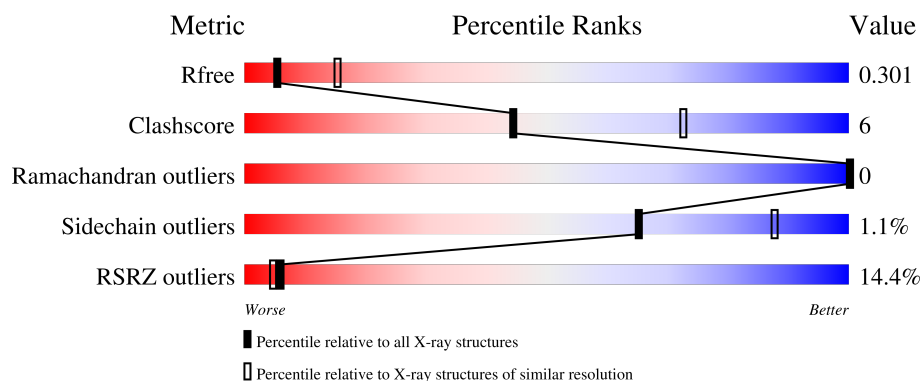
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	703	10% 81% 15% .
1	B	703	16% 81% 12% 6%
2	C	44	16% 34% 5% 61%
2	D	44	18% 34% 5% 61%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22372 atoms, of which 11256 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 SISTER CHROMATID COHESION PROTEIN PDS5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	677	Total	C	H	N	O	S	0	0	0
			11045	3526	5551	914	1041	13			
1	B	660	Total	C	H	N	O	S	0	0	0
			10805	3455	5441	889	1009	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q04264
A	0	ALA	-	expression tag	UNP Q04264
B	-1	GLY	-	expression tag	UNP Q04264
B	0	ALA	-	expression tag	UNP Q04264

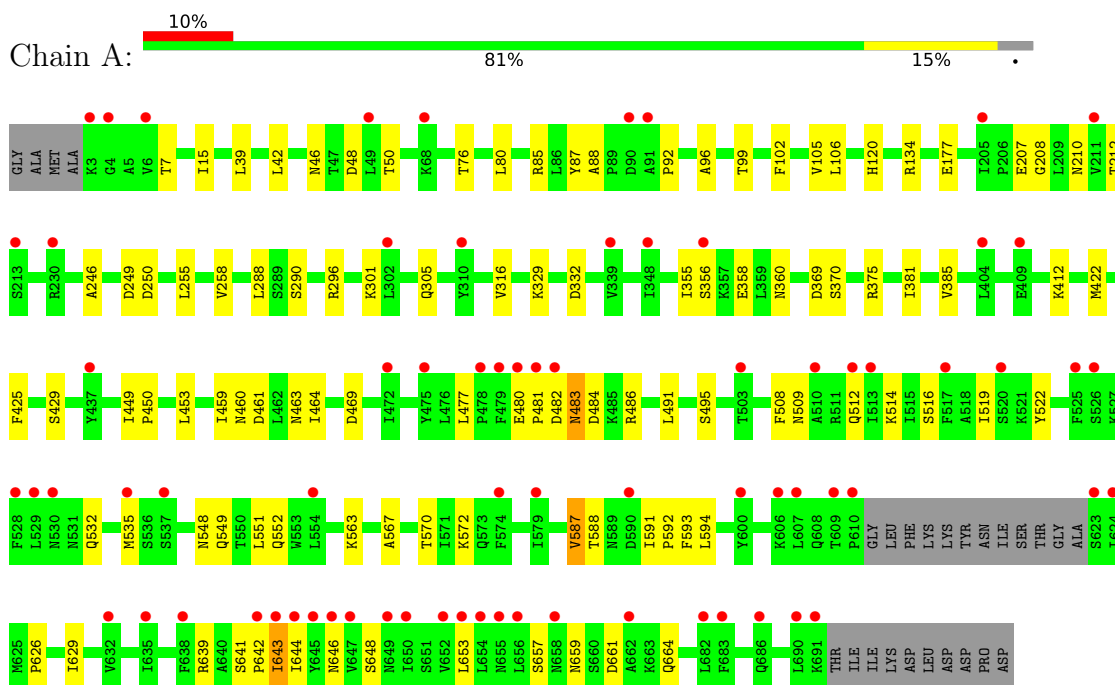
- Molecule 2 is a protein called MCD1-LIKE PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	17	Total	C	H	N	O	S	0	0	0
			261	81	132	20	27	1			
2	D	17	Total	C	H	N	O	S	0	0	0
			261	81	132	20	27	1			

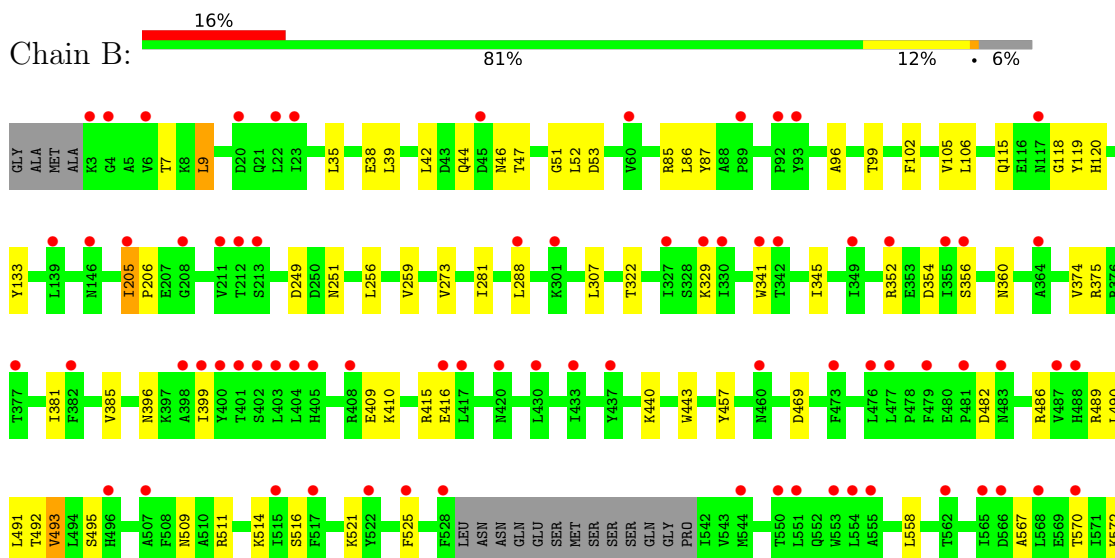
3 Residue-property plots

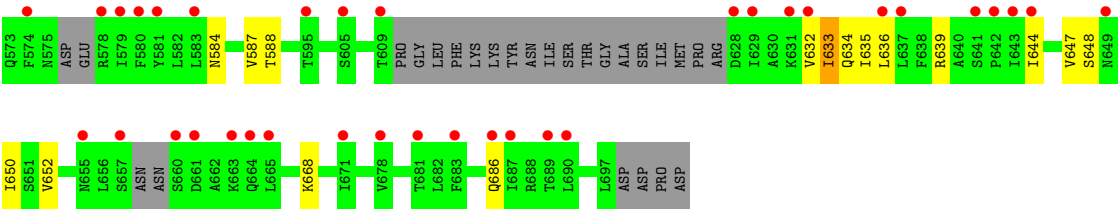
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SISTER CHROMATID COHESION PROTEIN PDS5

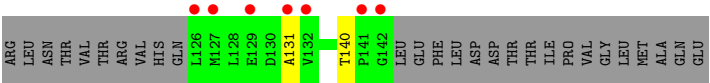


• Molecule 1: SISTER CHROMATID COHESION PROTEIN PDS5

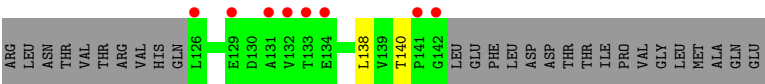




● Molecule 2: MCD1-LIKE PROTEIN



● Molecule 2: MCD1-LIKE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.23Å 62.56Å 155.94Å 90.00° 103.91° 90.00°	Depositor
Resolution (Å)	48.22 – 2.90 48.22 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.22-2.90) 96.3 (48.22-2.90)	Depositor EDS
R_{merge}	0.50	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.266 , 0.298 0.270 , 0.301	Depositor DCC
R_{free} test set	3021 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22372	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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	0.44	0/5600	0.73	7/7597 (0.1%)
1	B	0.37	0/5464	0.70	3/7408 (0.0%)
2	C	0.45	0/129	0.76	1/175 (0.6%)
2	D	0.32	0/129	0.78	0/175
All	All	0.41	0/11322	0.72	11/15355 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	ASP	N-CA-C	7.82	119.88	111.36
1	A	208	GLY	N-CA-C	7.76	121.50	112.50
1	B	205	ILE	CA-C-N	-7.54	111.99	119.90
1	B	205	ILE	C-N-CA	-7.54	111.99	119.90
1	B	44	GLN	N-CA-C	6.16	117.99	111.28
1	A	477	LEU	CA-C-N	-6.13	114.42	120.98
1	A	477	LEU	C-N-CA	-6.13	114.42	120.98
1	A	460	ASN	N-CA-C	5.95	119.77	111.74
1	A	483	ASN	N-CA-C	5.62	117.21	111.14
1	A	88	ALA	C-N-CD	5.14	131.90	120.60
2	C	131	ALA	N-CA-C	5.03	118.97	111.87

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	5494	5551	5551	71	1
1	B	5364	5441	5435	66	1
2	C	129	132	132	1	0
2	D	129	132	132	2	0
All	All	11116	11256	11250	135	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 (135) 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:42:LEU:O	1:A:85:ARG:NH2	2.06	0.89
1:A:486:ARG:NH1	1:A:593:PHE:CD2	2.43	0.86
1:A:642:PRO:C	1:A:643:ILE:HD12	2.08	0.77
1:A:369:ASP:O	1:A:375:ARG:NH1	2.17	0.76
1:A:482:ASP:OD1	1:A:483:ASN:N	2.21	0.72
1:A:643:ILE:HD12	1:A:643:ILE:N	2.05	0.71
1:B:51:GLY:O	1:B:52:LEU:HD12	1.90	0.71
1:B:51:GLY:C	1:B:52:LEU:HD12	2.17	0.70
1:B:85:ARG:HD2	1:B:133:TYR:CD1	2.28	0.68
1:B:558:LEU:HD22	1:B:635:ILE:HD13	1.74	0.68
1:A:459:ILE:HD11	1:A:461:ASP:HB3	1.76	0.68
1:A:288:LEU:O	1:A:329:LYS:NZ	2.25	0.67
1:A:482:ASP:O	1:A:486:ARG:HG3	1.94	0.67
1:A:486:ARG:CD	1:A:593:PHE:CE2	2.78	0.66
1:B:514:LYS:NZ	2:D:140:THR:O	2.28	0.65
1:A:516:SER:OG	1:A:587:VAL:O	2.15	0.65
1:B:567:ALA:O	1:B:570:THR:OG1	2.14	0.65
1:A:486:ARG:HD3	1:A:593:PHE:CE2	2.33	0.64
1:A:459:ILE:O	1:B:115:GLN:NE2	2.31	0.64
1:A:296:ARG:NH2	1:A:332:ASP:OD1	2.31	0.63
1:A:514:LYS:NZ	2:C:140:THR:O	2.31	0.63
1:B:558:LEU:HD22	1:B:635:ILE:CD1	2.29	0.63
1:A:567:ALA:O	1:A:570:THR:OG1	2.16	0.62
1:B:584:ASN:OD1	1:B:588:THR:OG1	2.18	0.62
1:B:652:VAL:HG12	1:B:668:LYS:HG3	1.83	0.61
1:A:7:THR:OG1	1:A:46:ASN:O	2.18	0.60
1:A:469:ASP:OD2	1:A:639:ARG:NE	2.35	0.59
1:A:532:GLN:OE1	1:A:535:MET:N	2.36	0.59
1:B:288:LEU:O	1:B:329:LYS:NZ	2.26	0.59
1:A:486:ARG:CZ	1:A:593:PHE:CD2	2.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:SER:O	1:B:360:ASN:ND2	2.36	0.58
1:A:356:SER:O	1:A:360:ASN:ND2	2.37	0.56
1:A:512:GLN:HG2	1:A:639:ARG:O	2.06	0.56
1:B:35:LEU:HD11	1:B:39:LEU:HD11	1.87	0.56
1:B:85:ARG:HD2	1:B:133:TYR:CG	2.40	0.56
1:B:85:ARG:NH2	1:B:86:LEU:HD21	2.21	0.56
1:A:87:TYR:CD2	1:A:92:PRO:HB3	2.42	0.55
1:B:118:GLY:C	1:B:119:TYR:CD1	2.85	0.54
1:A:459:ILE:HD11	1:A:461:ASP:CB	2.38	0.54
1:B:307:LEU:O	1:B:352:ARG:HD3	2.08	0.53
1:A:461:ASP:OD1	1:A:463:ASN:N	2.42	0.53
1:B:85:ARG:HD2	1:B:133:TYR:CE1	2.44	0.53
1:A:643:ILE:N	1:A:643:ILE:CD1	2.72	0.53
1:B:511:ARG:HD3	2:D:138:LEU:O	2.08	0.53
1:A:482:ASP:O	1:A:486:ARG:CG	2.56	0.52
1:A:661:ASP:OD2	1:A:664:GLN:NE2	2.42	0.52
1:A:480:GLU:CB	1:A:481:PRO:HA	2.39	0.52
1:B:558:LEU:CD2	1:B:635:ILE:CD1	2.88	0.51
1:B:352:ARG:NH2	1:B:354:ASP:OD2	2.43	0.50
1:B:102:PHE:O	1:B:105:VAL:HG12	2.11	0.50
1:B:119:TYR:CD1	1:B:119:TYR:N	2.79	0.50
1:B:85:ARG:HG3	1:B:133:TYR:HB3	1.93	0.50
1:B:486:ARG:NH2	1:B:648:SER:OG	2.45	0.50
1:A:486:ARG:NH2	1:A:648:SER:OG	2.45	0.50
1:B:53:ASP:OD1	1:B:87:TYR:OH	2.25	0.50
1:A:96:ALA:O	1:A:99:THR:OG1	2.29	0.50
1:B:375:ARG:NH1	1:B:409:GLU:OE1	2.44	0.49
1:B:7:THR:CG2	1:B:47:THR:HA	2.43	0.49
1:B:96:ALA:O	1:B:99:THR:OG1	2.28	0.49
1:A:102:PHE:O	1:A:105:VAL:HG12	2.12	0.49
1:A:626:PRO:O	1:A:629:ILE:N	2.45	0.49
1:B:491:LEU:O	1:B:495:SER:N	2.45	0.49
1:A:594:LEU:C	1:A:594:LEU:HD13	2.38	0.49
1:A:591:ILE:O	1:A:646:ASN:ND2	2.46	0.49
1:A:641:SER:OG	1:A:643:ILE:HD11	2.12	0.49
1:A:657:SER:OG	1:A:659:ASN:O	2.29	0.49
1:B:489:ARG:O	1:B:492:THR:OG1	2.19	0.48
1:A:301:LYS:O	1:A:305:GLN:HG3	2.14	0.48
1:A:134:ARG:NH1	1:A:177:GLU:OE1	2.48	0.47
1:B:632:VAL:O	1:B:635:ILE:HG13	2.15	0.46
1:B:9:LEU:HD12	1:B:38:GLU:CD	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASP:OD1	1:A:50:THR:N	2.48	0.46
1:B:205:ILE:N	1:B:206:PRO:CD	2.79	0.46
1:A:591:ILE:HG22	1:A:592:PRO:O	2.16	0.46
1:A:255:LEU:O	1:A:258:VAL:HG22	2.16	0.46
1:A:212:THR:CG2	1:B:416:GLU:CD	2.90	0.45
1:B:102:PHE:HA	1:B:105:VAL:HG12	1.98	0.45
1:B:440:LYS:HA	1:B:443:TRP:HB2	1.98	0.45
1:A:483:ASN:HA	1:A:486:ARG:NH1	2.32	0.45
1:A:509:ASN:CG	1:A:644:ILE:HD11	2.42	0.45
1:B:647:VAL:O	1:B:650:ILE:HG13	2.17	0.45
1:B:102:PHE:O	1:B:106:LEU:HG	2.17	0.44
1:A:480:GLU:HB2	1:A:481:PRO:CA	2.47	0.44
1:A:491:LEU:O	1:A:495:SER:N	2.51	0.44
1:B:39:LEU:HA	1:B:42:LEU:HG	2.00	0.44
1:A:246:ALA:CB	1:A:258:VAL:HG21	2.48	0.44
1:B:35:LEU:CD1	1:B:39:LEU:HD11	2.47	0.44
1:B:46:ASN:O	1:B:47:THR:OG1	2.35	0.44
1:B:9:LEU:CD1	1:B:38:GLU:CD	2.90	0.44
1:B:281:ILE:HG13	1:B:322:THR:HG21	2.00	0.44
1:B:457:TYR:OH	1:B:469:ASP:OD1	2.36	0.44
1:B:584:ASN:O	1:B:588:THR:OG1	2.35	0.44
1:A:369:ASP:OD1	1:A:370:SER:N	2.51	0.43
1:B:307:LEU:O	1:B:352:ARG:CD	2.66	0.43
1:A:76:THR:HG22	1:A:80:LEU:CD1	2.49	0.43
1:A:449:ILE:N	1:A:450:PRO:HD2	2.33	0.43
1:B:341:TRP:CH2	1:B:345:ILE:HD11	2.53	0.43
1:A:207:GLU:OE2	1:A:210:ASN:OD1	2.37	0.43
1:A:249:ASP:OD1	1:A:250:ASP:N	2.51	0.43
1:A:459:ILE:CD1	1:A:461:ASP:CB	2.97	0.43
1:A:316:VAL:HG11	1:A:355:ILE:HD11	2.00	0.43
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.84	0.43
1:A:480:GLU:HB2	1:A:481:PRO:HA	2.00	0.43
1:B:469:ASP:OD2	1:B:639:ARG:NE	2.52	0.43
1:B:633:ILE:HD12	1:B:634:GLN:N	2.33	0.43
1:A:508:PHE:O	1:A:512:GLN:HG3	2.18	0.43
1:B:410:LYS:O	1:B:415:ARG:NH2	2.52	0.43
1:A:102:PHE:O	1:A:106:LEU:HG	2.19	0.42
1:A:548:ASN:O	1:A:551:LEU:HG	2.19	0.42
1:B:588:THR:O	1:B:588:THR:HG22	2.19	0.42
1:B:256:LEU:HA	1:B:259:VAL:HG12	2.00	0.42
1:B:381:ILE:O	1:B:385:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ILE:HG23	1:A:358:GLU:OE1	2.18	0.42
1:A:519:ILE:HA	1:A:522:TYR:HB3	2.02	0.42
1:B:509:ASN:HD21	1:B:644:ILE:HD11	1.85	0.42
1:A:422:MET:HE3	1:A:453:LEU:HD12	2.02	0.41
1:A:425:PHE:O	1:A:429:SER:N	2.51	0.41
1:A:591:ILE:O	1:A:592:PRO:C	2.63	0.41
1:B:490:LEU:O	1:B:493:VAL:HG22	2.20	0.41
1:B:396:ASN:HB3	1:B:399:ILE:HG12	2.03	0.41
1:B:482:ASP:O	1:B:486:ARG:HG3	2.20	0.41
1:A:381:ILE:O	1:A:385:VAL:HG12	2.20	0.41
1:A:549:GLN:O	1:A:552:GLN:HG2	2.21	0.41
1:B:492:THR:O	1:B:495:SER:OG	2.28	0.41
1:B:521:LYS:O	1:B:525:PHE:N	2.53	0.41
1:B:516:SER:OG	1:B:587:VAL:O	2.32	0.41
1:A:461:ASP:HB3	1:A:464:ILE:HB	2.03	0.40
1:B:635:ILE:HD12	1:B:636:LEU:N	2.36	0.40
1:A:15:ILE:O	1:A:15:ILE:HG22	2.21	0.40
1:A:290:SER:O	1:A:296:ARG:HD3	2.21	0.40
1:B:249:ASP:O	1:B:251:ASN:N	2.51	0.40
1:B:273:VAL:HG23	1:B:273:VAL:O	2.21	0.40
1:B:42:LEU:O	1:B:85:ARG:NH2	2.54	0.40
1:A:482:ASP:CG	1:A:483:ASN:N	2.78	0.40
1:B:516:SER:HA	1:B:587: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:657:SER:O	1:B:686:GLN:NE2[2_556]	2.17	0.03

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	673/703 (96%)	633 (94%)	40 (6%)	0	100	100
1	B	650/703 (92%)	615 (95%)	35 (5%)	0	100	100
2	C	15/44 (34%)	14 (93%)	1 (7%)	0	100	100
2	D	15/44 (34%)	15 (100%)	0	0	100	100
All	All	1353/1494 (91%)	1277 (94%)	76 (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	629/650 (97%)	621 (99%)	8 (1%)	61	86
1	B	611/650 (94%)	605 (99%)	6 (1%)	68	89
2	C	15/40 (38%)	15 (100%)	0	100	100
2	D	15/40 (38%)	15 (100%)	0	100	100
All	All	1270/1380 (92%)	1256 (99%)	14 (1%)	65	88

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	412	LYS
1	A	563	LYS
1	A	572	LYS
1	A	587	VAL
1	A	588	THR
1	A	643	ILE
1	A	653	LEU
1	B	9	LEU
1	B	120	HIS
1	B	374	VAL
1	B	493	VAL
1	B	572	LYS

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Mol	Chain	Res	Type
1	B	633	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	122	GLN
1	A	160	ASN
1	A	248	ASN
1	A	347	GLN
1	A	483	ASN
1	A	539	GLN
1	A	573	GLN
1	A	598	ASN
1	A	601	ASN
1	A	655	ASN
1	B	44	GLN
1	B	120	HIS
1	B	122	GLN
1	B	160	ASN
1	B	460	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](#)

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	677/703 (96%)	0.82	73 (10%) 11 9	52, 102, 180, 211	0
1	B	660/703 (93%)	1.07	110 (16%) 4 3	50, 109, 179, 200	0
2	C	17/44 (38%)	1.45	7 (41%) 0 0	109, 140, 171, 178	0
2	D	17/44 (38%)	2.50	8 (47%) 0 0	131, 159, 187, 187	0
All	All	1371/1494 (91%)	0.97	198 (14%) 6 5	50, 108, 179, 211	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	657	SER	6.9
1	A	68	LYS	6.4
1	A	610	PRO	6.0
2	D	131	ALA	5.5
1	B	403	LEU	5.3
1	B	417	LEU	5.1
1	A	4	GLY	5.1
1	A	480	GLU	5.0
1	B	399	ILE	4.9
1	B	574	PHE	4.7
2	D	126	LEU	4.7
1	B	683	PHE	4.6
1	B	92	PRO	4.6
1	B	212	THR	4.5
1	B	628	ASP	4.4
1	B	643	ILE	4.4
1	A	650	ILE	4.3
1	B	580	PHE	4.3
1	B	631	LYS	4.3
1	B	632	VAL	4.3
1	B	6	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	478	PRO	4.1
1	A	513	ILE	4.0
1	B	553	TRP	4.0
1	B	663	LYS	4.0
1	B	689	THR	3.9
1	B	664	GLN	3.9
1	A	91	ALA	3.7
1	B	364	ALA	3.6
2	D	142	GLY	3.6
1	A	658	ASN	3.6
1	B	401	THR	3.6
1	B	4	GLY	3.6
1	B	433	ILE	3.6
1	A	3	LYS	3.6
1	B	213	SER	3.6
1	A	517	PHE	3.5
1	B	579	ILE	3.5
1	A	205	ILE	3.5
2	C	142	GLY	3.5
1	A	682	LEU	3.4
1	A	645	TYR	3.4
1	A	437	TYR	3.4
1	A	686	GLN	3.4
1	B	211	VAL	3.4
1	B	405	HIS	3.4
1	A	644	ILE	3.4
1	B	327	ILE	3.3
1	A	607	LEU	3.3
1	B	22	LEU	3.3
1	B	554	LEU	3.3
2	D	129	GLU	3.3
1	B	665	LEU	3.3
2	C	126	LEU	3.3
1	B	437	TYR	3.3
1	A	656	LEU	3.3
1	B	550	THR	3.3
1	A	635	ILE	3.2
1	A	590	ASP	3.2
1	B	637	LEU	3.2
1	A	537	SER	3.1
1	B	408	ARG	3.1
1	B	660	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	655	ASN	3.1
1	A	481	PRO	3.1
1	B	649	ASN	3.1
1	A	643	ILE	3.1
1	A	404	LEU	3.1
2	D	134	GLU	3.1
1	B	609	THR	3.1
1	A	654	LEU	3.0
2	D	133	THR	3.0
1	A	6	VAL	3.0
1	B	644	ILE	3.0
1	B	595	THR	3.0
1	A	646	ASN	3.0
2	C	131	ALA	2.9
1	B	205	ILE	2.9
1	A	482	ASP	2.9
1	A	520	SER	2.9
1	A	512	GLN	2.9
1	A	525	PHE	2.9
1	A	624	ILE	2.9
1	B	377	THR	2.9
1	B	93	TYR	2.8
1	A	479	PHE	2.8
1	B	641	SER	2.8
1	B	342	THR	2.8
1	A	579	ILE	2.8
1	B	355	ILE	2.8
1	B	562	THR	2.8
1	B	356	SER	2.8
2	D	141	PRO	2.8
1	A	632	VAL	2.7
1	A	647	VAL	2.7
1	A	609	THR	2.7
1	B	566	ASP	2.7
1	B	473	PHE	2.7
1	A	690	LEU	2.7
1	B	349	ILE	2.7
1	B	661	ASP	2.7
1	B	629	ILE	2.6
1	A	638	PHE	2.6
1	A	652	VAL	2.6
1	B	329	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	213	SER	2.6
1	A	356	SER	2.6
1	B	330	ILE	2.6
1	A	662	ALA	2.6
1	B	488	HIS	2.6
2	D	132	VAL	2.6
1	A	528	PHE	2.6
1	A	574	PHE	2.6
1	B	578	ARG	2.6
1	B	481	PRO	2.6
1	B	45	ASP	2.6
1	B	678	VAL	2.5
1	A	526	SER	2.5
1	A	653	LEU	2.5
1	A	535	MET	2.5
1	B	565	ILE	2.5
1	B	517	PHE	2.5
1	B	496	HIS	2.5
1	A	642	PRO	2.5
1	B	507	ALA	2.5
1	B	687	ILE	2.5
1	B	487	VAL	2.5
1	B	581	TYR	2.5
1	B	352	ARG	2.5
1	B	555	ALA	2.5
1	A	49	LEU	2.4
1	A	90	ASP	2.4
1	B	341	TRP	2.4
1	A	600	TYR	2.4
1	A	503	THR	2.4
1	B	117	ASN	2.4
1	A	230	ARG	2.4
2	C	129	GLU	2.4
1	B	551	LEU	2.4
1	A	348	ILE	2.4
1	A	211	VAL	2.3
1	B	544	MET	2.3
1	B	3	LYS	2.3
1	B	382	PHE	2.3
1	B	671	ILE	2.3
1	B	208	GLY	2.3
1	B	483	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	683	PHE	2.3
1	B	686	GLN	2.3
1	A	623	SER	2.3
1	B	570	THR	2.3
1	B	522	TYR	2.3
1	B	420	ASN	2.3
1	B	476	LEU	2.3
1	B	636	LEU	2.3
1	B	479	PHE	2.2
1	A	649	ASN	2.2
1	A	302	LEU	2.2
1	B	288	LEU	2.2
1	B	89	PRO	2.2
1	A	529	LEU	2.2
1	B	416	GLU	2.2
1	B	301	LYS	2.2
1	B	460	ASN	2.2
1	B	583	LEU	2.2
1	B	690	LEU	2.2
1	B	402	SER	2.2
2	C	127	MET	2.2
1	B	139	LEU	2.2
1	B	404	LEU	2.2
1	B	430	LEU	2.2
1	B	146	ASN	2.2
1	B	515	ILE	2.2
2	C	141	PRO	2.2
1	B	568	LEU	2.2
1	A	530	ASN	2.2
1	B	642	PRO	2.2
1	A	691	LYS	2.2
1	B	398	ALA	2.1
1	B	605	SER	2.1
1	A	339	VAL	2.1
2	C	132	VAL	2.1
1	A	606	LYS	2.1
1	B	477	LEU	2.1
1	B	23	ILE	2.1
1	B	60	VAL	2.1
1	B	525	PHE	2.1
1	B	528	PHE	2.1
1	B	655	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	681	THR	2.1
1	A	472	ILE	2.1
1	A	310	TYR	2.1
1	A	554	LEU	2.0
1	A	510	ALA	2.0
1	B	20	ASP	2.0
1	A	409	GLU	2.0
1	A	475	TYR	2.0
1	B	400	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.