



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:52 AM UTC

PDB ID : 7EQC / pdb_00007eqc
Title : Crystal structure of the mini-centralspindlin complex
Authors : Chen, Z.; Pan, H.
Deposited on : 2021-05-01
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

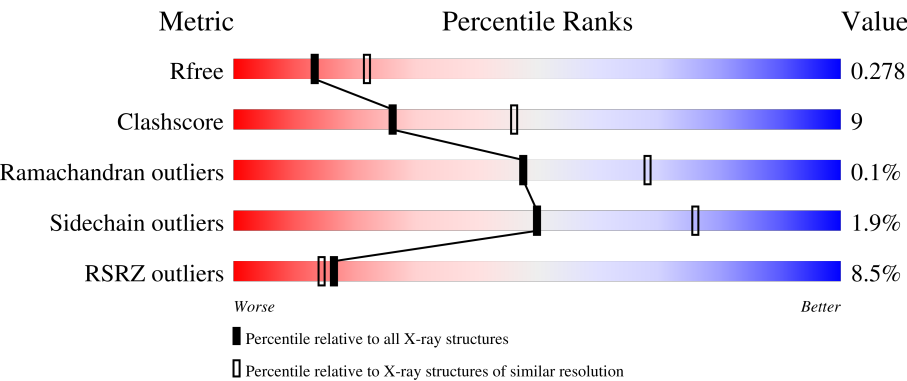
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



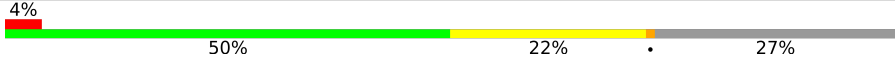
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	B	124	2% 65% 15% • 19%
1	C	124	6% 69% 16% 15%
1	D	124	8% 70% 11% 19%
1	G	124	6% 68% 19% 14%
2	E	134	7% 45% 14% • 40%

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Mol	Chain	Length	Quality of chain
2	F	134	
2	I	134	
2	J	134	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6720 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 CYtoKinesis defect.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	101	Total	C	N	O	S	0	1	0
			845	528	157	154	6			
1	C	106	Total	C	N	O	S	0	0	0
			883	551	162	164	6			
1	D	101	Total	C	N	O	S	0	0	0
			837	526	150	155	6			
1	G	107	Total	C	N	O	S	0	0	0
			892	557	164	165	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q9XUS9
B	-2	ALA	-	expression tag	UNP Q9XUS9
B	-1	GLY	-	expression tag	UNP Q9XUS9
B	0	SER	-	expression tag	UNP Q9XUS9
C	-3	GLY	-	expression tag	UNP Q9XUS9
C	-2	ALA	-	expression tag	UNP Q9XUS9
C	-1	GLY	-	expression tag	UNP Q9XUS9
C	0	SER	-	expression tag	UNP Q9XUS9
D	-3	GLY	-	expression tag	UNP Q9XUS9
D	-2	ALA	-	expression tag	UNP Q9XUS9
D	-1	GLY	-	expression tag	UNP Q9XUS9
D	0	SER	-	expression tag	UNP Q9XUS9
G	-3	GLY	-	expression tag	UNP Q9XUS9
G	-2	ALA	-	expression tag	UNP Q9XUS9
G	-1	GLY	-	expression tag	UNP Q9XUS9
G	0	SER	-	expression tag	UNP Q9XUS9

- Molecule 2 is a protein called Kinesin-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	109	Total	C	N	O	S	0	0	0
			881	542	151	179	9			
2	F	98	Total	C	N	O	S	0	0	0
			809	506	139	155	9			
2	E	81	Total	C	N	O	S	0	0	0
			671	417	116	133	5			
2	I	107	Total	C	N	O	S	0	0	0
			864	530	149	177	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	422	GLY	-	expression tag	UNP G5EG83
J	423	HIS	-	expression tag	UNP G5EG83
J	424	MET	-	expression tag	UNP G5EG83
J	425	GLY	-	expression tag	UNP G5EG83
J	426	SER	-	expression tag	UNP G5EG83
J	427	SER	-	expression tag	UNP G5EG83
J	428	GLY	-	expression tag	UNP G5EG83
J	429	GLY	-	expression tag	UNP G5EG83
F	422	GLY	-	expression tag	UNP G5EG83
F	423	HIS	-	expression tag	UNP G5EG83
F	424	MET	-	expression tag	UNP G5EG83
F	425	GLY	-	expression tag	UNP G5EG83
F	426	SER	-	expression tag	UNP G5EG83
F	427	SER	-	expression tag	UNP G5EG83
F	428	GLY	-	expression tag	UNP G5EG83
F	429	GLY	-	expression tag	UNP G5EG83
E	422	GLY	-	expression tag	UNP G5EG83
E	423	HIS	-	expression tag	UNP G5EG83
E	424	MET	-	expression tag	UNP G5EG83
E	425	GLY	-	expression tag	UNP G5EG83
E	426	SER	-	expression tag	UNP G5EG83
E	427	SER	-	expression tag	UNP G5EG83
E	428	GLY	-	expression tag	UNP G5EG83
E	429	GLY	-	expression tag	UNP G5EG83
I	422	GLY	-	expression tag	UNP G5EG83
I	423	HIS	-	expression tag	UNP G5EG83
I	424	MET	-	expression tag	UNP G5EG83
I	425	GLY	-	expression tag	UNP G5EG83
I	426	SER	-	expression tag	UNP G5EG83
I	427	SER	-	expression tag	UNP G5EG83
I	428	GLY	-	expression tag	UNP G5EG83
I	429	GLY	-	expression tag	UNP G5EG83

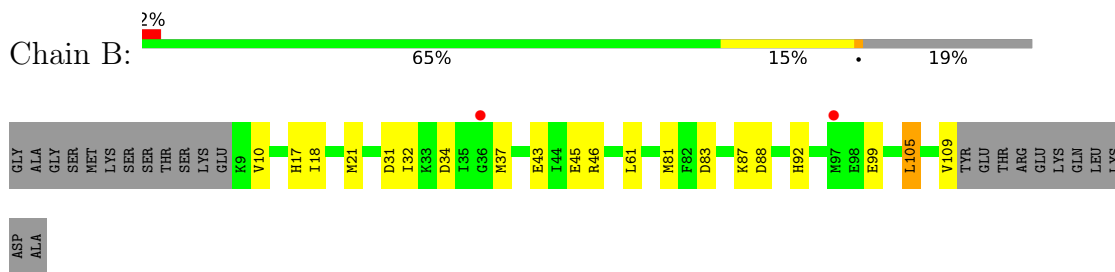
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	O 2	0	0
3	C	5	Total 5	O 5	0	0
3	J	12	Total 12	O 12	0	0
3	F	4	Total 4	O 4	0	0
3	D	7	Total 7	O 7	0	0
3	E	1	Total 1	O 1	0	0
3	G	3	Total 3	O 3	0	0
3	I	4	Total 4	O 4	0	0

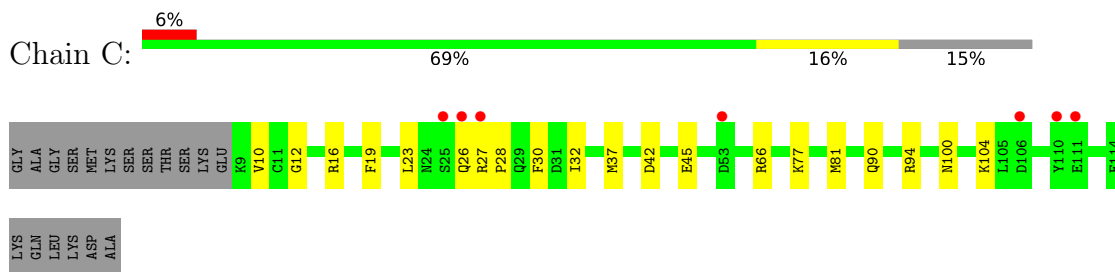
3 Residue-property plots [i](#)

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.

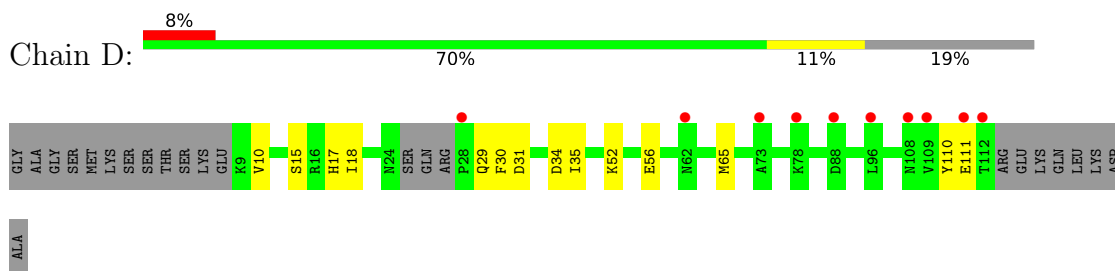
- Molecule 1: CYtoKinesis defect



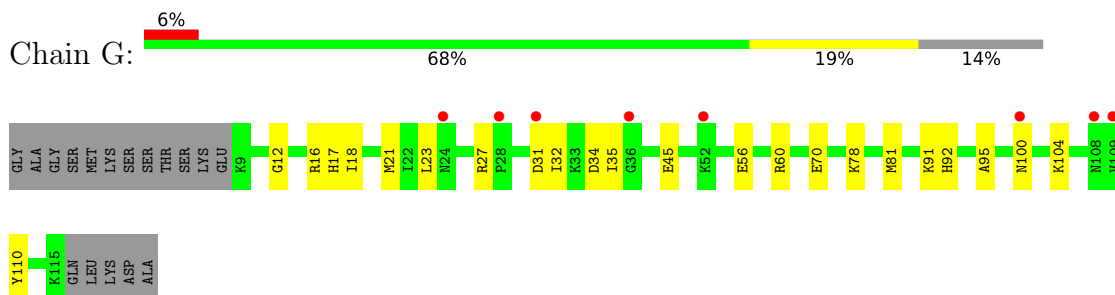
- Molecule 1: CYtoKinesis defect



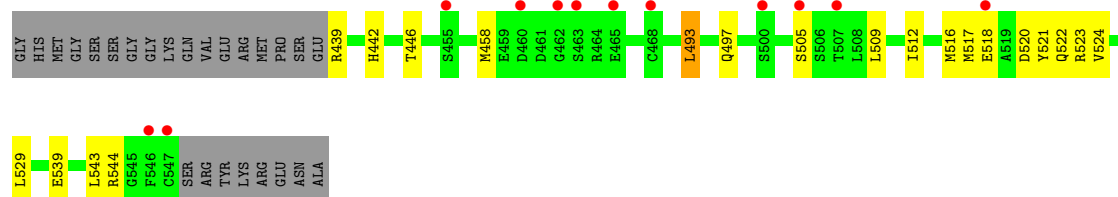
- Molecule 1: CYtoKinesis defect



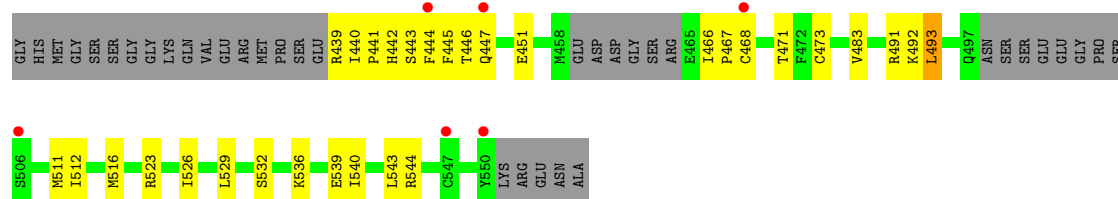
- Molecule 1: CYtoKinesis defect



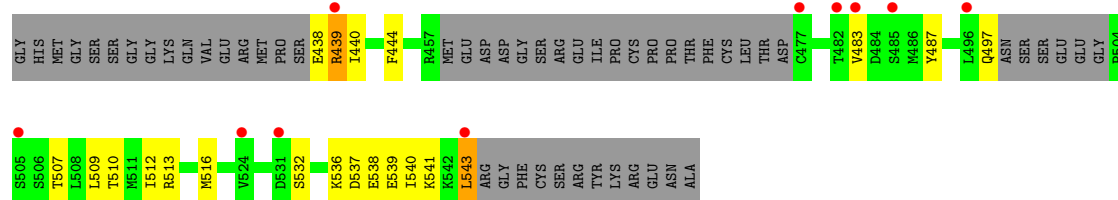
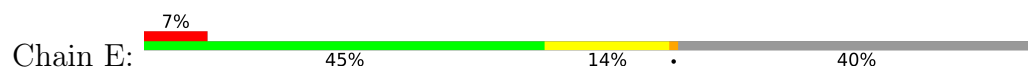
• Molecule 2: Kinesin-like protein



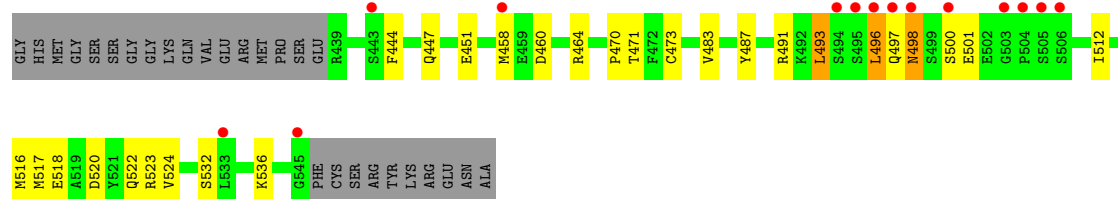
• Molecule 2: Kinesin-like protein



• Molecule 2: Kinesin-like protein



• Molecule 2: Kinesin-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.76Å 65.41Å 75.79Å 96.42° 92.24° 105.03°	Depositor
Resolution (Å)	41.65 – 2.50 41.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.0 (41.65-2.50) 95.9 (41.65-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.238 , 0.277 0.239 , 0.278	Depositor DCC
R_{free} test set	2005 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6720	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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	B	0.22	0/855	0.53	1/1137 (0.1%)
1	C	0.18	0/893	0.48	0/1188
1	D	0.20	0/846	0.45	0/1124
1	G	0.17	0/902	0.44	0/1199
2	E	0.24	0/679	0.51	0/906
2	F	0.28	0/822	0.56	0/1101
2	I	0.24	0/878	0.59	1/1180 (0.1%)
2	J	0.23	0/896	0.51	0/1204
All	All	0.22	0/6771	0.51	2/9039 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	LEU	CA-CB-CG	-6.08	95.00	116.30
2	I	496	LEU	CA-CB-CG	-5.27	97.86	116.30

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	B	845	0	867	16	0
1	C	883	0	902	24	0
1	D	837	0	857	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	892	0	915	16	0
2	E	671	0	661	19	0
2	F	809	0	794	34	0
2	I	864	0	833	36	0
2	J	881	0	847	22	0
3	B	2	0	0	0	0
3	C	5	0	0	0	0
3	D	7	0	0	0	0
3	E	1	0	0	1	0
3	F	4	0	0	1	0
3	G	3	0	0	0	0
3	I	4	0	0	1	0
3	J	12	0	0	1	0
All	All	6720	0	6676	125	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 9.

All (125) 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)
2:I:496:LEU:HD23	2:I:497:GLN:HG3	1.47	0.94
1:B:31:ASP:CG	2:I:498:ASN:HD21	1.82	0.88
1:C:26:GLN:H	2:I:464:ARG:HH21	1.27	0.82
1:C:30:PHE:O	2:E:497:GLN:NE2	2.11	0.82
2:E:538:GLU:HA	2:E:541:LYS:HB2	1.61	0.82
2:F:523:ARG:NH2	3:F:601:HOH:O	2.15	0.80
1:B:43:GLU:OE1	1:B:46:ARG:NH1	2.17	0.77
1:C:19:PHE:HB2	2:E:516:MET:HE1	1.67	0.76
2:J:521:TYR:CG	2:F:440:ILE:HD12	2.21	0.75
2:E:438:GLU:N	2:I:518:GLU:OE1	2.21	0.74
2:J:497:GLN:NE2	1:D:30:PHE:O	2.23	0.71
2:E:439:ARG:NH2	3:E:601:HOH:O	2.23	0.71
2:J:539:GLU:OE2	2:F:544:ARG:NH2	2.23	0.71
2:F:493:LEU:HB3	1:G:32:ILE:HD13	1.71	0.71
2:F:440:ILE:HG21	2:F:444:PHE:CD2	2.26	0.70
2:J:439:ARG:NH2	3:J:601:HOH:O	2.23	0.70
2:I:497:GLN:O	2:I:501:GLU:N	2.22	0.69
2:I:496:LEU:O	2:I:500:SER:HB3	1.93	0.69
1:B:99:GLU:HG2	1:C:100:ASN:HD21	1.59	0.68
1:C:28:PRO:HG2	2:I:497:GLN:CD	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ASP:OD1	2:I:498:ASN:ND2	2.27	0.66
2:J:516:MET:HE1	1:D:18:ILE:HB	1.76	0.66
1:B:32:ILE:HD13	2:I:493:LEU:HB3	1.77	0.65
1:B:18:ILE:HB	2:I:516:MET:HE1	1.79	0.65
1:C:28:PRO:HG2	2:I:497:GLN:NE2	2.11	0.65
1:C:30:PHE:HZ	2:I:497:GLN:HB2	1.61	0.64
1:C:90:GLN:OE1	1:C:94:ARG:NH2	2.32	0.63
2:J:517:MET:SD	2:F:445:PHE:HD1	2.23	0.62
1:C:26:GLN:N	2:I:464:ARG:HH21	1.94	0.62
2:I:496:LEU:HD23	2:I:497:GLN:CG	2.25	0.61
2:E:440:ILE:HD12	2:I:517:MET:HE3	1.83	0.61
2:J:521:TYR:CD2	2:F:440:ILE:HD12	2.35	0.60
2:J:458:MET:HB3	1:G:27:ARG:NH2	2.17	0.60
2:I:523:ARG:NH2	3:I:601:HOH:O	2.35	0.59
1:B:45:GLU:HB2	2:I:483:VAL:HG11	1.85	0.59
2:J:517:MET:SD	2:F:445:PHE:CD1	2.97	0.58
2:F:512:ILE:O	2:F:516:MET:HG3	2.04	0.58
1:B:31:ASP:HB3	1:B:34:ASP:HB2	1.86	0.56
2:I:497:GLN:O	2:I:500:SER:N	2.38	0.56
2:F:444:PHE:CE1	1:D:10:VAL:HG13	2.40	0.56
2:F:443:SER:O	2:F:447:GLN:HB2	2.07	0.55
1:G:92:HIS:NE2	2:I:460:ASP:HB3	2.23	0.54
2:I:518:GLU:OE2	2:I:522:GLN:NE2	2.40	0.54
1:G:56:GLU:HB3	1:G:60:ARG:HH12	1.73	0.54
2:I:471:THR:HG22	2:I:473:CYS:H	1.73	0.53
2:E:537:ASP:O	2:E:541:LYS:N	2.38	0.53
1:C:30:PHE:CZ	2:I:497:GLN:HB2	2.43	0.52
2:J:520:ASP:HA	2:J:523:ARG:HH11	1.75	0.52
1:D:111:GLU:OE2	2:I:451:GLU:N	2.42	0.52
2:F:516:MET:HE1	1:G:18:ILE:HB	1.91	0.52
1:G:100:ASN:OD1	1:G:104:LYS:HE2	2.09	0.52
1:C:32:ILE:HG23	1:C:37:MET:HB2	1.92	0.52
1:B:31:ASP:HA	2:I:498:ASN:ND2	2.25	0.51
2:J:521:TYR:CD1	2:F:440:ILE:HG23	2.46	0.51
2:J:521:TYR:CE1	2:F:441:PRO:HD2	2.45	0.51
2:J:544:ARG:NH2	2:F:539:GLU:OE2	2.40	0.51
2:F:447:GLN:O	2:F:451:GLU:HB2	2.10	0.51
1:G:78:LYS:HD3	1:G:81:MET:HE3	1.92	0.51
1:G:31:ASP:HB3	1:G:34:ASP:HB2	1.92	0.50
2:I:447:GLN:O	2:I:451:GLU:HB2	2.12	0.50
1:C:26:GLN:H	2:I:464:ARG:NH2	2.04	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:512:ILE:O	2:I:516:MET:HG3	2.12	0.49
2:F:493:LEU:HD21	1:D:35:ILE:HB	1.93	0.49
2:E:538:GLU:HG2	2:E:541:LYS:HD2	1.93	0.48
2:J:493:LEU:HD21	1:G:35:ILE:HB	1.95	0.48
2:F:439:ARG:O	2:F:440:ILE:HD13	2.13	0.48
1:B:32:ILE:HG23	1:B:37:MET:HG3	1.95	0.48
2:E:532:SER:O	2:E:536:LYS:HG2	2.13	0.48
1:C:27:ARG:HB2	1:C:28:PRO:C	2.39	0.48
1:B:83:ASP:OD2	1:B:87:LYS:NZ	2.47	0.48
2:E:512:ILE:O	2:E:516:MET:HG3	2.13	0.48
2:E:536:LYS:O	2:E:540:ILE:HG13	2.14	0.48
2:F:467:PRO:HG3	2:F:492:LYS:HE3	1.95	0.47
1:D:31:ASP:HB3	1:D:34:ASP:HB2	1.95	0.47
2:J:512:ILE:O	2:J:516:MET:HG3	2.15	0.47
2:F:466:ILE:HD12	1:D:29:GLN:O	2.15	0.47
1:G:95:ALA:HB1	2:I:458:MET:SD	2.55	0.47
1:C:28:PRO:HD3	2:I:501:GLU:HG2	1.97	0.46
1:C:77:LYS:HE2	1:C:81:MET:HE2	1.97	0.46
1:B:31:ASP:CG	2:I:498:ASN:ND2	2.63	0.46
2:I:520:ASP:HA	2:I:523:ARG:HH11	1.81	0.46
2:J:505:SER:O	2:J:509:LEU:HD23	2.16	0.46
2:F:440:ILE:HG22	2:F:441:PRO:CD	2.45	0.45
1:D:110:TYR:CD1	1:G:110:TYR:HB3	2.51	0.45
2:E:507:THR:HA	2:E:510:THR:HG22	1.98	0.45
2:J:442:HIS:O	2:J:446:THR:HG23	2.16	0.45
2:F:442:HIS:O	2:F:446:THR:HG23	2.17	0.45
2:F:540:ILE:O	2:F:544:ARG:HG2	2.16	0.45
1:B:88:ASP:O	1:B:92[A]:HIS:ND1	2.43	0.45
1:C:42:ASP:OD1	2:E:487:TYR:OH	2.24	0.45
2:E:439:ARG:HG2	2:E:439:ARG:O	2.17	0.45
1:B:81:MET:HG2	2:F:468:CYS:SG	2.56	0.45
2:J:521:TYR:CD2	2:F:440:ILE:CD1	3.00	0.45
2:J:518:GLU:O	2:J:522:GLN:HG3	2.16	0.45
1:G:12:GLY:O	1:G:16:ARG:HG3	2.18	0.44
2:F:471:THR:HG22	2:F:473:CYS:H	1.82	0.44
2:I:498:ASN:OD1	2:I:498:ASN:C	2.59	0.44
1:C:10:VAL:HG13	2:I:444:PHE:CE2	2.52	0.44
2:J:543:LEU:HB3	2:F:543:LEU:HB3	1.99	0.44
2:F:440:ILE:CG2	2:F:441:PRO:HD2	2.48	0.44
2:E:537:ASP:OD1	2:I:536:LYS:NZ	2.39	0.44
2:E:539:GLU:O	2:E:543:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:HIS:NE2	1:G:21:MET:HE3	2.33	0.43
2:I:532:SER:O	2:I:536:LYS:HG3	2.18	0.43
1:C:100:ASN:OD1	1:C:104:LYS:HE2	2.17	0.43
1:D:65:MET:HE3	1:D:65:MET:HB2	1.87	0.43
2:F:532:SER:O	2:F:536:LYS:HG3	2.19	0.43
2:F:511:MET:HE1	1:D:17:HIS:ND1	2.34	0.43
2:F:483:VAL:HG11	1:G:45:GLU:HB2	2.01	0.43
2:F:440:ILE:HG22	2:F:441:PRO:HD2	2.01	0.42
1:B:10:VAL:HG13	2:E:444:PHE:CE1	2.55	0.41
1:D:52:LYS:O	1:D:56:GLU:HG2	2.20	0.41
2:E:509:LEU:O	2:E:513:ARG:HG3	2.21	0.41
1:B:17:HIS:NE2	1:B:21:MET:HE3	2.35	0.41
1:G:23:LEU:HD23	1:G:23:LEU:HA	1.94	0.41
2:I:487:TYR:HB3	2:I:491:ARG:NH1	2.35	0.41
1:C:90:GLN:HB3	1:C:94:ARG:NH2	2.36	0.41
1:C:26:GLN:HE22	1:G:91:LYS:HD3	1.86	0.41
1:C:23:LEU:HD23	1:C:23:LEU:HA	1.83	0.41
1:C:66:ARG:HH11	1:C:66:ARG:HD2	1.77	0.41
2:J:529:LEU:HD12	2:F:526:ILE:HD13	2.02	0.41
2:F:440:ILE:HG22	2:F:441:PRO:N	2.36	0.41
1:C:12:GLY:O	1:C:16:ARG:HG3	2.21	0.41
1:C:45:GLU:HB2	2:E:483:VAL:HG11	2.02	0.41
2:J:516:MET:CE	1:D:15:SER:HA	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	100/124 (81%)	97 (97%)	3 (3%)	0	100	100
1	C	104/124 (84%)	104 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	97/124 (78%)	97 (100%)	0	0	100	100
1	G	105/124 (85%)	104 (99%)	1 (1%)	0	100	100
2	E	75/134 (56%)	75 (100%)	0	0	100	100
2	F	92/134 (69%)	91 (99%)	1 (1%)	0	100	100
2	I	105/134 (78%)	102 (97%)	2 (2%)	1 (1%)	12	24
2	J	107/134 (80%)	106 (99%)	1 (1%)	0	100	100
All	All	785/1032 (76%)	776 (99%)	8 (1%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	470	PRO

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	B	92/110 (84%)	89 (97%)	3 (3%)	33	61
1	C	96/110 (87%)	96 (100%)	0	100	100
1	D	91/110 (83%)	91 (100%)	0	100	100
1	G	97/110 (88%)	96 (99%)	1 (1%)	68	86
2	E	77/122 (63%)	75 (97%)	2 (3%)	40	68
2	F	93/122 (76%)	90 (97%)	3 (3%)	34	62
2	I	100/122 (82%)	97 (97%)	3 (3%)	36	64
2	J	102/122 (84%)	100 (98%)	2 (2%)	48	75
All	All	748/928 (81%)	734 (98%)	14 (2%)	50	76

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

Mol	Chain	Res	Type
1	B	61	LEU

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Mol	Chain	Res	Type
1	B	105	LEU
1	B	109	VAL
2	J	493	LEU
2	J	524	VAL
2	F	491	ARG
2	F	493	LEU
2	F	529	LEU
2	E	439	ARG
2	E	543	LEU
1	G	70	GLU
2	I	493	LEU
2	I	498	ASN
2	I	524	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	100	ASN
2	I	498	ASN

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 [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	B	101/124 (81%)	0.75	2 (1%) 65 61	30, 80, 115, 160	1 (0%)
1	C	106/124 (85%)	0.79	7 (6%) 24 21	51, 83, 120, 168	0
1	D	101/124 (81%)	0.76	10 (9%) 13 11	42, 73, 107, 138	0
1	G	107/124 (86%)	0.70	8 (7%) 20 18	47, 75, 103, 129	0
2	E	81/134 (60%)	1.02	10 (12%) 8 7	46, 91, 138, 147	0
2	F	98/134 (73%)	0.77	6 (6%) 27 23	50, 76, 137, 159	0
2	I	107/134 (79%)	1.08	14 (13%) 7 6	52, 76, 145, 167	0
2	J	109/134 (81%)	0.93	12 (11%) 10 8	40, 78, 128, 157	0
All	All	810/1032 (78%)	0.85	69 (8%) 16 14	30, 79, 132, 168	1 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	503	GLY	6.3
2	I	545	GLY	5.2
2	I	505	SER	5.0
2	J	462	GLY	4.4
1	C	25	SER	4.4
2	I	498	ASN	4.0
2	F	468	CYS	4.0
2	I	500	SER	4.0
2	I	494	SER	3.8
2	E	483	VAL	3.7
1	B	36	GLY	3.7
2	E	543	LEU	3.6
1	D	88	ASP	3.6
1	D	112	THR	3.5
2	J	505	SER	3.4
2	I	504	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	J	546	PHE	3.2
2	J	460	ASP	3.1
2	I	506	SER	3.0
1	G	108	ASN	3.0
2	J	465	GLU	3.0
2	E	505	SER	3.0
2	I	443	SER	3.0
2	I	495	SER	3.0
1	D	62	ASN	2.9
1	C	26	GLN	2.9
1	C	106	ASP	2.8
1	G	28	PRO	2.8
2	J	463	SER	2.8
1	D	28	PRO	2.7
2	E	531	ASP	2.7
1	G	109	VAL	2.7
1	D	108	ASN	2.7
1	C	53	ASP	2.6
1	D	78	LYS	2.6
1	C	27	ARG	2.5
2	J	507	THR	2.5
2	F	506	SER	2.5
2	J	518	GLU	2.5
2	E	524	VAL	2.5
2	F	550	TYR	2.5
2	I	533	LEU	2.5
1	D	73	ALA	2.5
2	J	500	SER	2.5
2	J	547	CYS	2.4
2	E	482	THR	2.4
2	E	485	SER	2.4
2	I	496	LEU	2.4
2	E	439	ARG	2.4
1	G	31	ASP	2.4
1	C	110	TYR	2.4
2	I	458	MET	2.4
1	D	109	VAL	2.3
2	J	468	CYS	2.3
1	C	111	GLU	2.3
1	D	111	GLU	2.3
2	F	547	CYS	2.3
2	F	447	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	497	GLN	2.2
1	G	24	ASN	2.2
1	G	100	ASN	2.2
1	G	52	LYS	2.2
2	E	477	CYS	2.2
1	G	36	GLY	2.2
2	E	496	LEU	2.2
2	J	455	SER	2.1
2	F	444	PHE	2.1
1	D	96	LEU	2.0
1	B	97	MET	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.