Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2022 – 02:10 PM JST

PDB ID	:	7EQC
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 following versions of software and data (see references ⓘ) were used in the production of this report:

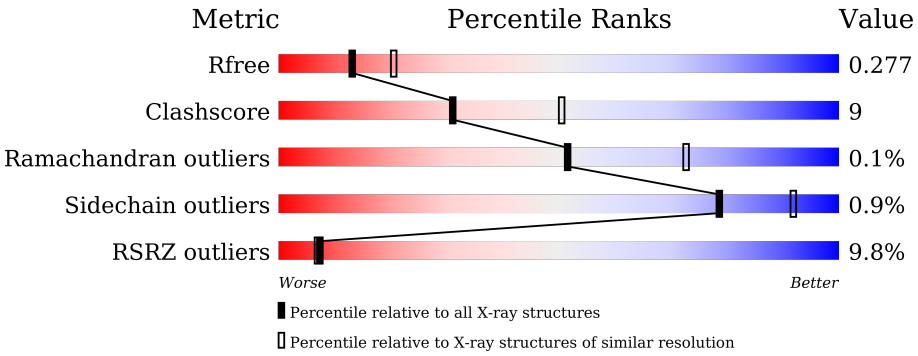
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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.



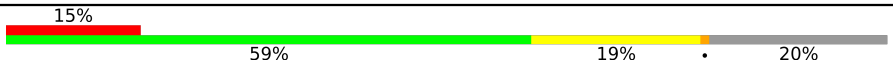
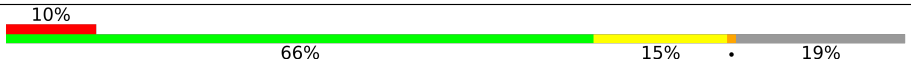
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	4% 67% 14% • 19%
1	C	124	9% 71% 15% 15%
1	D	124	6% 72% 10% 19%
1	G	124	2% 69% 17% 14%
2	E	134	9% 46% 13% • 40%
2	F	134	7% 51% 22% • 27%

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

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

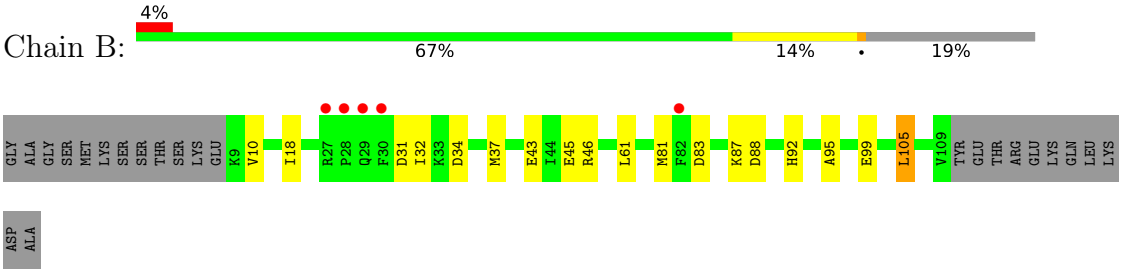
- Molecule 3 is water.

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

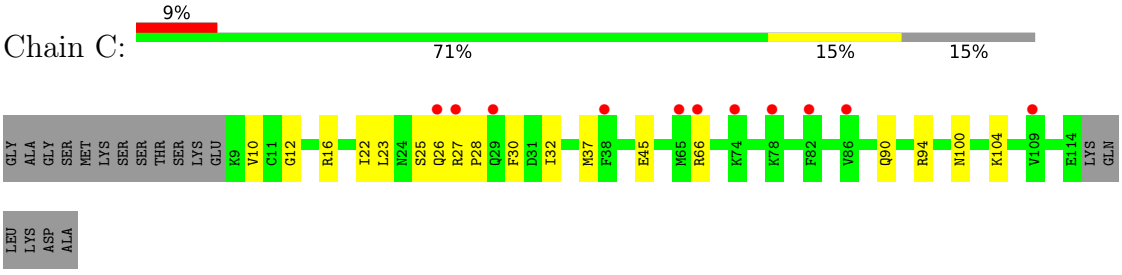
3 Residue-property plots (i)

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.

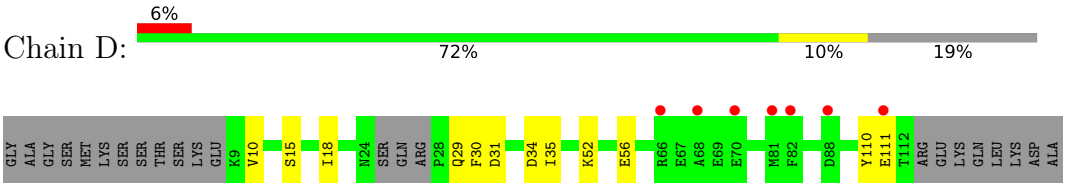
• Molecule 1: CYtoKinesis defect



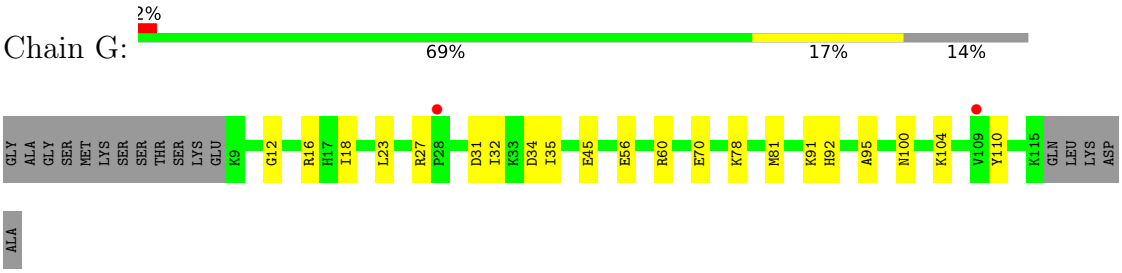
• Molecule 1: CYtoKinesis defect



• Molecule 1: CYtoKinesis defect

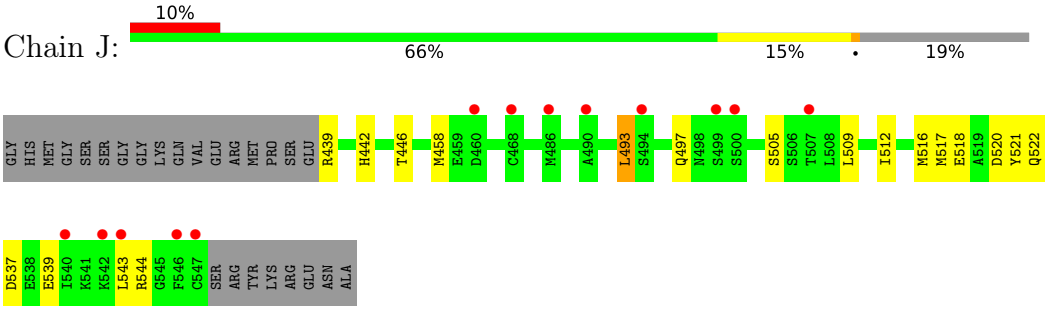


• Molecule 1: CYtoKinesis defect



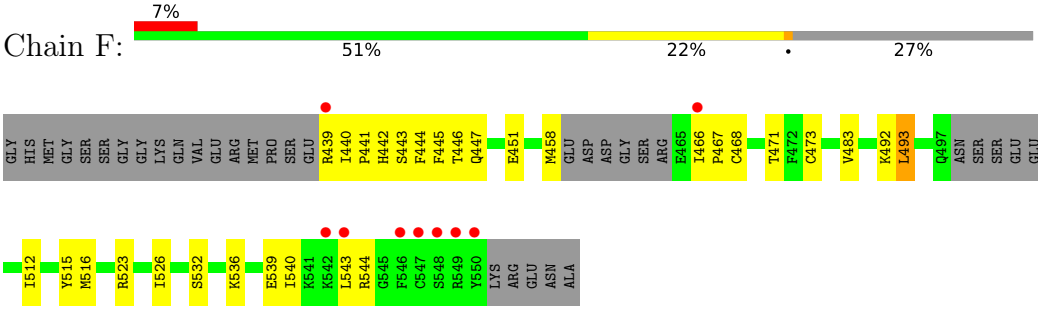
• Molecule 2: Kinesin-like protein

Chain J:



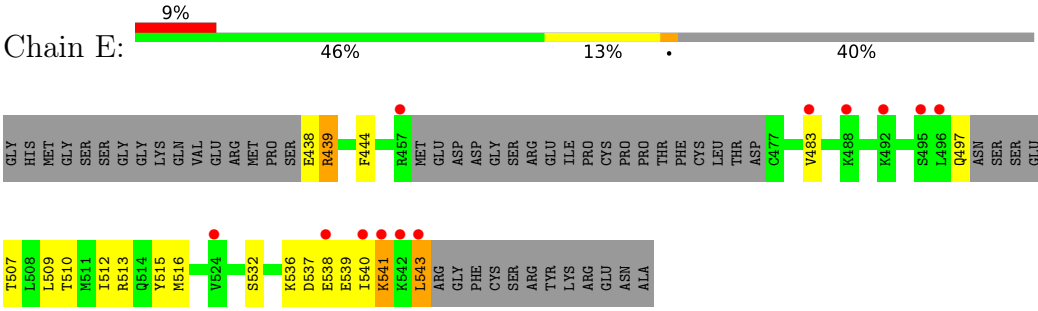
- Molecule 2: Kinesin-like protein

Chain F:



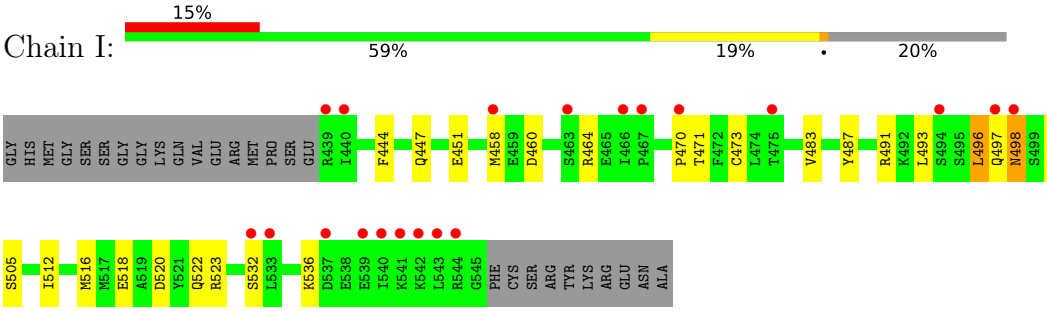
- Molecule 2: Kinesin-like protein

Chain E:



- Molecule 2: Kinesin-like protein

Chain I:



4 Data and refinement statistics (i)

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) 96.0 (41.65-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.238 , 0.277 0.238 , 0.277	Depositor DCC
R_{free} test set	1636 reflections (4.14%)	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)	0.33 , 59.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	B	0.30	0/855	0.57	1/1137 (0.1%)
1	C	0.26	0/893	0.43	0/1188
1	D	0.31	0/846	0.45	0/1124
1	G	0.27	0/902	0.44	0/1199
2	E	0.30	0/679	0.50	2/906 (0.2%)
2	F	0.33	0/822	0.49	0/1101
2	I	0.31	0/878	0.54	1/1180 (0.1%)
2	J	0.30	0/896	0.49	0/1204
All	All	0.30	0/6771	0.49	4/9039 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	105	LEU	CA-CB-CG	-8.82	95.00	115.30
2	I	496	LEU	CA-CB-CG	-7.58	97.86	115.30
2	E	543	LEU	CA-CB-CG	5.83	128.72	115.30
2	E	541	LYS	CD-CE-NZ	5.23	123.72	111.70

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	B	845	0	867	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	883	0	902	22	0
1	D	837	0	857	10	0
1	G	892	0	915	15	0
2	E	671	0	661	17	0
2	F	809	0	794	36	0
2	I	864	0	833	36	0
2	J	881	0	847	24	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	122	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 (122) 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	0.83
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ASP:OD1	2:I:498:ASN:ND2	2.27	0.66
1:B:32:ILE:HD13	2:I:493:LEU:HB3	1.77	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
1:C:28:PRO:HG2	2:I:497:GLN:CD	2.21	0.60
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:B:18:ILE:HB	2:I:516:MET:HE1	1.89	0.54
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
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:F:516:MET:HE1	1:G:18:ILE:HB	1.91	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: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
2:E:515:TYR:CZ	2:I:516:MET:HE2	2.48	0.49
2:I:512:ILE:O	2:I:516:MET:HG3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:516:MET:HE2	2:F:515:TYR:CZ	2.48	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
2:J:516:MET:HE1	1:D:15:SER:HA	1.95	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: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
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:J:537:ASP:OD1	2:F:536:LYS:NZ	2.40	0.45
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:E:439:ARG:HG2	2:E:439:ARG:O	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
2:I:496:LEU:O	2:I:496:LEU:HG	2.11	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
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:J:516:MET:HE1	1:D:18:ILE:HB	2.00	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
1:G:78:LYS:HD3	1:G:81:MET:HE3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:532:SER:O	2:I:536:LYS:HG3	2.18	0.43
1:C:27:ARG:HB2	1:C:28:PRO:C	2.39	0.43
1:C:100:ASN:OD1	1:C:104:LYS:HE2	2.17	0.43
1:C:22:ILE:O	1:C:25:SER:OG	2.23	0.43
2:F:532:SER:O	2:F:536:LYS:HG3	2.19	0.43
2:F:483:VAL:HG11	1:G:45:GLU:HB2	2.01	0.43
2:I:502:GLU:HA	2:I:505:SER:HG	1.83	0.42
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: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
1:B:95:ALA:HB1	2:F:458:MET:HE3	2.04	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
1	D	97/124 (78%)	97 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	15 28
2	J	107/134 (80%)	106 (99%)	1 (1%)	0	100 100
All	All	785/1032 (76%)	776 (99%)	8 (1%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	470	PRO

5.3.2 Protein sidechains (i)

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%)	90 (98%)	2 (2%)	52 77
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%)	76 90
2	E	77/122 (63%)	76 (99%)	1 (1%)	69 87
2	F	93/122 (76%)	92 (99%)	1 (1%)	73 89
2	I	100/122 (82%)	99 (99%)	1 (1%)	76 90
2	J	102/122 (84%)	101 (99%)	1 (1%)	76 90
All	All	748/928 (81%)	741 (99%)	7 (1%)	78 92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	61	LEU
1	B	105	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	493	LEU
2	F	493	LEU
2	E	439	ARG
1	G	70	GLU
2	I	498	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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 monosaccharides 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, 95^{th} 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%)	0.48	5 (4%) 28 30	53, 80, 115, 160	0
1	C	106/124 (85%)	0.72	11 (10%) 6 6	51, 83, 120, 168	0
1	D	101/124 (81%)	0.51	7 (6%) 16 17	42, 73, 107, 138	0
1	G	107/124 (86%)	0.46	2 (1%) 66 69	47, 75, 103, 129	0
2	E	81/134 (60%)	0.94	12 (14%) 2 2	46, 91, 138, 147	0
2	F	98/134 (73%)	0.58	9 (9%) 9 9	50, 76, 137, 159	0
2	I	107/134 (79%)	1.10	20 (18%) 1 1	52, 76, 145, 167	0
2	J	109/134 (81%)	0.93	13 (11%) 4 4	40, 78, 128, 157	0
All	All	810/1032 (78%)	0.71	79 (9%) 7 7	40, 79, 132, 168	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	546	PHE	6.0
2	E	541	LYS	5.9
2	E	540	ILE	5.8
1	C	27	ARG	5.8
2	I	544	ARG	5.5
2	E	543	LEU	5.3
2	J	547	CYS	4.7
2	I	543	LEU	4.7
2	F	546	PHE	4.4
1	D	66	ARG	4.4
2	I	539	GLU	4.3
2	I	541	LYS	4.2
2	F	550	TYR	4.2
2	I	533	LEU	4.0
1	G	109	VAL	3.8
2	E	483	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	498	ASN	3.8
2	E	496	LEU	3.8
2	E	488	LYS	3.8
2	F	547	CYS	3.7
2	I	439	ARG	3.6
2	E	542	LYS	3.5
2	I	542	LYS	3.4
1	B	27	ARG	3.4
2	J	543	LEU	3.2
2	E	457	ARG	3.1
1	B	29	GLN	3.1
1	D	111	GLU	2.9
2	J	460	ASP	2.9
2	I	463	SER	2.9
1	C	66	ARG	2.8
1	C	29	GLN	2.8
2	I	537	ASP	2.7
2	E	524	VAL	2.7
1	B	82	PHE	2.7
2	J	499	SER	2.7
1	D	70	GLU	2.7
2	F	548	SER	2.6
1	B	30	PHE	2.6
2	J	500	SER	2.6
2	I	466	ILE	2.6
2	F	549	ARG	2.6
1	C	38	PHE	2.6
2	J	542	LYS	2.6
2	E	495	SER	2.5
2	J	468	CYS	2.5
2	I	497	GLN	2.5
1	D	88	ASP	2.5
1	C	65	MET	2.5
2	I	470	PRO	2.4
2	F	466	ILE	2.4
2	I	540	ILE	2.4
2	E	492	LYS	2.4
1	C	74	LYS	2.4
1	C	78	LYS	2.3
1	D	81	MET	2.3
2	J	507	THR	2.3
1	C	109	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	543	LEU	2.3
1	B	28	PRO	2.3
1	C	86	VAL	2.2
2	I	475	THR	2.2
2	F	542	LYS	2.2
2	J	540	ILE	2.2
2	I	467	PRO	2.2
2	J	494	SER	2.2
1	C	26	GLN	2.2
2	J	490	ALA	2.2
2	I	440	ILE	2.2
1	G	28	PRO	2.2
2	I	494	SER	2.2
2	J	486	MET	2.1
1	D	68	ALA	2.1
1	C	82	PHE	2.1
1	D	82	PHE	2.1
2	I	532	SER	2.1
2	I	458	MET	2.1
2	E	538	GLU	2.0
2	F	439	ARG	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 monosaccharides 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.