



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:12 am BST

PDB ID : 5Z38
Title : Crystal structure of CsrA bound to CesT
Authors : Ye, F.; Yang, F.; Yu, R.; Lin, X.; Qi, J.; Chen, Z.; Gao, G.F.; Lu, G.
Deposited on : 2018-01-05
Resolution : 2.29 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	:	2.11
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)	:	2.11

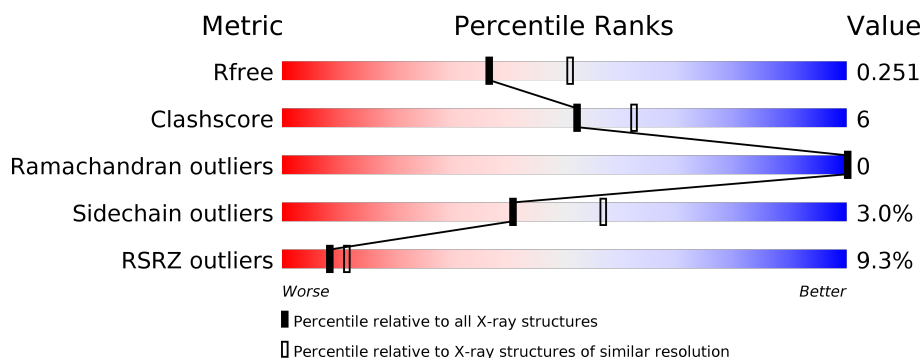
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	158	<div> <div>7%</div> <div>85% 11% ..</div> </div>
1	B	158	<div> <div>%</div> <div>79% 16% ..</div> </div>
1	C	158	<div> <div>6%</div> <div>83% 14% ..</div> </div>
1	D	158	<div> <div>18%</div> <div>78% 16% 5%</div> </div>
2	E	49	<div> <div></div> <div>78% .. 16%</div> </div>
2	G	49	<div> <div>12%</div> <div>65% 18% 16%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	49	<div> <div>12%</div> <div>73%</div> <div>14%</div> <div>12%</div> </div>
2	K	49	<div> <div>31%</div> <div>73%</div> <div>10%</div> <div>16%</div> </div>
3	F	71	<div> <div>6%</div> <div>70%</div> <div>11%</div> <div>18%</div> </div>
3	H	71	<div> <div>4%</div> <div>73%</div> <div>6%</div> <div>21%</div> </div>
3	J	71	<div> <div>1%</div> <div>58%</div> <div>17%</div> <div>23%</div> </div>
3	L	71	<div> <div>8%</div> <div>69%</div> <div>7%</div> <div>24%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7968 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 CesT protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1228	781	194	245	8			
1	B	154	Total	C	N	O	S	0	0	0
			1228	781	194	245	8			
1	C	155	Total	C	N	O	S	0	0	0
			1232	783	195	246	8			
1	D	150	Total	C	N	O	S	0	0	0
			1197	764	190	236	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q5WMC8
A	0	PRO	-	expression tag	UNP Q5WMC8
B	-1	GLY	-	expression tag	UNP Q5WMC8
B	0	PRO	-	expression tag	UNP Q5WMC8
C	-1	GLY	-	expression tag	UNP Q5WMC8
C	0	PRO	-	expression tag	UNP Q5WMC8
D	-1	GLY	-	expression tag	UNP Q5WMC8
D	0	PRO	-	expression tag	UNP Q5WMC8

- Molecule 2 is a protein called Truncated-CsrA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	41	Total	C	N	O	S	0	0	0
			299	188	54	55	2			
2	G	41	Total	C	N	O	S	0	0	0
			299	188	54	55	2			
2	I	43	Total	C	N	O	S	0	0	0
			312	196	57	57	2			
2	K	41	Total	C	N	O	S	0	0	0
			299	188	54	55	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	GLY	-	expression tag	UNP B7UHB4
E	-3	PRO	-	expression tag	UNP B7UHB4
E	-2	LEU	-	expression tag	UNP B7UHB4
E	-1	GLY	-	expression tag	UNP B7UHB4
E	0	SER	-	expression tag	UNP B7UHB4
G	-4	GLY	-	expression tag	UNP B7UHB4
G	-3	PRO	-	expression tag	UNP B7UHB4
G	-2	LEU	-	expression tag	UNP B7UHB4
G	-1	GLY	-	expression tag	UNP B7UHB4
G	0	SER	-	expression tag	UNP B7UHB4
I	-4	GLY	-	expression tag	UNP B7UHB4
I	-3	PRO	-	expression tag	UNP B7UHB4
I	-2	LEU	-	expression tag	UNP B7UHB4
I	-1	GLY	-	expression tag	UNP B7UHB4
I	0	SER	-	expression tag	UNP B7UHB4
K	-4	GLY	-	expression tag	UNP B7UHB4
K	-3	PRO	-	expression tag	UNP B7UHB4
K	-2	LEU	-	expression tag	UNP B7UHB4
K	-1	GLY	-	expression tag	UNP B7UHB4
K	0	SER	-	expression tag	UNP B7UHB4

- Molecule 3 is a protein called wild type CsrA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	58	Total	C	N	O	S	0	0	0
			445	276	83	84	2			
3	H	56	Total	C	N	O	S	0	0	0
			437	272	81	82	2			
3	J	55	Total	C	N	O	S	0	0	0
			431	269	80	80	2			
3	L	54	Total	C	N	O	S	0	0	0
			423	264	79	79	1			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	GLY	-	linker	UNP B7UHB4
F	-8	GLY	-	linker	UNP B7UHB4
F	-7	GLY	-	linker	UNP B7UHB4
F	-6	GLY	-	linker	UNP B7UHB4
F	-5	SER	-	linker	UNP B7UHB4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	GLY	-	linker	UNP B7UHB4
F	-3	GLY	-	linker	UNP B7UHB4
F	-2	GLY	-	linker	UNP B7UHB4
F	-1	GLY	-	linker	UNP B7UHB4
F	0	SER	-	linker	UNP B7UHB4
H	-9	GLY	-	linker	UNP B7UHB4
H	-8	GLY	-	linker	UNP B7UHB4
H	-7	GLY	-	linker	UNP B7UHB4
H	-6	GLY	-	linker	UNP B7UHB4
H	-5	SER	-	linker	UNP B7UHB4
H	-4	GLY	-	linker	UNP B7UHB4
H	-3	GLY	-	linker	UNP B7UHB4
H	-2	GLY	-	linker	UNP B7UHB4
H	-1	GLY	-	linker	UNP B7UHB4
H	0	SER	-	linker	UNP B7UHB4
J	-9	GLY	-	linker	UNP B7UHB4
J	-8	GLY	-	linker	UNP B7UHB4
J	-7	GLY	-	linker	UNP B7UHB4
J	-6	GLY	-	linker	UNP B7UHB4
J	-5	SER	-	linker	UNP B7UHB4
J	-4	GLY	-	linker	UNP B7UHB4
J	-3	GLY	-	linker	UNP B7UHB4
J	-2	GLY	-	linker	UNP B7UHB4
J	-1	GLY	-	linker	UNP B7UHB4
J	0	SER	-	linker	UNP B7UHB4
L	-9	GLY	-	linker	UNP B7UHB4
L	-8	GLY	-	linker	UNP B7UHB4
L	-7	GLY	-	linker	UNP B7UHB4
L	-6	GLY	-	linker	UNP B7UHB4
L	-5	SER	-	linker	UNP B7UHB4
L	-4	GLY	-	linker	UNP B7UHB4
L	-3	GLY	-	linker	UNP B7UHB4
L	-2	GLY	-	linker	UNP B7UHB4
L	-1	GLY	-	linker	UNP B7UHB4
L	0	SER	-	linker	UNP B7UHB4

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	27	Total O 27 27	0	0

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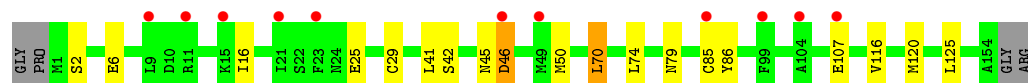
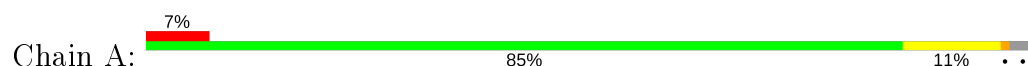
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	15	Total 15	O 15	0	0
4	D	16	Total 16	O 16	0	0
4	E	12	Total 12	O 12	0	0
4	F	11	Total 11	O 11	0	0
4	G	8	Total 8	O 8	0	0
4	H	9	Total 9	O 9	0	0
4	I	8	Total 8	O 8	0	0
4	J	8	Total 8	O 8	0	0
4	K	7	Total 7	O 7	0	0
4	L	6	Total 6	O 6	0	0

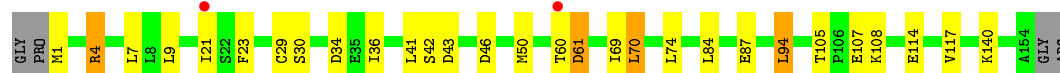
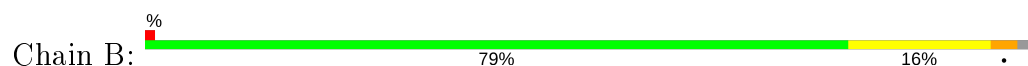
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

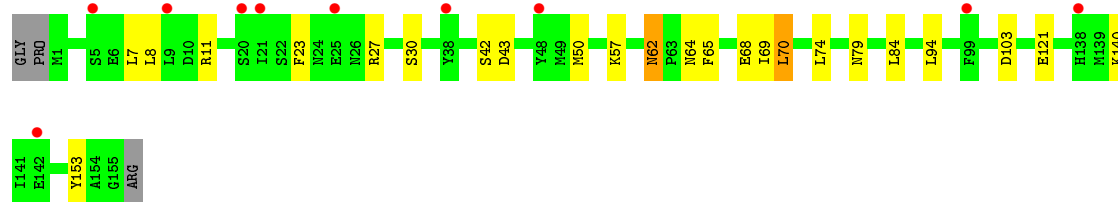
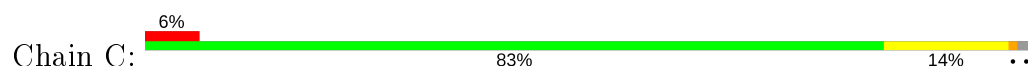
• Molecule 1: CesT protein



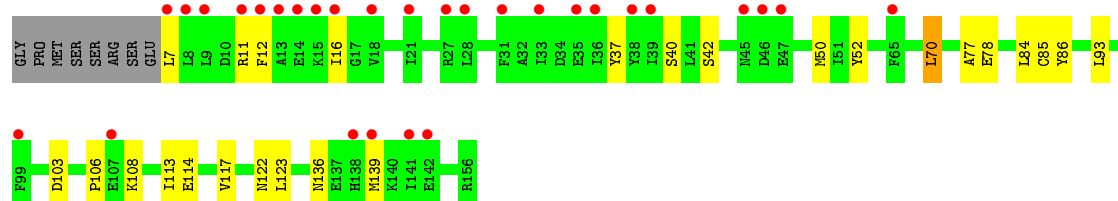
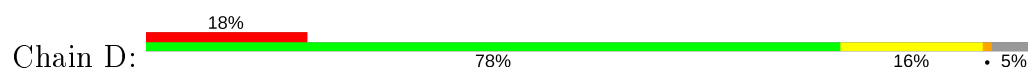
• Molecule 1: CesT protein




• Molecule 1: CesT protein



• Molecule 1: CesT protein



• Molecule 2: Truncated-CsrA

Chain E:  78% 16%




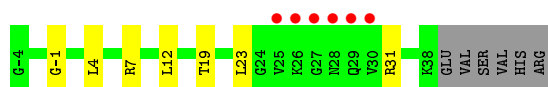
- Molecule 2: Truncated-CsrA

Chain G:  12% 65% 18% 16%




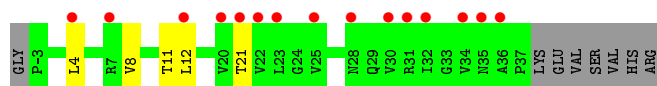
- Molecule 2: Truncated-CsrA

Chain I:  12% 73% 14% 12%



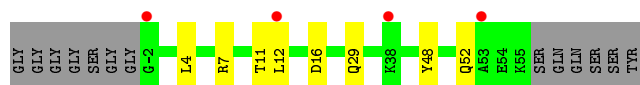
- Molecule 2: Truncated-CsrA

Chain K:  31% 73% 10% 16%




- Molecule 3: wild type CsrA

Chain F:  6% 70% 11% 18%



- Molecule 3: wild type CsrA

Chain H:  4% 73% 6% 21%



- Molecule 3: wild type CsrA

Chain J:  % 58% 17% 23%



- Molecule 3: wild type CsrA

GLY
GLY
GLY
GLY
SER
GLY
GLY
GLY
GLY
SER
MET
L2
L3
L4
R7
V25
K26
G27
N28
Q29
V30
K38
R50
K55
SER
GLN
SER
SER
TYR

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	252.75Å 52.55Å 93.36Å 90.00° 96.73° 90.00°	Depositor
Resolution (Å)	49.35 – 2.29 49.35 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.35-2.29) 98.8 (49.35-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.233 , 0.251 0.234 , 0.251	Depositor DCC
R_{free} test set	2677 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7968	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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	0.26	0/1253	0.42	0/1696
1	B	0.42	0/1253	0.50	0/1696
1	C	0.28	0/1257	0.42	0/1701
1	D	0.29	0/1222	0.46	0/1655
2	E	0.25	0/300	0.55	0/405
2	G	0.25	0/300	0.55	0/405
2	I	0.26	0/313	0.48	0/422
2	K	0.24	0/300	0.54	0/405
3	F	0.27	0/447	0.48	0/600
3	H	0.25	0/439	0.48	0/590
3	J	0.25	0/433	0.48	0/582
3	L	0.25	0/425	0.46	0/572
All	All	0.30	0/7942	0.47	0/10729

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	1228	0	1179	16	0
1	B	1228	0	1179	22	0
1	C	1232	0	1182	19	0
1	D	1197	0	1149	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	299	0	329	4	0
2	G	299	0	329	5	0
2	I	312	0	345	4	0
2	K	299	0	329	3	0
3	F	445	0	472	5	0
3	H	437	0	466	2	0
3	J	431	0	461	9	0
3	L	423	0	449	3	0
4	A	11	0	0	0	0
4	B	27	0	0	2	0
4	C	15	0	0	2	0
4	D	16	0	0	2	0
4	E	12	0	0	0	0
4	F	11	0	0	0	0
4	G	8	0	0	0	0
4	H	9	0	0	0	0
4	I	8	0	0	0	0
4	J	8	0	0	0	0
4	K	7	0	0	0	0
4	L	6	0	0	1	0
All	All	7968	0	7869	87	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 6.

All (87) 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:121:GLU:OE1	2:E:4:LEU:HA	1.66	0.94
1:B:87:GLU:HB2	1:B:94:LEU:HD21	1.57	0.86
1:D:84:LEU:HD21	1:D:123:LEU:HD11	1.66	0.78
2:G:7:ARG:HG2	3:H:29:GLN:HG2	1.65	0.78
1:B:61:ASP:N	1:B:61:ASP:OD1	2.13	0.76
1:D:42:SER:HB3	1:D:50:MET:HB2	1.71	0.72
3:F:4:LEU:HD11	3:F:12:LEU:HD13	1.72	0.71
1:D:122:ASN:OD1	3:J:44:ARG:NH1	2.24	0.70
1:A:42:SER:HB3	1:A:50:MET:HB2	1.76	0.68
2:G:17:GLU:HG3	2:G:37:PRO:HB3	1.77	0.66
1:B:30:SER:HB3	1:B:140:LYS:HD2	1.79	0.65
1:C:7:LEU:HD21	1:C:11:ARG:HH21	1.64	0.63
1:D:7:LEU:N	4:D:202:HOH:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ARG:HD2	1:C:43:ASP:HB3	1.82	0.61
2:E:7:ARG:HD2	3:F:29:GLN:HB3	1.83	0.60
1:A:86:TYR:HB3	1:C:70:LEU:HB3	1.84	0.60
1:B:42:SER:HB3	1:B:50:MET:HB2	1.84	0.58
1:A:74:LEU:HD21	1:C:94:LEU:HD11	1.86	0.58
3:L:25:VAL:HG22	3:L:30:VAL:HG22	1.85	0.58
3:L:7:ARG:NH1	4:L:101:HOH:O	2.37	0.58
1:B:105:THR:HB	1:B:108:LYS:HG3	1.85	0.57
2:G:18:VAL:HG11	3:H:14:ILE:HG21	1.86	0.57
2:I:-1:GLY:HA2	3:J:38:LYS:HG3	1.86	0.56
2:K:11:THR:HG23	2:K:21:THR:HG22	1.85	0.56
2:E:29:GLN:HG2	3:F:7:ARG:HG2	1.87	0.56
1:B:70:LEU:HB3	1:D:86:TYR:HB3	1.88	0.55
2:I:23:LEU:HB2	2:I:31:ARG:HG2	1.89	0.54
1:C:23:PHE:HB3	1:C:27:ARG:HA	1.89	0.54
1:A:2:SER:HB3	1:A:6:GLU:HB2	1.90	0.54
1:B:70:LEU:HD13	1:D:70:LEU:HD13	1.90	0.53
3:J:25:VAL:HG12	3:J:30:VAL:HG22	1.90	0.53
3:J:6:ARG:HD2	3:J:12:LEU:HB3	1.91	0.53
1:B:4:ARG:NH1	1:B:46:ASP:O	2.41	0.53
1:A:79:ASN:ND2	1:C:153:TYR:O	2.37	0.52
1:D:11:ARG:HG3	1:D:106:PRO:HG2	1.92	0.51
1:A:45:ASN:OD1	1:A:46:ASP:N	2.43	0.51
1:D:114:GLU:HA	1:D:117:VAL:HG22	1.92	0.51
2:K:4:LEU:HD11	2:K:12:LEU:HG	1.91	0.51
1:A:25:GLU:H	1:A:25:GLU:CD	2.15	0.50
1:B:114:GLU:HA	1:B:117:VAL:HG22	1.92	0.50
1:B:105:THR:HG22	1:B:107:GLU:H	1.76	0.50
1:A:125:LEU:HD12	2:G:4:LEU:HD21	1.95	0.49
1:B:69:ILE:HG23	1:B:84:LEU:HD13	1.96	0.48
3:J:1:MET:N	3:J:1:MET:SD	2.86	0.46
1:B:29:CYS:SG	1:B:41:LEU:HB2	2.56	0.46
1:A:107:GLU:N	1:A:107:GLU:OE1	2.48	0.46
1:A:70:LEU:HD22	1:C:70:LEU:HD22	1.98	0.46
1:C:79:ASN:ND2	4:C:204:HOH:O	2.42	0.46
1:B:1:MET:N	4:B:202:HOH:O	2.34	0.46
2:I:4:LEU:HD13	2:I:12:LEU:HD22	1.98	0.45
2:G:-2:LEU:HD12	2:G:3:ILE:HD11	1.98	0.45
3:J:46:GLU:HG2	3:J:47:ILE:N	2.31	0.45
1:B:60:THR:O	1:B:60:THR:OG1	2.34	0.44
1:B:70:LEU:HD22	1:D:70:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HA	1:A:16:ILE:HD13	1.83	0.44
1:B:23:PHE:CE1	1:B:43:ASP:HB2	2.53	0.44
3:F:48:TYR:O	3:F:52:GLN:HG2	2.18	0.44
1:C:30:SER:HB2	1:C:140:LYS:HD3	2.00	0.44
1:D:77:ALA:O	4:D:201:HOH:O	2.21	0.43
1:D:136:ASN:OD1	1:D:139:MET:HG3	2.18	0.43
2:I:31:ARG:HD3	3:J:3:ILE:HD11	2.01	0.43
1:C:69:ILE:HG23	1:C:84:LEU:HD13	2.00	0.43
1:D:12:PHE:O	1:D:16:ILE:HG13	2.18	0.43
1:B:74:LEU:HG	1:D:85:CYS:HB3	1.99	0.43
1:A:116:VAL:O	1:A:120:MET:HG3	2.18	0.43
1:B:9:LEU:HD21	1:B:21:ILE:HG22	2.01	0.42
1:C:42:SER:OG	1:C:50:MET:HB2	2.19	0.42
1:D:113:ILE:O	1:D:117:VAL:HG13	2.19	0.42
1:A:29:CYS:SG	1:A:41:LEU:HB2	2.60	0.42
1:B:34:ASP:O	1:B:36:ILE:HG13	2.20	0.42
1:D:103:ASP:O	1:D:108:LYS:NZ	2.41	0.42
2:K:8:VAL:HG23	3:L:28:ASN:HB2	2.02	0.41
1:B:23:PHE:CZ	1:B:43:ASP:HB2	2.55	0.41
1:B:9:LEU:HD22	1:B:23:PHE:CE2	2.55	0.41
3:F:16:ASP:N	3:F:16:ASP:OD1	2.53	0.41
1:B:4:ARG:H	1:B:4:ARG:HG3	1.57	0.41
1:C:103:ASP:OD1	4:C:201:HOH:O	2.22	0.41
1:A:85:CYS:HB3	1:C:74:LEU:HG	2.02	0.41
1:D:40:SER:HB2	1:D:52:TYR:HB2	2.02	0.41
3:J:18:VAL:HA	3:J:35:ASN:O	2.21	0.41
1:C:121:GLU:OE1	2:E:4:LEU:CA	2.54	0.41
3:J:19:THR:OG1	3:J:35:ASN:HB2	2.21	0.41
1:A:86:TYR:CB	1:C:70:LEU:HB3	2.51	0.41
1:C:62:ASN:HB3	1:C:65:PHE:HB2	2.03	0.41
1:C:64:ASN:O	1:C:68:GLU:HG2	2.21	0.40
4:B:205:HOH:O	1:D:78:GLU:HG3	2.21	0.40
1:A:70:LEU:HD13	1:C:70:LEU:HD13	2.03	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	152/158 (96%)	146 (96%)	6 (4%)	0	100	100
1	B	152/158 (96%)	145 (95%)	7 (5%)	0	100	100
1	C	153/158 (97%)	147 (96%)	6 (4%)	0	100	100
1	D	148/158 (94%)	142 (96%)	6 (4%)	0	100	100
2	E	39/49 (80%)	38 (97%)	1 (3%)	0	100	100
2	G	39/49 (80%)	38 (97%)	1 (3%)	0	100	100
2	I	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
2	K	39/49 (80%)	39 (100%)	0	0	100	100
3	F	56/71 (79%)	55 (98%)	1 (2%)	0	100	100
3	H	54/71 (76%)	54 (100%)	0	0	100	100
3	J	53/71 (75%)	48 (91%)	5 (9%)	0	100	100
3	L	52/71 (73%)	52 (100%)	0	0	100	100
All	All	978/1112 (88%)	943 (96%)	35 (4%)	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	136/138 (99%)	134 (98%)	2 (2%)	65	79
1	B	136/138 (99%)	131 (96%)	5 (4%)	34	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	136/138 (99%)	132 (97%)	4 (3%)	42	58
1	D	131/138 (95%)	128 (98%)	3 (2%)	50	67
2	E	34/41 (83%)	33 (97%)	1 (3%)	42	58
2	G	34/41 (83%)	32 (94%)	2 (6%)	19	27
2	I	35/41 (85%)	33 (94%)	2 (6%)	20	28
2	K	34/41 (83%)	34 (100%)	0	100	100
3	F	49/56 (88%)	48 (98%)	1 (2%)	55	72
3	H	49/56 (88%)	47 (96%)	2 (4%)	30	43
3	J	48/56 (86%)	45 (94%)	3 (6%)	18	24
3	L	47/56 (84%)	46 (98%)	1 (2%)	53	70
All	All	869/940 (92%)	843 (97%)	26 (3%)	41	57

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	70	LEU
1	B	4	ARG
1	B	7	LEU
1	B	61	ASP
1	B	70	LEU
1	B	94	LEU
1	C	8	LEU
1	C	57	LYS
1	C	62	ASN
1	C	70	LEU
1	D	37	TYR
1	D	70	LEU
1	D	93	LEU
2	E	7	ARG
3	F	11	THR
2	G	2	LEU
2	G	26	LYS
3	H	16	ASP
3	H	19	THR
2	I	7	ARG
2	I	19	THR
3	J	1	MET

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Mol	Chain	Res	Type
3	J	2	LEU
3	J	35	ASN
3	L	50	ARG

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

Mol	Chain	Res	Type
2	G	35	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 carbohydrates 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	154/158 (97%)	0.89	11 (7%) 16 21	57, 81, 121, 141	0
1	B	154/158 (97%)	0.34	2 (1%) 77 81	49, 76, 113, 176	0
1	C	155/158 (98%)	0.70	10 (6%) 18 24	55, 89, 135, 167	0
1	D	150/158 (94%)	1.00	29 (19%) 1 1	55, 90, 148, 196	0
2	E	41/49 (83%)	0.33	0 100 100	47, 61, 91, 117	0
2	G	41/49 (83%)	0.74	6 (14%) 2 3	54, 65, 108, 139	0
2	I	43/49 (87%)	0.96	6 (13%) 2 4	66, 86, 127, 139	0
2	K	41/49 (83%)	1.52	15 (36%) 0 0	49, 98, 142, 192	0
3	F	58/71 (81%)	0.44	4 (6%) 16 22	46, 68, 114, 159	0
3	H	56/71 (78%)	0.70	3 (5%) 25 32	50, 73, 110, 125	0
3	J	55/71 (77%)	0.55	1 (1%) 68 74	65, 90, 133, 141	0
3	L	54/71 (76%)	0.66	6 (11%) 5 7	55, 91, 123, 134	0
All	All	1002/1112 (90%)	0.72	93 (9%) 8 11	46, 82, 134, 196	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	30	VAL	5.8
2	K	12	LEU	5.5
1	B	60	THR	5.3
2	I	27	GLY	5.1
1	D	46	ASP	4.9
1	D	9	LEU	4.8
2	K	25	VAL	4.8
2	K	22	VAL	4.6
1	A	9	LEU	4.5
1	D	138	HIS	4.4
1	A	21	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	11	ARG	4.2
2	I	26	LYS	4.1
2	G	-3	PRO	4.1
1	D	38	TYR	4.0
3	L	3	ILE	3.8
1	D	141	ILE	3.8
1	D	31	PHE	3.7
1	D	18	VAL	3.7
1	D	14	GLU	3.7
2	K	20	VAL	3.7
1	D	139	MET	3.7
1	C	21	ILE	3.6
2	I	25	VAL	3.6
2	K	31	ARG	3.6
1	D	142	GLU	3.6
1	D	12	PHE	3.4
2	I	28	ASN	3.4
1	A	104	ALA	3.4
1	D	16	ILE	3.3
3	H	11	THR	3.1
1	C	9	LEU	3.1
3	F	53	ALA	3.1
1	A	11	ARG	3.0
1	B	21	ILE	3.0
1	C	138	HIS	2.9
1	A	46	ASP	2.9
1	A	23	PHE	2.9
1	C	38	TYR	2.9
2	K	36	ALA	2.9
3	L	29	GLN	2.9
3	F	-2	GLY	2.9
1	D	8	LEU	2.9
2	K	4	LEU	2.9
3	J	2	LEU	2.8
2	K	23	LEU	2.8
1	C	25	GLU	2.8
2	K	7	ARG	2.8
3	H	12	LEU	2.8
1	D	21	ILE	2.7
1	A	85	CYS	2.7
3	L	25	VAL	2.7
1	D	47	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	28	LEU	2.7
2	K	32	ILE	2.6
1	D	36	ILE	2.6
1	C	99	PHE	2.6
1	A	15	LYS	2.5
1	C	142	GLU	2.5
3	H	53	ALA	2.5
1	D	45	ASN	2.5
2	G	12	LEU	2.5
1	D	99	PHE	2.4
2	I	30	VAL	2.4
1	A	99	PHE	2.4
1	D	65	PHE	2.4
3	L	38	LYS	2.3
2	I	29	GLN	2.3
3	L	4	LEU	2.3
1	D	7	LEU	2.3
2	G	2	LEU	2.2
1	D	107	GLU	2.2
1	D	15	LYS	2.2
2	K	35	ASN	2.2
2	K	34	VAL	2.2
2	K	21	THR	2.2
3	L	26	LYS	2.2
1	C	5	SER	2.2
1	A	49	MET	2.2
1	D	33	ILE	2.2
2	G	3	ILE	2.2
2	G	4	LEU	2.2
3	F	12	LEU	2.2
1	A	107	GLU	2.1
1	D	39	ILE	2.1
1	D	27	ARG	2.1
1	D	13	ALA	2.1
3	F	38	LYS	2.1
2	G	32	ILE	2.1
1	C	48	TYR	2.1
1	D	35	GLU	2.0
1	C	20	SER	2.0
2	K	28	ASN	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 carbohydrates 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.