Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2022 – 12:01 PM EDT

PDB ID	:	8D06
Title	:	Hallucinated C3 protein assembly HALC3_104
Authors	:	Ragotte, R.J.; Bera, A.K.; Wicky, B.I.M.; Milles, L.F.; Baker, D.
Deposited on	:	2022-05-25
Resolution	:	3.40 Å(reported)

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

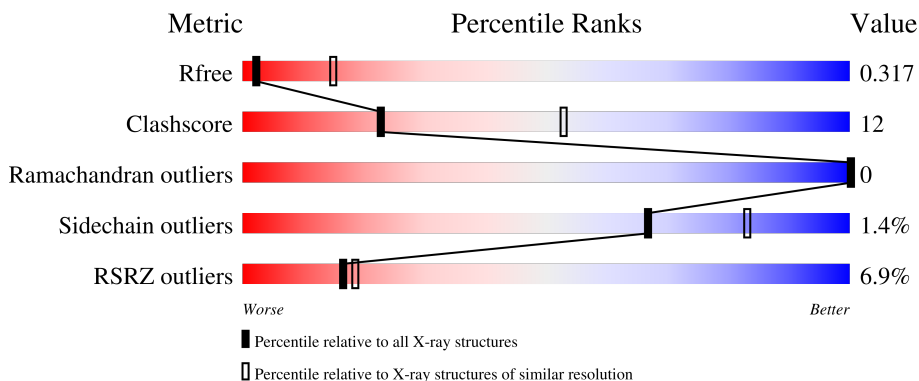|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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	A	70	3% / 73% 19% 9%
1	B	70	4% / 77% 19% •
1	C	70	80% 16% •
1	D	70	.% / 59% 34% 7%
1	E	70	6% / 43% 51% 6%

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Mol	Chain	Length	Quality of chain
1	F	70	4% 67% 27% 6%
1	G	70	23% 46% 39% 14%
1	H	70	13% 73% 19% 9%
1	I	70	10% 50% 34% 16%
1	J	70	3% 70% 24% 6%
1	K	70	3% 61% 33% 6%
1	L	70	7% 77% 19%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 6341 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 HALC3_104.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	S	0	0	0
			525	334	82	107	2			
1	B	67	Total	C	N	O	S	0	0	0
			542	344	86	110	2			
1	C	67	Total	C	N	O	S	0	0	0
			542	344	86	110	2			
1	D	65	Total	C	N	O	S	0	0	0
			534	340	84	108	2			
1	E	66	Total	C	N	O	S	0	0	0
			538	342	85	109	2			
1	F	66	Total	C	N	O	S	0	0	0
			538	342	85	109	2			
1	H	64	Total	C	N	O	S	0	0	0
			525	334	82	107	2			
1	G	60	Total	C	N	O	S	0	0	0
			491	315	74	100	2			
1	I	59	Total	C	N	O	S	0	0	0
			488	313	77	96	2			
1	L	67	Total	C	N	O	S	0	0	0
			542	344	86	110	2			
1	K	66	Total	C	N	O	S	0	0	0
			538	342	85	109	2			
1	J	66	Total	C	N	O	S	0	0	0
			538	342	85	109	2			

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: HALC3_104

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- Molecule 1: HALC3_104

Chain F:

4%

67% 27% 6%

MET SER G3 I6 D7 E8 I9 K12 L13 K14 H15 L16 E17 E18 L23 M27 M30 L31 E32 L33 S38 Y47 E55 L58 K59 T62 I68 GLY SER

• Molecule 1: HALC3_104

Chain H:

13%

73% 19% 9%

MET SER GLY LYS R5 I6 D7 E10 L13 K14 F19 T20 L23 L26 E32 L33 L34 K35 L36 S42 D43 Y47 L58 A61 T62 E63 K67 I68 GLY SER

• Molecule 1: HALC3_104

Chain G:

23%

46% 39% • 14%

MET SER GLY LYS ARG I6 I9 E10 L13 K14 H15 L16 E17 E18 F19 T20 T21 H22 L23 I24 K25 L26 M27 E28 T29 M30 L31 E32 L33 L34 K35 L36 V37 S38 D39 G40 LYS SER ASP S44 Y47 L50 A54 Y57 Q60 A64 A65 K66 K67 I68 GLY SER

• Molecule 1: HALC3_104

Chain I:

10%

50% 34% 16%

MET SER GLY LYS R5 I9 E10 S11 K12 L13 K14 H15 L16 F19 T20 T21 I24 K25 L26 M27 M30 L31 E32 L36 V37 K41 ASP SER GLU E46 Y47 K48 E49 K53 A54 E55 E56 Y57 A61 A64 K67 ILE GLY SER

• Molecule 1: HALC3_104

Chain L:

7%

77% 19% •

MET SER G3 I6 E10 L13 K14 H15 E18 F19 T20 L23 L26 L34 K35 L36 V37 S38 K41 Y47 E55 K59 G69 SER

• Molecule 1: HALC3_104

Chain K:

3%

61% 33% 6%

MET SER G3 I6 D7 E8 I9 E10 S11 K12 L13 L16 E17 E18 F19 T20 L23 I24 M27 L31 E32 L33 L34 K35 S38 Y47 E52 E55 T62 E63 A64 K66 K67 I68 GLY SER

• Molecule 1: HALC3_104

Chain J:

3%

70% 24% 6%

MET SER GLY K4 R5 I6 D7 E8 I9 E10 S11 K12 L13 K14 H15 F19 L23 I26 M30 L33 V37 S38 S42 D43 I68 G69 SER

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	107.50Å 107.50Å 111.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.45 – 3.40 77.45 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (77.45-3.40) 99.4 (77.45-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.284 , 0.309 0.281 , 0.317	Depositor DCC
R_{free} test set	1005 reflections (5.75%)	wwPDB-VP
Wilson B-factor (Å^2)	118.2	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 90.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-l,-k 0.000 for -h,l,k 0.000 for l,-k,h 0.016 for -l,-k,-h 0.047 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6341	wwPDB-VP
Average B, all atoms (Å^2)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	A	0.24	0/529	0.38	0/704
1	B	0.26	0/546	0.40	0/725
1	C	0.25	0/546	0.42	0/725
1	D	0.25	0/538	0.42	0/715
1	E	0.27	0/542	0.50	0/720
1	F	0.25	0/542	0.41	0/720
1	G	0.25	0/494	0.44	0/657
1	H	0.24	0/529	0.39	0/704
1	I	0.24	0/491	0.46	0/651
1	J	0.24	0/542	0.41	0/720
1	K	0.24	0/542	0.40	0/720
1	L	0.26	0/546	0.41	0/725
All	All	0.25	0/6387	0.42	0/8486

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 ⓘ

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	525	0	544	10	0
1	B	542	0	563	10	0
1	C	542	0	563	9	0
1	D	534	0	557	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	538	0	560	33	0
1	F	538	0	560	16	0
1	G	491	0	508	21	0
1	H	525	0	544	11	0
1	I	488	0	512	18	0
1	J	538	0	560	15	0
1	K	538	0	560	18	0
1	L	542	0	563	10	0
All	All	6341	0	6594	149	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 12.

All (149) 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:D:16:LEU:HD21	1:F:16:LEU:HD21	1.57	0.86
1:G:32:GLU:HA	1:G:35:LYS:HD2	1.65	0.76
1:G:64:ALA:HA	1:G:67:LYS:HD2	1.74	0.70
1:G:18:GLU:O	1:G:22:HIS:ND1	2.21	0.68
1:K:13:LEU:HD11	1:J:9:ILE:HG23	1.77	0.65
1:L:23:LEU:HD21	1:K:23:LEU:HD21	1.81	0.62
1:G:16:LEU:O	1:G:20:THR:HG23	2.00	0.61
1:H:19:PHE:HE1	1:H:61:ALA:HB1	1.65	0.61
1:H:32:GLU:HA	1:H:35:LYS:HD2	1.83	0.60
1:C:8:GLU:O	1:C:12:LYS:HG2	2.02	0.59
1:G:13:LEU:HD11	1:I:9:ILE:HG23	1.85	0.59
1:E:18:GLU:O	1:E:22:HIS:ND1	2.36	0.59
1:A:58:LEU:O	1:A:62:THR:HG23	2.03	0.59
1:F:23:LEU:O	1:F:27:MET:HG2	2.02	0.59
1:I:20:THR:O	1:I:24:ILE:HG13	2.04	0.58
1:K:31:LEU:HA	1:K:34:LEU:HD12	1.86	0.58
1:J:30:MET:HA	1:J:33:LEU:HD12	1.85	0.58
1:I:26:LEU:O	1:I:30:MET:HG2	2.04	0.58
1:F:12:LYS:HD3	1:F:68:ILE:HG23	1.86	0.58
1:I:11:SER:O	1:I:15:HIS:ND1	2.38	0.57
1:E:59:LYS:O	1:E:63:GLU:OE1	2.22	0.57
1:E:52:GLU:O	1:E:56:GLU:HG3	2.04	0.56
1:E:21:THR:O	1:E:25:LYS:HG2	2.04	0.56
1:G:37:VAL:HG11	1:I:37:VAL:HG22	1.87	0.56
1:I:16:LEU:O	1:I:20:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:GLU:HA	1:E:35:LYS:HD2	1.86	0.56
1:E:65:ALA:O	1:E:68:ILE:HG22	2.07	0.55
1:K:23:LEU:O	1:K:27:MET:HG2	2.06	0.55
1:K:31:LEU:O	1:K:35:LYS:HG3	2.07	0.55
1:J:8:GLU:O	1:J:12:LYS:HG2	2.05	0.55
1:G:31:LEU:HD21	1:I:55:GLU:HB2	1.88	0.55
1:E:32:GLU:HG3	1:E:50:LEU:HD21	1.89	0.55
1:K:18:GLU:HG3	1:K:64:ALA:HB1	1.88	0.54
1:E:55:GLU:O	1:E:59:LYS:HE2	2.08	0.54
1:B:14:LYS:HE3	1:B:15:HIS:CE1	2.43	0.54
1:E:14:LYS:O	1:E:17:GLU:HG3	2.09	0.53
1:F:15:HIS:HB2	1:F:68:ILE:HG13	1.90	0.53
1:H:58:LEU:HD22	1:I:31:LEU:HD21	1.91	0.52
1:D:22:HIS:HA	1:D:25:LYS:HD2	1.92	0.52
1:I:26:LEU:HD13	1:I:57:TYR:HB2	1.91	0.52
1:L:36:LEU:HD22	1:L:41:LYS:HD2	1.90	0.52
1:E:56:GLU:O	1:E:60:GLN:HG3	2.09	0.52
1:D:24:ILE:HD11	1:E:65:ALA:HB3	1.90	0.52
1:K:62:THR:HG22	1:K:66:LYS:HE3	1.90	0.52
1:D:31:LEU:HD21	1:E:58:LEU:HD13	1.92	0.52
1:F:30:MET:HA	1:F:33:LEU:HD12	1.92	0.51
1:J:6:ILE:O	1:J:10:GLU:HG3	2.10	0.51
1:A:55:GLU:HG2	1:C:31:LEU:HD11	1.92	0.51
1:D:21:THR:O	1:D:25:LYS:HG3	2.10	0.51
1:L:6:ILE:O	1:L:10:GLU:HG3	2.12	0.50
1:J:43:ASP:OD1	1:J:43:ASP:N	2.44	0.50
1:J:15:HIS:HB2	1:J:68:ILE:HD13	1.94	0.50
1:H:14:LYS:NZ	1:J:10:GLU:OE1	2.44	0.49
1:H:19:PHE:CE1	1:H:61:ALA:HB1	2.46	0.49
1:D:13:LEU:HD11	1:E:9:ILE:HG23	1.94	0.49
1:E:26:LEU:O	1:E:30:MET:HG3	2.11	0.49
1:K:16:LEU:O	1:K:20:THR:HG23	2.12	0.49
1:A:35:LYS:HG2	1:B:51:LEU:HD21	1.95	0.48
1:D:26:LEU:O	1:D:30:MET:HG3	2.14	0.48
1:L:47:TYR:CE1	1:J:38:SER:HB2	2.49	0.48
1:G:36:LEU:HB3	1:G:47:TYR:CZ	2.49	0.48
1:E:45:GLU:O	1:E:49:GLU:HG3	2.14	0.48
1:E:49:GLU:O	1:E:53:LYS:HG2	2.14	0.47
1:G:15:HIS:CG	1:G:68:ILE:HD11	2.50	0.47
1:B:45:GLU:OE1	1:B:45:GLU:N	2.47	0.47
1:D:63:GLU:O	1:D:67:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:PHE:CE1	1:I:61:ALA:HB1	2.49	0.47
1:C:21:THR:HG22	1:C:25:LYS:HE2	1.96	0.47
1:G:21:THR:HA	1:G:24:ILE:HD12	1.96	0.47
1:G:31:LEU:HG	1:G:35:LYS:HE3	1.96	0.47
1:G:22:HIS:HD2	1:G:60:GLN:HB3	1.80	0.47
1:D:21:THR:HG22	1:D:25:LYS:HE3	1.96	0.46
1:D:6:ILE:O	1:D:10:GLU:HG3	2.16	0.46
1:E:33:LEU:O	1:E:37:VAL:HG23	2.16	0.46
1:E:67:LYS:HE2	1:E:67:LYS:HB2	1.71	0.46
1:L:34:LEU:HD13	1:K:33:LEU:HD13	1.98	0.46
1:A:13:LEU:HD11	1:B:9:ILE:HG23	1.97	0.46
1:D:31:LEU:CD2	1:E:58:LEU:HD13	2.46	0.46
1:A:16:LEU:O	1:A:20:THR:HG23	2.14	0.46
1:L:13:LEU:HD11	1:K:9:ILE:HG23	1.97	0.46
1:K:24:ILE:HD11	1:J:19:PHE:HE1	1.81	0.46
1:A:9:ILE:HG23	1:C:13:LEU:HD11	1.98	0.46
1:B:21:THR:O	1:B:25:LYS:HG2	2.16	0.46
1:I:49:GLU:O	1:I:53:LYS:HG2	2.16	0.46
1:D:16:LEU:HD13	1:E:16:LEU:HD13	1.97	0.46
1:H:13:LEU:HD11	1:G:13:LEU:HD21	1.98	0.46
1:D:14:LYS:O	1:D:18:GLU:HG3	2.16	0.46
1:G:19:PHE:HE2	1:G:65:ALA:HB2	1.80	0.46
1:E:60:GLN:HA	1:E:63:GLU:OE1	2.15	0.45
1:H:20:THR:O	1:H:23:LEU:HB3	2.17	0.45
1:E:31:LEU:HD13	1:F:58:LEU:HD22	1.99	0.45
1:H:67:LYS:HA	1:H:67:LYS:HD2	1.78	0.45
1:K:6:ILE:HA	1:K:9:ILE:HD12	1.98	0.45
1:E:13:LEU:HD11	1:F:9:ILE:HG23	1.98	0.45
1:J:4:LYS:O	1:J:8:GLU:HG3	2.16	0.45
1:E:38:SER:HB3	1:F:47:TYR:HE2	1.82	0.44
1:F:8:GLU:O	1:F:12:LYS:HG2	2.17	0.44
1:A:23:LEU:HD23	1:B:19:PHE:HZ	1.82	0.44
1:H:10:GLU:HG2	1:G:9:ILE:HD11	1.99	0.44
1:D:30:MET:HB3	1:E:30:MET:HE1	2.00	0.44
1:D:30:MET:HB3	1:D:30:MET:HE2	1.80	0.44
1:I:32:GLU:O	1:I:36:LEU:HG	2.17	0.44
1:A:23:LEU:HD21	1:C:23:LEU:HD21	2.00	0.44
1:E:24:ILE:HG22	1:E:28:GLU:OE2	2.18	0.43
1:I:21:THR:HA	1:I:24:ILE:HD12	2.00	0.43
1:A:39:ASP:HB2	1:A:41:LYS:HE2	2.00	0.43
1:B:23:LEU:HD21	1:C:23:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:SER:HB2	1:K:47:TYR:CE2	2.53	0.43
1:G:10:GLU:HG2	1:I:5:ARG:HH22	1.83	0.43
1:K:62:THR:O	1:K:66:LYS:HG3	2.18	0.43
1:K:52:GLU:HA	1:K:55:GLU:OE1	2.19	0.43
1:G:66:LYS:HD2	1:G:66:LYS:HA	1.79	0.43
1:F:14:LYS:O	1:F:18:GLU:HG2	2.18	0.43
1:E:13:LEU:HD23	1:E:16:LEU:HD12	2.01	0.43
1:G:47:TYR:CD1	1:G:50:LEU:HD12	2.54	0.43
1:I:13:LEU:HA	1:I:16:LEU:HG	2.00	0.43
1:J:10:GLU:HA	1:J:13:LEU:HG	2.01	0.42
1:D:25:LYS:HG3	1:D:25:LYS:H	1.69	0.42
1:H:19:PHE:CE2	1:I:20:THR:HB	2.53	0.42
1:K:23:LEU:HD23	1:J:19:PHE:CZ	2.54	0.42
1:L:23:LEU:HD21	1:J:23:LEU:HD21	2.02	0.42
1:A:24:ILE:HD11	1:B:65:ALA:HB3	2.01	0.42
1:D:34:LEU:HD11	1:E:30:MET:HE3	2.01	0.42
1:J:33:LEU:O	1:J:37:VAL:HG23	2.18	0.42
1:I:53:LYS:HA	1:I:53:LYS:HD3	1.84	0.42
1:L:55:GLU:HG3	1:L:59:LYS:HE2	2.02	0.42
1:G:26:LEU:HD13	1:G:57:TYR:HB2	2.02	0.42
1:G:10:GLU:OE2	1:I:12:LYS:NZ	2.50	0.42
1:C:16:LEU:O	1:C:20:THR:HG23	2.19	0.42
1:D:5:ARG:O	1:D:8:GLU:HG2	2.19	0.42
1:H:26:LEU:HD12	1:H:26:LEU:HA	1.92	0.42
1:D:16:LEU:HD11	1:F:16:LEU:HD22	2.02	0.42
1:E:38:SER:HB3	1:F:47:TYR:CE2	2.54	0.41
1:E:59:LYS:O	1:E:62:THR:HB	2.20	0.41
1:F:55:GLU:O	1:F:59:LYS:NZ	2.48	0.41
1:L:15:HIS:HA	1:L:18:GLU:CD	2.41	0.41
1:D:58:LEU:HD23	1:F:31:LEU:HD12	2.03	0.41
1:B:31:LEU:HD12	1:C:58:LEU:HD22	2.03	0.41
1:D:9:ILE:O	1:D:13:LEU:HG	2.21	0.41
1:K:38:SER:HA	1:J:42:SER:HG	1.85	0.41
1:D:47:TYR:CE1	1:F:38:SER:HB2	2.55	0.41
1:D:34:LEU:HD13	1:E:33:LEU:HD13	2.03	0.41
1:G:17:GLU:O	1:G:21:THR:HG23	2.20	0.41
1:K:63:GLU:HA	1:K:66:LYS:HD2	2.03	0.41
1:D:19:PHE:CD2	1:D:65:ALA:HB2	2.56	0.41
1:C:4:LYS:HE2	1:C:4:LYS:HB3	1.87	0.40
1:E:15:HIS:CD2	1:E:67:LYS:HE3	2.56	0.40
1:E:24:ILE:HD12	1:F:62:THR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LYS:HA	1:B:56:GLU:HG2	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	62/70 (89%)	62 (100%)	0	0	100	100
1	B	65/70 (93%)	65 (100%)	0	0	100	100
1	C	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
1	D	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
1	E	64/70 (91%)	61 (95%)	3 (5%)	0	100	100
1	F	64/70 (91%)	61 (95%)	3 (5%)	0	100	100
1	G	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
1	H	62/70 (89%)	58 (94%)	4 (6%)	0	100	100
1	I	55/70 (79%)	55 (100%)	0	0	100	100
1	J	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
1	K	64/70 (91%)	64 (100%)	0	0	100	100
1	L	65/70 (93%)	63 (97%)	2 (3%)	0	100	100
All	All	749/840 (89%)	729 (97%)	20 (3%)	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	59/63 (94%)	58 (98%)	1 (2%)	60	80
1	B	60/63 (95%)	60 (100%)	0	100	100
1	C	60/63 (95%)	60 (100%)	0	100	100
1	D	60/63 (95%)	59 (98%)	1 (2%)	60	80
1	E	60/63 (95%)	59 (98%)	1 (2%)	60	80
1	F	60/63 (95%)	60 (100%)	0	100	100
1	G	55/63 (87%)	53 (96%)	2 (4%)	35	63
1	H	59/63 (94%)	58 (98%)	1 (2%)	60	80
1	I	54/63 (86%)	52 (96%)	2 (4%)	34	62
1	J	60/63 (95%)	60 (100%)	0	100	100
1	K	60/63 (95%)	58 (97%)	2 (3%)	38	66
1	L	60/63 (95%)	60 (100%)	0	100	100
All	All	707/756 (94%)	697 (99%)	10 (1%)	67	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	D	42	SER
1	E	4	LYS
1	H	47	TYR
1	G	38	SER
1	G	68	ILE
1	I	47	TYR
1	I	67	LYS
1	K	7	ASP
1	K	11	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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, 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(Å²)	Q<0.9
1	A	64/70 (91%)	0.65	2 (3%)	49	48	95, 111, 137, 162	0
1	B	67/70 (95%)	0.64	3 (4%)	33	33	98, 115, 145, 155	0
1	C	67/70 (95%)	0.48	0	100	100	89, 104, 122, 130	0
1	D	65/70 (92%)	0.44	1 (1%)	73	72	96, 115, 136, 144	0
1	E	66/70 (94%)	0.54	4 (6%)	21	22	115, 135, 164, 178	0
1	F	66/70 (94%)	0.45	3 (4%)	33	33	90, 126, 144, 160	0
1	G	60/70 (85%)	1.19	16 (26%)	0	0	181, 205, 234, 243	0
1	H	64/70 (91%)	0.84	9 (14%)	2	3	168, 189, 209, 214	0
1	I	59/70 (84%)	0.45	7 (11%)	4	5	170, 193, 231, 242	0
1	J	66/70 (94%)	0.57	2 (3%)	50	49	105, 122, 141, 152	0
1	K	66/70 (94%)	0.57	2 (3%)	50	49	102, 117, 140, 158	0
1	L	67/70 (95%)	0.62	5 (7%)	14	16	101, 124, 157, 170	0
All	All	777/840 (92%)	0.62	54 (6%)	16	18	89, 125, 212, 243	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	34	LEU	5.7
1	G	30	MET	4.6
1	H	19	PHE	4.3
1	L	19	PHE	4.1
1	E	68	ILE	4.0
1	H	33	LEU	3.9
1	I	30	MET	3.9
1	I	9	ILE	3.6
1	G	33	LEU	3.6
1	H	36	LEU	3.5
1	I	64	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	42	SER	3.5
1	H	47	TYR	3.4
1	I	31	LEU	3.2
1	I	36	LEU	3.1
1	G	54	ALA	3.0
1	G	35	LYS	2.9
1	I	27	MET	2.9
1	E	13	LEU	2.9
1	G	23	LEU	2.8
1	G	47	TYR	2.8
1	B	67	LYS	2.7
1	H	63	GLU	2.7
1	H	34	LEU	2.7
1	G	29	THR	2.7
1	G	24	ILE	2.7
1	G	22	HIS	2.7
1	G	13	LEU	2.6
1	L	20	THR	2.6
1	B	30	MET	2.5
1	J	43	ASP	2.5
1	A	33	LEU	2.4
1	H	43	ASP	2.4
1	F	13	LEU	2.4
1	D	19	PHE	2.4
1	G	26	LEU	2.4
1	F	6	ILE	2.3
1	G	10	GLU	2.3
1	B	68	ILE	2.2
1	G	27	MET	2.2
1	H	7	ASP	2.2
1	J	26	LEU	2.2
1	F	9	ILE	2.2
1	K	31	LEU	2.1
1	I	13	LEU	2.1
1	L	13	LEU	2.1
1	G	31	LEU	2.1
1	K	12	LYS	2.1
1	G	25	LYS	2.1
1	L	47	TYR	2.1
1	E	37	VAL	2.0
1	A	51	LEU	2.0
1	L	26	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	3	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.