



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 02:04 PM BST

PDB ID : 6S4L
Title : Structure of human KCTD1
Authors : Pinkas, D.M.; Bufton, J.C.; Fox, A.E.; Pike, A.C.W.; Newman, J.A.; Krojer, T.; Shrestha, L.; Burgess-Brown, N.A.; von Delft, F.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Bullock, A.N.
Deposited on : 2019-06-28
Resolution : 2.42 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	:	2.13
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)	:	2.13

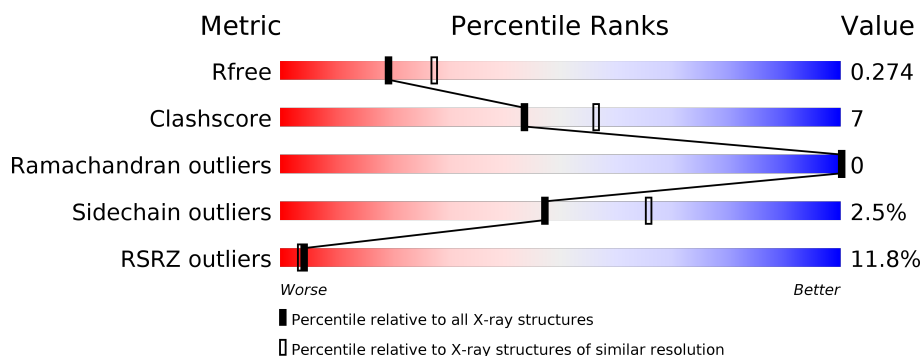
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	232	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	B	232	<div> <div>10%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 9%</div> </div> </div>
1	C	232	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 9%</div> </div> </div>
1	D	232	<div> <div>13%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>7%</div> </div> </div>
1	E	232	<div> <div>16%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>• 12%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8534 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 BTB/POZ domain-containing protein KCTD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1731	1100	305	317	9			
1	B	211	Total	C	N	O	S	0	0	0
			1684	1070	295	311	8			
1	C	212	Total	C	N	O	S	0	0	0
			1697	1078	296	315	8			
1	D	215	Total	C	N	O	S	0	0	0
			1712	1086	303	315	8			
1	E	205	Total	C	N	O	S	0	0	0
			1644	1043	287	306	8			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	SER	-	expression tag	UNP Q719H9
A	27	MET	-	expression tag	UNP Q719H9
A	64	ASP	GLU	conflict	UNP Q719H9
B	26	SER	-	expression tag	UNP Q719H9
B	27	MET	-	expression tag	UNP Q719H9
B	64	ASP	GLU	conflict	UNP Q719H9
C	26	SER	-	expression tag	UNP Q719H9
C	27	MET	-	expression tag	UNP Q719H9
C	64	ASP	GLU	conflict	UNP Q719H9
D	26	SER	-	expression tag	UNP Q719H9
D	27	MET	-	expression tag	UNP Q719H9
D	64	ASP	GLU	conflict	UNP Q719H9
E	26	SER	-	expression tag	UNP Q719H9
E	27	MET	-	expression tag	UNP Q719H9
E	64	ASP	GLU	conflict	UNP Q719H9

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total I 2 2	0	0

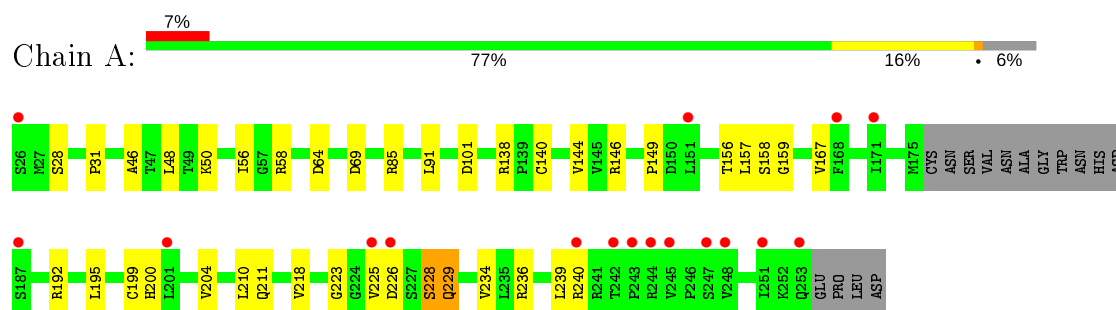
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	15	Total O 15 15	0	0
4	B	14	Total O 14 14	0	0
4	C	14	Total O 14 14	0	0
4	D	10	Total O 10 10	0	0
4	E	9	Total O 9 9	0	0

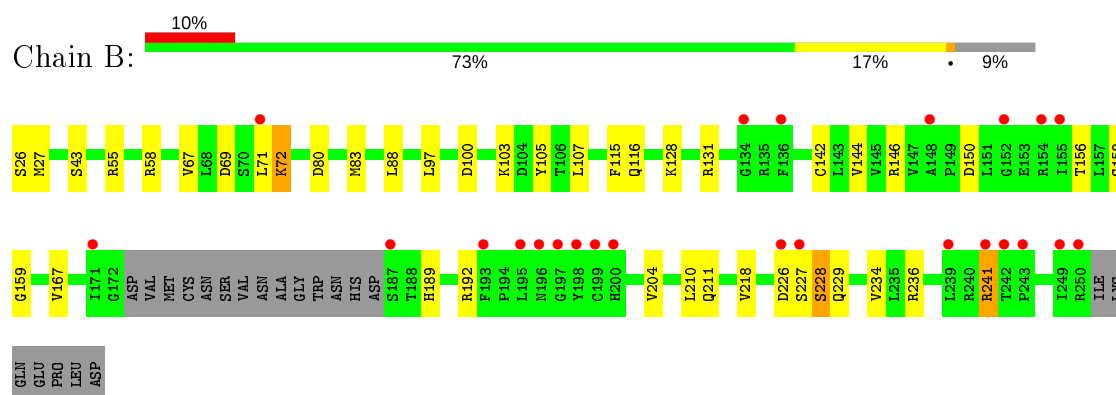
3 Residue-property plots [i](#)

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.

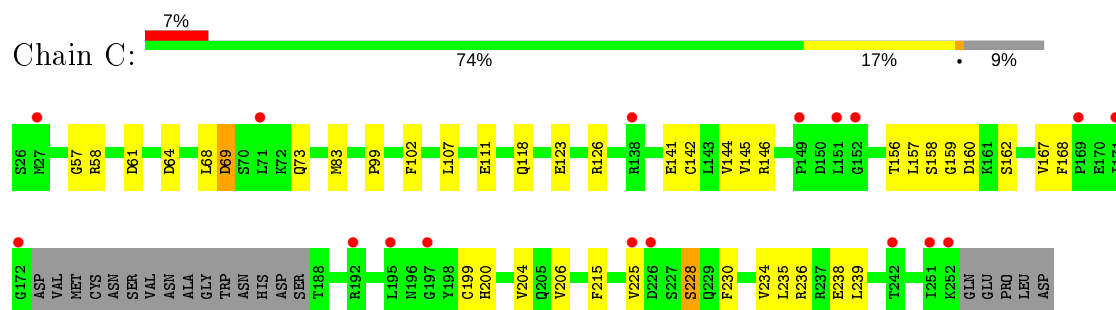
- Molecule 1: BTB/POZ domain-containing protein KCTD1



- Molecule 1: BTB/POZ domain-containing protein KCTD1

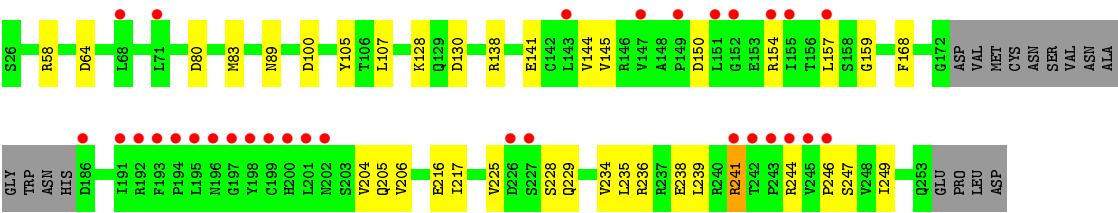


- Molecule 1: BTB/POZ domain-containing protein KCTD1

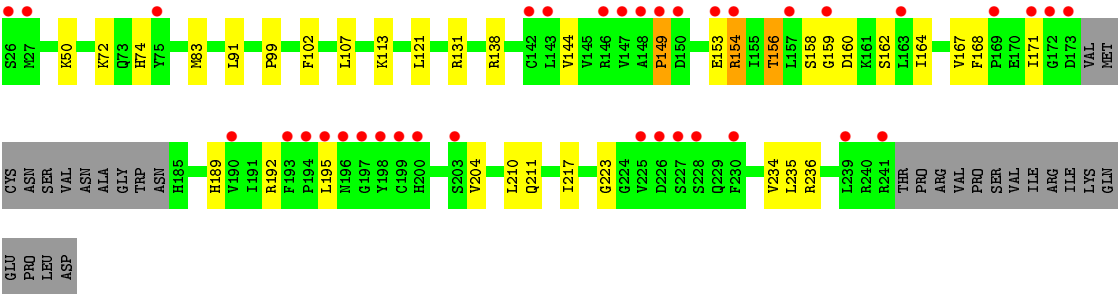


- Molecule 1: BTB/POZ domain-containing protein KCTD1





● Molecule 1: BTB/POZ domain-containing protein KCTD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.45Å 95.87Å 104.34Å 90.00° 92.16° 90.00°	Depositor
Resolution (Å)	70.57 – 2.42 70.57 – 2.41	Depositor EDS
% Data completeness (in resolution range)	59.0 (70.57-2.42) 59.0 (70.57-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.245 , 0.281 0.241 , 0.274	Depositor DCC
R_{free} test set	1420 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8534	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, IOD

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	0/1767	0.41	0/2387
1	B	0.24	0/1719	0.41	0/2323
1	C	0.24	0/1733	0.41	0/2343
1	D	0.24	0/1747	0.40	0/2362
1	E	0.24	0/1678	0.41	0/2265
All	All	0.24	0/8644	0.41	0/11680

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	1731	0	1699	29	0
1	B	1684	0	1658	33	0
1	C	1697	0	1659	25	0
1	D	1712	0	1668	21	0
1	E	1644	0	1597	26	0
2	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	15	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	0	1	0
4	C	14	0	0	1	0
4	D	10	0	0	0	0
4	E	9	0	0	2	0
All	All	8534	0	8281	112	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 7.

All (112) 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:E:168:PHE:HB2	1:E:171:ILE:HD11	1.68	0.76
1:A:58:ARG:NH2	1:A:64:ASP:OD2	2.20	0.74
1:D:216:GLU:OE2	1:E:138:ARG:NH1	2.27	0.67
1:B:71:LEU:HB2	1:B:72:LYS:HD3	1.77	0.66
1:A:211:GLN:NE2	1:B:142:CYS:SG	2.68	0.66
1:E:83:MET:HG3	1:E:107:LEU:HG	1.78	0.65
1:E:144:VAL:HB	1:E:158:SER:HB2	1.78	0.65
1:C:204:VAL:HG11	1:D:159:GLY:HA2	1.79	0.65
1:D:130:ASP:HB3	1:D:241:ARG:HH12	1.63	0.64
1:B:97:LEU:HB3	1:C:107:LEU:HG	1.81	0.63
1:B:58:ARG:NH2	1:B:116:GLN:OE1	2.32	0.62
1:A:199:CYS:SG	1:A:200:HIS:N	2.72	0.62
1:A:229:GLN:NE2	1:B:146:ARG:HH12	1.97	0.62
1:B:204:VAL:HG11	1:C:159:GLY:HA2	1.82	0.61
1:B:211:GLN:NE2	1:C:142:CYS:SG	2.73	0.61
1:C:236:ARG:NH2	1:C:238:GLU:OE2	2.32	0.61
1:A:156:THR:HG23	1:A:192:ARG:HA	1.83	0.60
1:B:58:ARG:NH1	4:B:401:HOH:O	2.34	0.60
1:D:204:VAL:HG21	1:E:159:GLY:HA2	1.83	0.60
1:D:58:ARG:NH1	1:D:64:ASP:OD2	2.34	0.60
1:B:144:VAL:HB	1:B:158:SER:HB2	1.84	0.59
1:D:144:VAL:HG22	1:D:234:VAL:HG22	1.84	0.59
1:A:159:GLY:HA2	1:E:204:VAL:HG11	1.85	0.58
1:E:171:ILE:HG12	1:E:195:LEU:HD11	1.85	0.58
1:A:138:ARG:HH21	1:A:236:ARG:HH22	1.52	0.58
1:E:167:VAL:HG11	1:E:210:LEU:HD23	1.85	0.58
1:A:144:VAL:HG22	1:A:234:VAL:HG22	1.86	0.57
1:A:229:GLN:HE22	1:B:146:ARG:HH12	1.51	0.57
1:E:149:PRO:HA	1:E:153:GLU:HA	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ASP:O	1:B:131:ARG:NH1	2.38	0.56
1:C:69:ASP:O	1:C:73:GLN:N	2.27	0.56
1:B:226:ASP:OD1	1:B:227:SER:N	2.39	0.56
1:C:58:ARG:NH1	1:C:64:ASP:OD2	2.39	0.55
1:A:144:VAL:HB	1:A:158:SER:HB2	1.87	0.55
1:A:28:SER:HB3	1:A:46:ALA:HB2	1.88	0.55
1:E:164:ILE:HG22	1:E:171:ILE:HD13	1.89	0.54
1:A:228:SER:O	1:A:228:SER:OG	2.23	0.54
1:B:167:VAL:HG11	1:B:210:LEU:HD23	1.91	0.53
1:C:141:GLU:HG3	1:C:239:LEU:HD11	1.90	0.53
1:B:144:VAL:HG22	1:B:234:VAL:HG22	1.90	0.53
1:C:160:ASP:OD2	1:C:162:SER:OG	2.22	0.53
1:C:199:CYS:SG	1:C:200:HIS:N	2.81	0.53
1:E:211:GLN:HE21	1:E:217:ILE:HG13	1.74	0.52
1:D:80:ASP:OD2	1:D:107:LEU:HD21	2.10	0.52
1:C:168:PHE:CZ	1:C:206:VAL:HG23	2.45	0.52
1:A:236:ARG:NH1	4:A:404:HOH:O	2.39	0.52
1:D:138:ARG:HH21	1:D:236:ARG:HH12	1.57	0.52
1:A:204:VAL:HG11	1:B:159:GLY:HA2	1.93	0.51
1:B:69:ASP:O	1:B:71:LEU:N	2.40	0.50
1:A:157:LEU:HD11	1:A:195:LEU:HD22	1.92	0.50
1:C:225:VAL:HG22	1:C:228:SER:HB3	1.93	0.50
1:E:72:LYS:NZ	4:E:303:HOH:O	2.43	0.50
1:D:141:GLU:HG3	1:D:239:LEU:HD11	1.94	0.50
1:A:146:ARG:HB2	1:A:156:THR:HB	1.94	0.49
1:D:138:ARG:NH2	1:D:238:GLU:OE2	2.46	0.49
1:C:144:VAL:HG22	1:C:234:VAL:HG22	1.95	0.48
1:A:50:LYS:HD3	1:A:91:LEU:O	2.13	0.47
1:E:217:ILE:HG12	1:E:235:LEU:HG	1.96	0.47
1:D:216:GLU:OE1	1:E:236:ARG:NH1	2.43	0.47
1:B:226:ASP:OD2	1:C:228:SER:HB2	2.14	0.47
1:B:55:ARG:HB3	1:B:115:PHE:HA	1.98	0.46
1:C:83:MET:HB2	1:C:111:GLU:HG3	1.97	0.46
1:B:43:SER:HB2	1:B:88:LEU:HD21	1.96	0.46
1:C:57:GLY:O	1:C:61:ASP:HB2	2.16	0.46
1:E:154:ARG:HE	1:E:156:THR:HG22	1.81	0.45
1:C:146:ARG:HB2	1:C:156:THR:OG1	2.16	0.45
1:B:226:ASP:N	1:C:228:SER:OG	2.49	0.45
1:A:239:LEU:H	1:A:239:LEU:HD23	1.82	0.45
1:B:241:ARG:HA	1:B:241:ARG:HD2	1.78	0.45
1:A:226:ASP:CB	1:B:228:SER:HB3	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HD22	1:A:56:ILE:HD11	1.99	0.44
1:C:167:VAL:HG23	1:C:168:PHE:CD2	2.52	0.44
1:D:168:PHE:HZ	1:D:206:VAL:HG13	1.83	0.44
1:C:123:GLU:OE1	1:C:126:ARG:NH1	2.51	0.44
1:E:50:LYS:HD2	1:E:91:LEU:O	2.18	0.44
1:A:85:ARG:NH2	1:B:80:ASP:OD2	2.51	0.43
1:E:144:VAL:HG22	1:E:234:VAL:HG22	1.99	0.43
1:C:118:GLN:NE2	4:C:301:HOH:O	2.35	0.43
1:D:150:ASP:OD2	1:D:154:ARG:HD3	2.18	0.43
1:A:167:VAL:HG11	1:A:210:LEU:HD23	2.01	0.43
1:D:225:VAL:HG22	1:D:228:SER:HB2	2.01	0.43
1:D:205:GLN:HE21	1:E:189:HIS:CD2	2.37	0.43
1:D:83:MET:HG3	1:D:107:LEU:HG	2.00	0.43
1:E:113:LYS:HA	1:E:121:LEU:HD11	2.01	0.43
1:E:131:ARG:NH1	4:E:305:HOH:O	2.51	0.43
1:A:149:PRO:HG2	1:B:192:ARG:HH21	1.82	0.42
1:A:229:GLN:HE21	1:A:229:GLN:HB2	1.60	0.42
1:C:99:PRO:HD2	1:C:102:PHE:CD1	2.55	0.42
1:B:226:ASP:HA	1:B:229:GLN:CD	2.40	0.42
1:C:144:VAL:HB	1:C:158:SER:HB2	2.01	0.42
1:B:150:ASP:OD1	1:B:150:ASP:N	2.52	0.42
1:C:215:PHE:HB3	1:C:235:LEU:HB3	2.01	0.42
1:E:160:ASP:O	1:E:164:ILE:HG13	2.19	0.42
1:A:31:PRO:HD3	1:B:67:VAL:HG11	2.02	0.42
1:C:145:VAL:HG22	1:C:157:LEU:HD13	2.02	0.42
1:E:168:PHE:HB2	1:E:171:ILE:CD1	2.46	0.41
1:A:218:VAL:HG13	1:E:217:ILE:HD12	2.02	0.41
1:B:105:TYR:CE2	1:B:128:LYS:HD2	2.55	0.41
1:A:140:CYS:HB2	1:A:236:ARG:HD3	2.02	0.41
1:B:26:SER:OG	1:B:27:MET:N	2.51	0.41
1:D:105:TYR:CE2	1:D:128:LYS:HD2	2.56	0.41
1:E:99:PRO:HD2	1:E:102:PHE:CD1	2.56	0.41
1:D:217:ILE:HG12	1:D:235:LEU:HG	2.02	0.41
1:A:101:ASP:OD2	1:B:103:LYS:HG2	2.21	0.41
1:D:244:ARG:C	1:D:246:PRO:HD3	2.41	0.41
1:D:145:VAL:HG22	1:D:157:LEU:HD13	2.02	0.41
1:A:223:GLY:HA3	1:E:223:GLY:HA2	2.03	0.40
1:B:83:MET:HG3	1:B:107:LEU:HG	2.02	0.40
1:B:146:ARG:HB2	1:B:156:THR:OG1	2.22	0.40
1:D:225:VAL:O	1:D:229:GLN:HG3	2.21	0.40
1:E:160:ASP:OD2	1:E:162:SER:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:HG11	1:B:236:ARG:HE	1.85	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	A	213/232 (92%)	201 (94%)	12 (6%)	0	100	100
1	B	207/232 (89%)	191 (92%)	16 (8%)	0	100	100
1	C	208/232 (90%)	189 (91%)	19 (9%)	0	100	100
1	D	211/232 (91%)	195 (92%)	16 (8%)	0	100	100
1	E	201/232 (87%)	187 (93%)	14 (7%)	0	100	100
All	All	1040/1160 (90%)	963 (93%)	77 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	A	188/211 (89%)	183 (97%)	5 (3%)	44	63
1	B	185/211 (88%)	181 (98%)	4 (2%)	52	69
1	C	186/211 (88%)	182 (98%)	4 (2%)	52	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	184/211 (87%)	179 (97%)	5 (3%)	44	63
1	E	178/211 (84%)	173 (97%)	5 (3%)	43	62
All	All	921/1055 (87%)	898 (98%)	23 (2%)	47	66

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASP
1	A	225	VAL
1	A	228	SER
1	A	229	GLN
1	A	240	ARG
1	B	72	LYS
1	B	189	HIS
1	B	228	SER
1	B	241	ARG
1	C	68	LEU
1	C	69	ASP
1	C	228	SER
1	C	230	PHE
1	D	89	ASN
1	D	100	ASP
1	D	241	ARG
1	D	247	SER
1	D	249	ILE
1	E	74	HIS
1	E	149	PRO
1	E	154	ARG
1	E	156	THR
1	E	192	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	229	GLN
1	B	211	GLN
1	D	39	HIS
1	E	39	HIS
1	E	73	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	189	HIS
1	E	229	GLN

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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å ²)	Q<0.9
1	A	217/232 (93%)	0.46	17 (7%) 13 11	14, 53, 107, 131	0
1	B	211/232 (90%)	0.56	24 (11%) 5 4	16, 53, 109, 145	0
1	C	212/232 (91%)	0.45	17 (8%) 12 11	18, 53, 100, 124	0
1	D	215/232 (92%)	0.83	31 (14%) 2 2	16, 56, 114, 181	0
1	E	205/232 (88%)	0.84	36 (17%) 1 1	12, 55, 115, 136	0
All	All	1060/1160 (91%)	0.63	125 (11%) 4 4	12, 55, 110, 181	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	171	ILE	15.1
1	D	198	TYR	11.4
1	D	245	VAL	9.9
1	B	195	LEU	8.7
1	B	226	ASP	8.1
1	A	151	LEU	7.9
1	D	199	CYS	7.5
1	E	195	LEU	7.4
1	B	250	ARG	7.4
1	E	198	TYR	7.0
1	A	253	GLN	6.9
1	D	197	GLY	6.6
1	B	198	TYR	6.5
1	A	248	VAL	6.3
1	E	148	ALA	6.3
1	A	226	ASP	6.0
1	E	225	VAL	6.0
1	D	201	LEU	5.8
1	E	26	SER	5.6
1	D	244	ARG	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	196	ASN	5.6
1	B	197	GLY	5.5
1	E	227	SER	5.4
1	E	150	ASP	5.3
1	D	195	LEU	5.3
1	D	151	LEU	5.1
1	B	134	GLY	5.1
1	D	243	PRO	5.0
1	C	27	MET	5.0
1	D	196	ASN	4.9
1	E	226	ASP	4.8
1	E	193	PHE	4.8
1	D	226	ASP	4.8
1	A	225	VAL	4.7
1	D	242	THR	4.7
1	B	243	PRO	4.6
1	D	246	PRO	4.5
1	D	194	PRO	4.5
1	C	242	THR	4.3
1	D	193	PHE	4.3
1	C	195	LEU	4.1
1	C	252	LYS	4.1
1	B	200	HIS	4.0
1	E	169	PRO	4.0
1	E	173	ASP	3.9
1	C	251	ILE	3.8
1	E	200	HIS	3.8
1	D	157	LEU	3.7
1	B	242	THR	3.7
1	C	169	PRO	3.7
1	D	192	ARG	3.7
1	D	200	HIS	3.5
1	D	241	ARG	3.5
1	B	193	PHE	3.5
1	E	147	VAL	3.5
1	E	190	VAL	3.4
1	C	151	LEU	3.4
1	D	202	ASN	3.4
1	C	171	ILE	3.3
1	E	172	GLY	3.3
1	A	251	ILE	3.2
1	D	227	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	155	ILE	3.2
1	C	149	PRO	3.2
1	A	245	VAL	3.2
1	D	154	ARG	3.1
1	B	171	ILE	3.1
1	D	71	LEU	3.1
1	D	186	ASP	3.1
1	B	199	CYS	3.0
1	B	71	LEU	3.0
1	B	249	ILE	2.9
1	A	242	THR	2.9
1	E	239	LEU	2.9
1	B	136	PHE	2.9
1	B	239	LEU	2.9
1	A	26	SER	2.9
1	B	154	ARG	2.8
1	E	199	CYS	2.8
1	D	143	LEU	2.8
1	A	171	ILE	2.7
1	B	155	ILE	2.7
1	D	149	PRO	2.7
1	E	27	MET	2.7
1	E	159	GLY	2.7
1	E	241	ARG	2.7
1	A	244	ARG	2.7
1	E	154	ARG	2.6
1	C	226	ASP	2.6
1	B	241	ARG	2.6
1	A	201	LEU	2.6
1	E	197	GLY	2.6
1	C	225	VAL	2.5
1	A	168	PHE	2.5
1	D	147	VAL	2.5
1	C	71	LEU	2.5
1	B	196	ASN	2.5
1	A	247	SER	2.4
1	D	68	LEU	2.4
1	E	228	SER	2.4
1	A	243	PRO	2.4
1	B	227	SER	2.4
1	E	143	LEU	2.4
1	A	187	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	191	ILE	2.3
1	E	194	PRO	2.3
1	E	153	GLU	2.3
1	E	75	TYR	2.3
1	E	142	CYS	2.3
1	C	172	GLY	2.3
1	E	157	LEU	2.3
1	E	149	PRO	2.2
1	C	138	ARG	2.2
1	C	197	GLY	2.2
1	E	163	LEU	2.2
1	B	148	ALA	2.1
1	C	152	GLY	2.1
1	C	192	ARG	2.1
1	E	230	PHE	2.1
1	A	240	ARG	2.1
1	B	152	GLY	2.1
1	D	152	GLY	2.1
1	B	187	SER	2.0
1	E	203	SER	2.0
1	E	146	ARG	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	A	302	1/1	0.80	0.23	43,43,43,43	0
2	NA	A	301	1/1	0.95	0.11	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	IOD	B	301	1/1	0.99	0.11	64,64,64,64	0
3	IOD	B	302	1/1	0.99	0.13	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.