



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 6S4L / pdb_00006s4l
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 types of validation reports are described at

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

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

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

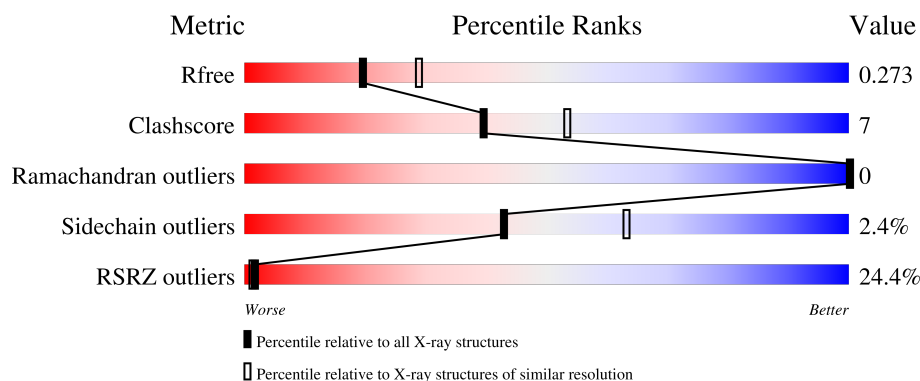
1 Overall quality at a glance

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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	21% 77% 16% • 6%
1	B	232	20% 73% 16% • 9%
1	C	232	20% 74% 16% • 9%
1	D	232	28% 77% 15% 7%
1	E	232	22% 72% 15% • 12%

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 (CCD ID: NA) (formula: Na).

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

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

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

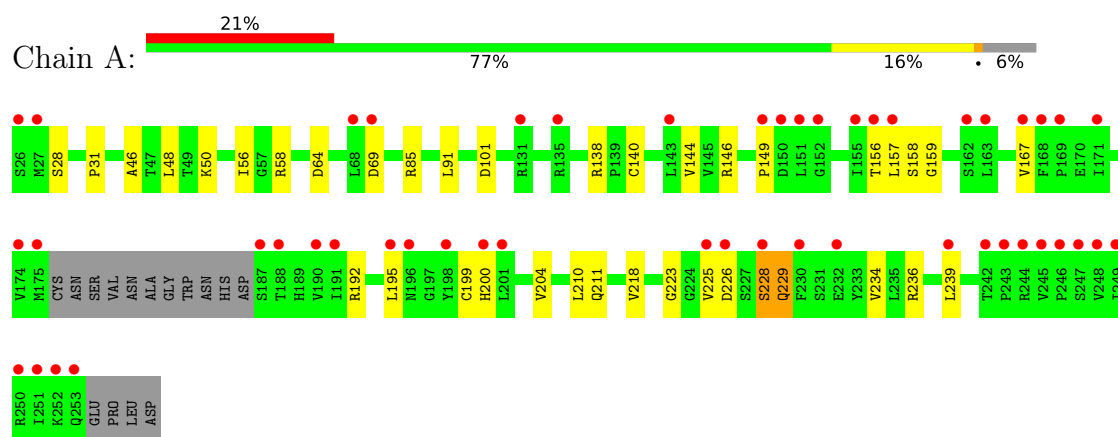
- Molecule 4 is water.

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

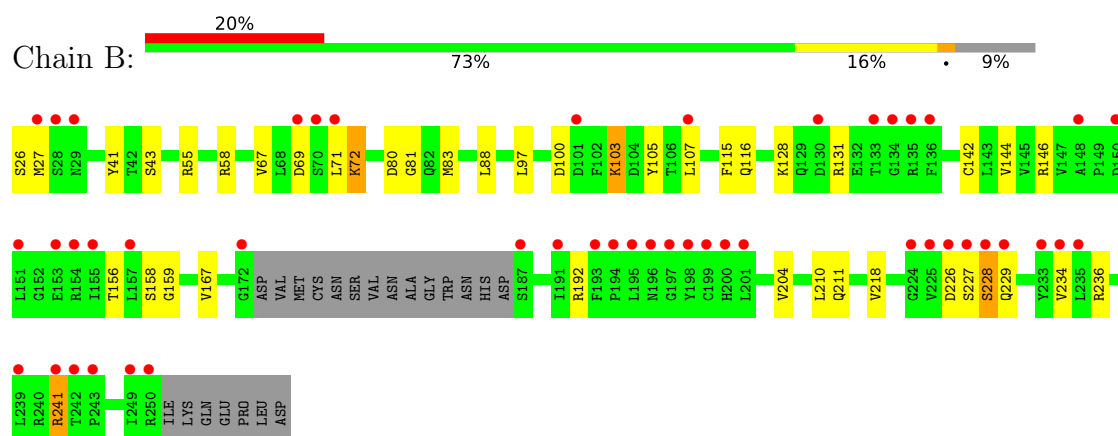
3 Residue-property plots

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.

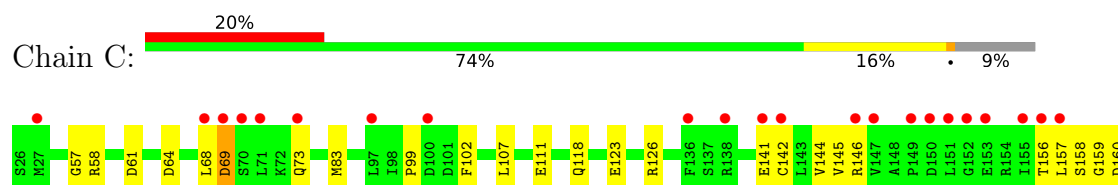
- Molecule 1: BTB/POZ domain-containing protein KCTD1

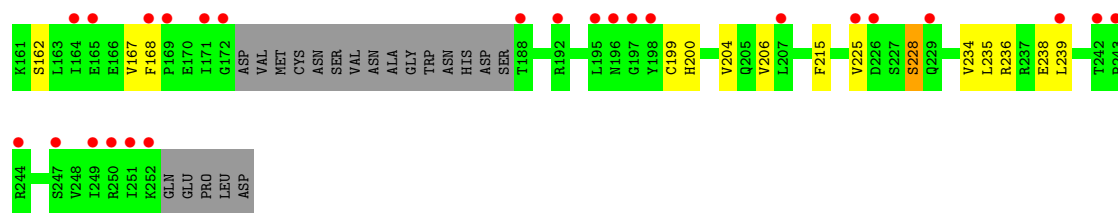


- Molecule 1: BTB/POZ domain-containing protein KCTD1

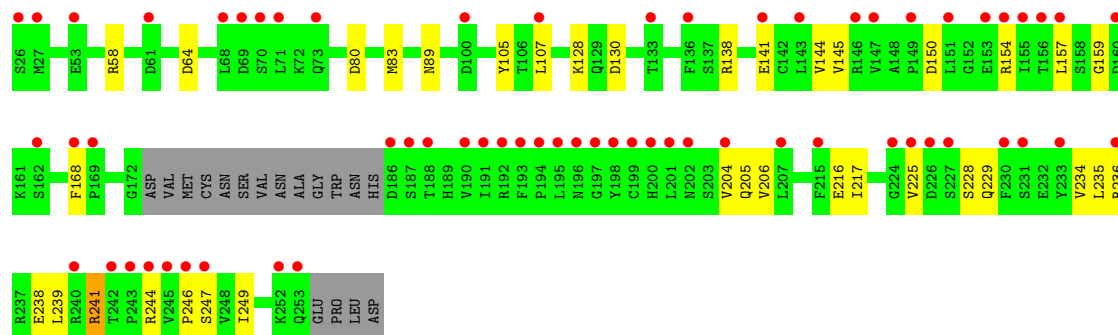
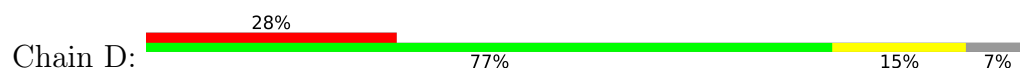


- Molecule 1: BTB/POZ domain-containing protein KCTD1

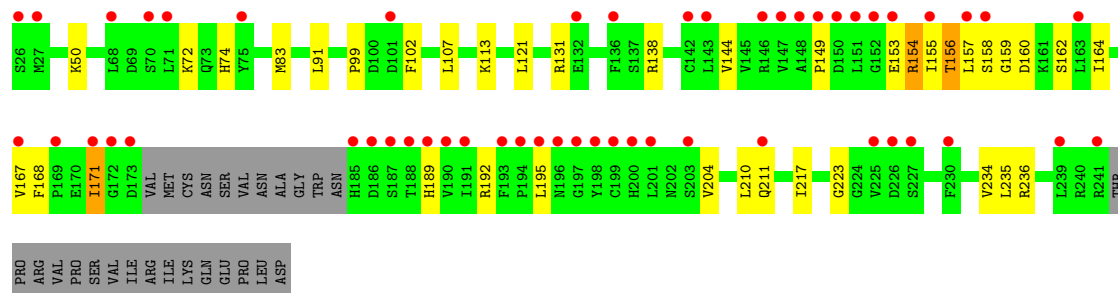
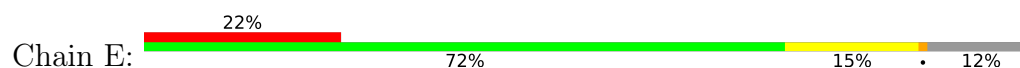




● Molecule 1: BTB/POZ domain-containing protein KCTD1



● 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 – 2.42	Depositor EDS
% Data completeness (in resolution range)	59.0 (70.57-2.42) 59.4 (70.57-2.42)	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 , 0.273	Depositor DCC
R_{free} test set	1420 reflections (2.77%)	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 , 40.6	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

5.1 Standard geometry

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

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	0.10	0/1767	0.28	0/2387
1	B	0.09	0/1719	0.28	0/2323
1	C	0.10	0/1733	0.26	0/2343
1	D	0.09	0/1747	0.27	0/2362
1	E	0.10	0/1678	0.27	0/2265
All	All	0.10	0/8644	0.27	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

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

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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

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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:28:SER:HB3	1:A:46:ALA:HB2	1.88	0.55
1:A:144:VAL:HB	1:A:158:SER:HB2	1.87	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:B:226:ASP:HA	1:B:229:GLN:CD	2.40	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:41:TYR:OH	1:B:81:GLY:O	2.27	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:D:244:ARG:C	1:D:246:PRO:HD3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LEU:H	1:A:239:LEU:HD23	1.82	0.45
1:B:241:ARG:HD2	1:B:241:ARG:HA	1.78	0.45
1:A:226:ASP:CB	1:B:228:SER:HB3	2.47	0.45
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:83:MET:HG3	1:D:107:LEU:HG	2.00	0.43
1:D:205:GLN:HE21	1:E:189:HIS:CD2	2.37	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:C:144:VAL:HB	1:C:158:SER:HB2	2.01	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: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

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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%)	184 (98%)	4 (2%)	47	67
1	B	185/211 (88%)	181 (98%)	4 (2%)	45	66
1	C	186/211 (88%)	183 (98%)	3 (2%)	55	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	184/211 (87%)	180 (98%)	4 (2%)	45	66
1	E	178/211 (84%)	171 (96%)	7 (4%)	28	46
All	All	921/1055 (87%)	899 (98%)	22 (2%)	43	63

All (22) 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	B	72	LYS
1	B	103	LYS
1	B	228	SER
1	B	241	ARG
1	C	68	LEU
1	C	69	ASP
1	C	228	SER
1	D	89	ASN
1	D	241	ARG
1	D	247	SER
1	D	249	ILE
1	E	74	HIS
1	E	154	ARG
1	E	155	ILE
1	E	156	THR
1	E	157	LEU
1	E	171	ILE
1	E	192	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	229	GLN
1	B	211	GLN
1	C	29	ASN
1	D	39	HIS
1	E	39	HIS
1	E	73	GLN

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

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	217/232 (93%)	1.15	49 (22%) 2 2	14, 53, 107, 131	0
1	B	211/232 (90%)	1.18	47 (22%) 2 2	16, 53, 109, 145	0
1	C	212/232 (91%)	1.22	47 (22%) 2 2	18, 53, 100, 124	0
1	D	215/232 (92%)	1.42	64 (29%) 1 1	16, 56, 114, 181	0
1	E	205/232 (88%)	1.36	52 (25%) 1 1	12, 55, 115, 136	0
All	All	1060/1160 (91%)	1.27	259 (24%) 2 1	12, 55, 110, 181	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	243	PRO	6.8
1	E	171	ILE	6.5
1	E	195	LEU	6.3
1	C	27	MET	6.3
1	E	26	SER	6.3
1	B	198	TYR	6.2
1	E	172	GLY	5.4
1	A	253	GLN	5.4
1	E	185	HIS	5.4
1	E	186	ASP	5.3
1	D	198	TYR	5.2
1	D	199	CYS	5.0
1	D	245	VAL	4.9
1	B	195	LEU	4.8
1	B	155	ILE	4.7
1	B	228	SER	4.7
1	A	243	PRO	4.6
1	A	228	SER	4.6
1	A	151	LEU	4.6
1	D	246	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	152	GLY	4.5
1	D	187	SER	4.5
1	E	239	LEU	4.5
1	D	201	LEU	4.4
1	D	195	LEU	4.4
1	A	245	VAL	4.4
1	B	250	ARG	4.4
1	A	251	ILE	4.3
1	D	193	PHE	4.3
1	E	193	PHE	4.3
1	C	251	ILE	4.3
1	E	173	ASP	4.3
1	D	200	HIS	4.2
1	C	242	THR	4.2
1	E	187	SER	4.1
1	A	248	VAL	4.1
1	C	195	LEU	4.1
1	D	155	ILE	4.0
1	A	187	SER	4.0
1	C	147	VAL	3.9
1	D	197	GLY	3.9
1	A	168	PHE	3.9
1	E	150	ASP	3.9
1	B	239	LEU	3.9
1	B	243	PRO	3.9
1	C	151	LEU	3.8
1	D	68	LEU	3.8
1	E	198	TYR	3.8
1	B	71	LEU	3.8
1	D	188	THR	3.8
1	A	175	MET	3.8
1	C	149	PRO	3.7
1	A	190	VAL	3.7
1	D	202	ASN	3.7
1	A	226	ASP	3.7
1	B	226	ASP	3.7
1	E	148	ALA	3.7
1	A	244	ARG	3.7
1	B	187	SER	3.6
1	D	231	SER	3.6
1	B	136	PHE	3.6
1	D	196	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	188	THR	3.6
1	D	27	MET	3.6
1	C	243	PRO	3.6
1	E	196	ASN	3.6
1	B	242	THR	3.5
1	E	190	VAL	3.5
1	A	242	THR	3.5
1	B	199	CYS	3.5
1	C	197	GLY	3.5
1	D	133	THR	3.5
1	B	227	SER	3.4
1	D	157	LEU	3.4
1	E	225	VAL	3.4
1	A	191	ILE	3.4
1	A	246	PRO	3.4
1	E	230	PHE	3.3
1	C	68	LEU	3.3
1	C	164	ILE	3.3
1	D	70	SER	3.3
1	C	69	ASP	3.3
1	D	149	PRO	3.3
1	D	151	LEU	3.3
1	A	167	VAL	3.3
1	D	192	ARG	3.3
1	E	226	ASP	3.3
1	D	253	GLN	3.3
1	B	193	PHE	3.3
1	C	226	ASP	3.3
1	D	186	ASP	3.3
1	C	169	PRO	3.3
1	D	194	PRO	3.3
1	E	142	CYS	3.2
1	A	152	GLY	3.2
1	C	97	LEU	3.2
1	D	233	TYR	3.2
1	B	134	GLY	3.2
1	B	135	ARG	3.2
1	D	154	ARG	3.2
1	E	136	PHE	3.2
1	E	75	TYR	3.2
1	A	225	VAL	3.2
1	B	172	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	199	CYS	3.2
1	E	27	MET	3.1
1	E	68	LEU	3.1
1	D	225	VAL	3.1
1	D	244	ARG	3.1
1	C	70	SER	3.1
1	D	168	PHE	3.1
1	E	169	PRO	3.1
1	D	242	THR	3.1
1	B	224	GLY	3.1
1	E	167	VAL	3.0
1	E	149	PRO	3.0
1	A	249	ILE	3.0
1	A	150	ASP	3.0
1	D	100	ASP	2.9
1	B	229	GLN	2.9
1	E	153	GLU	2.9
1	A	239	LEU	2.9
1	D	247	SER	2.9
1	C	138	ARG	2.9
1	A	195	LEU	2.9
1	E	241	ARG	2.9
1	E	201	LEU	2.9
1	D	147	VAL	2.8
1	D	160	ASP	2.8
1	B	241	ARG	2.8
1	D	26	SER	2.8
1	E	188	THR	2.8
1	B	69	ASP	2.8
1	B	196	ASN	2.8
1	D	190	VAL	2.8
1	C	192	ARG	2.8
1	B	101	ASP	2.8
1	B	249	ILE	2.7
1	D	207	LEU	2.7
1	D	69	ASP	2.7
1	D	230	PHE	2.7
1	A	169	PRO	2.7
1	B	225	VAL	2.7
1	C	198	TYR	2.7
1	D	227	SER	2.7
1	A	131	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	27	MET	2.7
1	A	196	ASN	2.7
1	E	203	SER	2.7
1	C	172	GLY	2.6
1	D	169	PRO	2.6
1	B	200	HIS	2.6
1	E	163	LEU	2.6
1	A	198	TYR	2.6
1	C	252	LYS	2.6
1	B	197	GLY	2.6
1	C	71	LEU	2.6
1	A	188	THR	2.6
1	D	61	ASP	2.6
1	C	136	PHE	2.6
1	A	171	ILE	2.5
1	D	53	GLU	2.5
1	C	239	LEU	2.5
1	A	26	SER	2.5
1	D	191	ILE	2.5
1	C	73	GLN	2.5
1	E	147	VAL	2.5
1	E	227	SER	2.5
1	E	101	ASP	2.5
1	A	155	ILE	2.5
1	E	155	ILE	2.5
1	A	163	LEU	2.5
1	D	136	PHE	2.5
1	A	149	PRO	2.5
1	C	171	ILE	2.5
1	C	196	ASN	2.5
1	C	142	CYS	2.4
1	B	150	ASP	2.4
1	B	107	LEU	2.4
1	B	151	LEU	2.4
1	E	200	HIS	2.4
1	B	27	MET	2.4
1	D	156	THR	2.4
1	D	226	ASP	2.4
1	A	156	THR	2.4
1	A	174	VAL	2.4
1	C	225	VAL	2.4
1	B	148	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	132	GLU	2.4
1	B	130	ASP	2.4
1	C	146	ARG	2.4
1	E	70	SER	2.3
1	B	201	LEU	2.3
1	D	204	VAL	2.3
1	B	133	THR	2.3
1	B	154	ARG	2.3
1	D	240	ARG	2.3
1	E	151	LEU	2.3
1	B	70	SER	2.3
1	E	157	LEU	2.3
1	D	215	PHE	2.3
1	B	153	GLU	2.3
1	C	244	ARG	2.3
1	A	230	PHE	2.3
1	A	250	ARG	2.3
1	A	200	HIS	2.2
1	E	189	HIS	2.2
1	E	197	GLY	2.2
1	A	252	LYS	2.2
1	B	191	ILE	2.2
1	E	71	LEU	2.2
1	E	194	PRO	2.2
1	E	143	LEU	2.2
1	D	153	GLU	2.2
1	B	233	TYR	2.2
1	C	229	GLN	2.2
1	A	201	LEU	2.2
1	C	150	ASP	2.2
1	D	141	GLU	2.2
1	C	250	ARG	2.2
1	B	29	ASN	2.2
1	A	143	LEU	2.2
1	D	71	LEU	2.2
1	E	191	ILE	2.2
1	A	247	SER	2.2
1	C	247	SER	2.2
1	E	158	SER	2.2
1	A	232	GLU	2.2
1	C	141	GLU	2.2
1	C	156	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	107	LEU	2.1
1	E	146	ARG	2.1
1	C	100	ASP	2.1
1	B	194	PRO	2.1
1	E	211	GLN	2.1
1	A	68	LEU	2.1
1	B	157	LEU	2.1
1	C	207	LEU	2.1
1	C	153	GLU	2.1
1	A	69	ASP	2.1
1	B	234	VAL	2.1
1	D	143	LEU	2.1
1	D	252	LYS	2.1
1	A	162	SER	2.1
1	B	28	SER	2.1
1	A	157	LEU	2.1
1	C	157	LEU	2.1
1	C	152	GLY	2.1
1	D	224	GLY	2.1
1	C	249	ILE	2.1
1	A	135	ARG	2.0
1	D	146	ARG	2.0
1	B	235	LEU	2.0
1	C	165	GLU	2.0
1	C	155	ILE	2.0
1	D	162	SER	2.0
1	D	73	GLN	2.0
1	C	168	PHE	2.0
1	D	236	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	NA	A	302	1/1	0.59	0.25	43,43,43,43	0
2	NA	A	301	1/1	0.94	0.13	59,59,59,59	0
3	IOD	B	301	1/1	0.96	0.05	64,64,64,64	0
3	IOD	B	302	1/1	0.99	0.03	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.