



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:50 PM UTC

PDB ID : 3DRX / pdb_00003drx
Title : X-ray crystal structure of human KCTD5 protein crystallized in high-salt buffer
Authors : Tereshko, V.; Dementieva, I.; Goldstein, S.A.N.
Deposited on : 2008-07-11
Resolution : 3.11 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

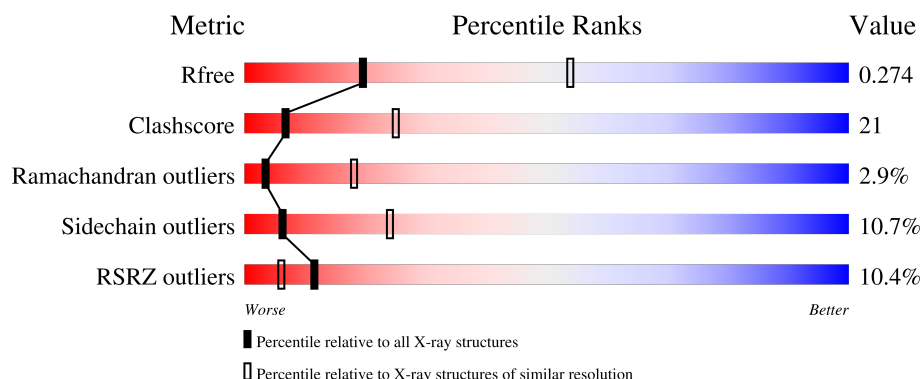
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	202	10% 43% 30% 7% 20%
1	B	202	14% 54% 24% 6% 15%
1	C	202	4% 48% 29% 11% 12%
1	D	202	10% 58% 26% • 12%
1	E	202	5% 50% 26% 7% 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6907 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 KCTD5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1306	831	223	246	6			
1	B	172	Total	C	N	O	S	0	0	0
			1385	874	236	269	6			
1	C	177	Total	C	N	O	S	0	0	0
			1430	902	243	279	6			
1	D	177	Total	C	N	O	S	0	0	0
			1427	901	243	277	6			
1	E	169	Total	C	N	O	S	0	0	0
			1359	860	232	261	6			

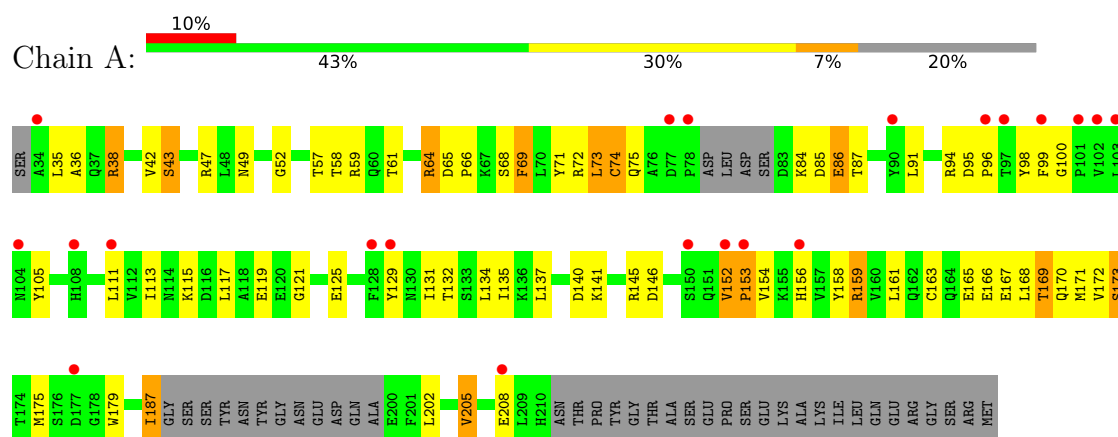
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	SER	-	expression tag	UNP Q9NXV2
B	33	SER	-	expression tag	UNP Q9NXV2
C	33	SER	-	expression tag	UNP Q9NXV2
D	33	SER	-	expression tag	UNP Q9NXV2
E	33	SER	-	expression tag	UNP Q9NXV2

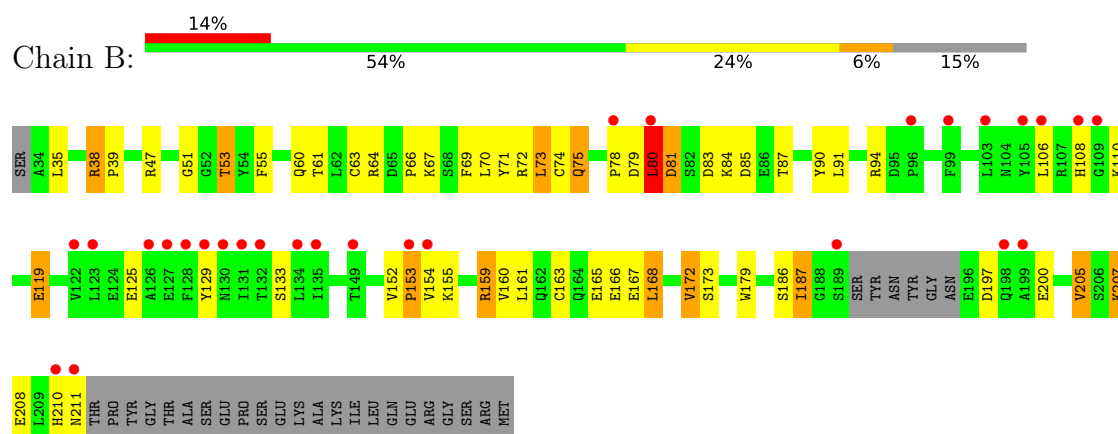
3 Residue-property plots [i](#)

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.

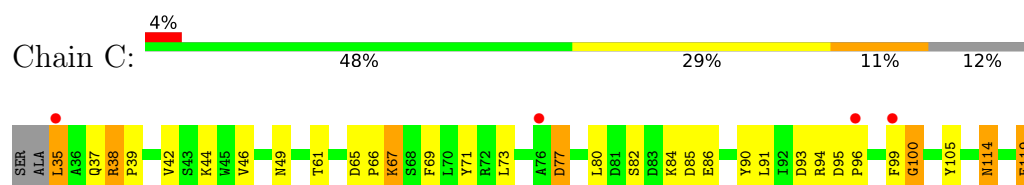
- Molecule 1: BTB/POZ domain-containing protein KCTD5

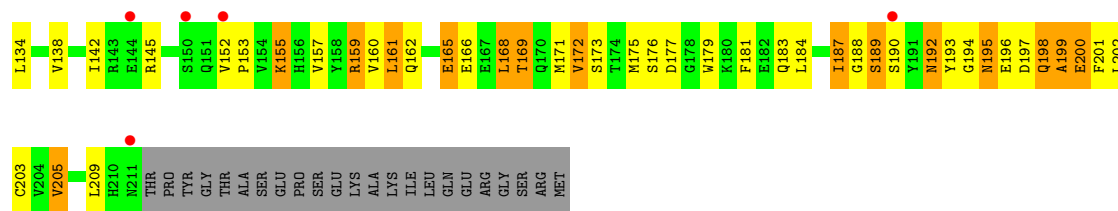


- Molecule 1: BTB/POZ domain-containing protein KCTD5

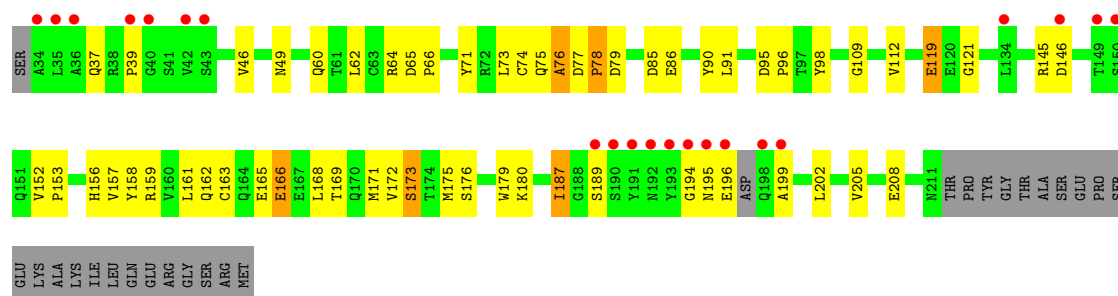


- Molecule 1: BTB/POZ domain-containing protein KCTD5

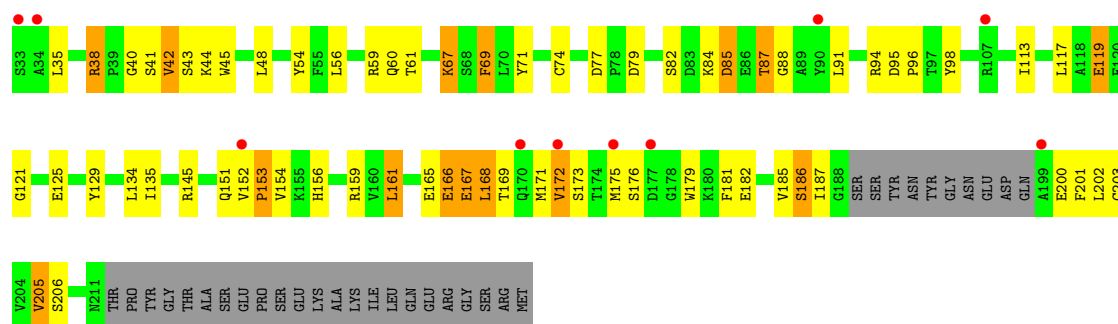




● Molecule 1: BTB/POZ domain-containing protein KCTD5



● Molecule 1: BTB/POZ domain-containing protein KCTD5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.86Å 128.58Å 152.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.11 20.00 – 3.11	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.11) 98.5 (20.00-3.11)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.227 , 0.275 0.225 , 0.274	Depositor DCC
R_{free} test set	1321 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6907	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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	0.47	0/1329	0.81	2/1793 (0.1%)
1	B	0.53	0/1409	0.85	1/1903 (0.1%)
1	C	0.55	0/1457	0.95	6/1970 (0.3%)
1	D	0.51	0/1453	0.82	2/1963 (0.1%)
1	E	0.54	0/1383	0.84	1/1868 (0.1%)
All	All	0.52	0/7031	0.86	12/9497 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	ARG	CA-C-N	12.24	135.14	119.84
1	C	38	ARG	C-N-CA	12.24	135.14	119.84
1	B	80	LEU	N-CA-C	-9.44	102.86	114.75
1	E	41	SER	N-CA-C	-7.79	104.20	112.93
1	C	152	VAL	N-CA-C	6.95	116.60	108.96
1	D	189	SER	N-CA-C	6.48	119.42	110.35
1	D	152	VAL	N-CA-C	5.69	114.53	108.95
1	C	197	ASP	N-CA-C	-5.45	106.95	113.21
1	C	77	ASP	CA-C-N	5.43	124.77	118.85
1	C	77	ASP	C-N-CA	5.43	124.77	118.85
1	A	152	VAL	CA-C-N	5.21	126.36	119.84
1	A	152	VAL	C-N-CA	5.21	126.36	119.84

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	1306	0	1309	69	0
1	B	1385	0	1371	48	0
1	C	1430	0	1405	72	0
1	D	1427	0	1405	50	0
1	E	1359	0	1353	67	0
All	All	6907	0	6843	294	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 21.

All (294) 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:152:VAL:CG1	1:E:153:PRO:HD2	1.77	1.13
1:E:38:ARG:HG2	1:E:38:ARG:HH11	1.09	1.07
1:E:152:VAL:HG12	1:E:153:PRO:HD2	1.37	1.03
1:E:165:GLU:O	1:E:168:LEU:HB2	1.69	0.92
1:A:72:ARG:HG3	1:A:73:LEU:HD13	1.49	0.91
1:C:165:GLU:N	1:C:200:GLU:HG3	1.86	0.91
1:A:38:ARG:H	1:A:38:ARG:HH11	1.16	0.90
1:E:154:VAL:O	1:E:154:VAL:HG23	1.71	0.89
1:B:172:VAL:HG21	1:C:160:VAL:HG23	1.55	0.86
1:C:165:GLU:H	1:C:200:GLU:HG3	1.39	0.86
1:D:172:VAL:HA	1:D:175:MET:CE	2.07	0.85
1:E:152:VAL:HG12	1:E:153:PRO:CD	2.06	0.85
1:D:85:ASP:HB3	1:D:91:LEU:HD21	1.57	0.84
1:E:38:ARG:HG2	1:E:38:ARG:NH1	1.85	0.84
1:E:152:VAL:HG13	1:E:153:PRO:HD2	1.59	0.84
1:C:38:ARG:HD3	1:C:38:ARG:N	1.93	0.84
1:E:171:MET:HE1	1:E:203:CYS:SG	2.19	0.83
1:E:159:ARG:HD3	1:E:179:TRP:CH2	2.15	0.81
1:E:84:LYS:HE3	1:E:88:GLY:O	1.82	0.80
1:A:69:PHE:O	1:A:72:ARG:HG2	1.84	0.78
1:B:152:VAL:CG1	1:B:153:PRO:HD2	2.15	0.77
1:D:169:THR:O	1:D:173:SER:HB2	1.86	0.76
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.16	0.76
1:B:163:CYS:HB2	1:B:167:GLU:HG3	1.68	0.75
1:D:37:GLN:O	1:D:39:PRO:HD3	1.86	0.75
1:B:47:ARG:NH2	1:B:87:THR:HB	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:SER:C	1:E:187:ILE:HG13	2.12	0.73
1:E:159:ARG:HD3	1:E:179:TRP:CZ3	2.24	0.73
1:C:195:ASN:O	1:C:198:GLN:HB2	1.89	0.73
1:C:142:ILE:HG23	1:C:145:ARG:HH12	1.54	0.72
1:E:85:ASP:OD2	1:E:85:ASP:C	2.32	0.71
1:D:194:GLY:O	1:D:196:GLU:N	2.20	0.71
1:E:151:GLN:HE22	1:E:154:VAL:HG12	1.54	0.71
1:D:163:CYS:SG	1:D:171:MET:HE2	2.31	0.71
1:A:71:TYR:O	1:A:74:CYS:HB3	1.90	0.71
1:B:75:GLN:HA	1:B:75:GLN:HE21	1.57	0.70
1:B:38:ARG:HG3	1:B:39:PRO:HD2	1.72	0.69
1:E:165:GLU:HG3	1:E:166:GLU:N	2.08	0.69
1:D:194:GLY:O	1:D:196:GLU:HG2	1.93	0.69
1:B:85:ASP:HB3	1:B:91:LEU:HD21	1.75	0.69
1:A:59:ARG:NH1	1:A:73:LEU:O	2.26	0.68
1:A:163:CYS:HB2	1:A:167:GLU:HG3	1.74	0.68
1:E:166:GLU:C	1:E:168:LEU:H	2.02	0.68
1:B:152:VAL:HG13	1:B:153:PRO:HD2	1.76	0.68
1:B:173:SER:HB3	1:C:159:ARG:HH21	1.58	0.67
1:A:66:PRO:HA	1:A:71:TYR:CD1	2.30	0.67
1:C:172:VAL:HA	1:C:175:MET:CE	2.24	0.67
1:D:172:VAL:HA	1:D:175:MET:HE3	1.77	0.67
1:C:198:GLN:O	1:C:199:ALA:CB	2.43	0.66
1:E:151:GLN:NE2	1:E:154:VAL:HG12	2.11	0.66
1:D:64:ARG:HH12	1:D:109:GLY:HA2	1.60	0.66
1:C:192:ASN:HB3	1:C:198:GLN:CD	2.20	0.66
1:A:38:ARG:H	1:A:38:ARG:NH1	1.94	0.65
1:C:165:GLU:H	1:C:200:GLU:CG	2.08	0.65
1:E:166:GLU:HG3	1:E:167:GLU:H	1.60	0.65
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.79	0.65
1:C:85:ASP:HB3	1:C:91:LEU:HD21	1.79	0.65
1:C:172:VAL:HA	1:C:175:MET:HE3	1.78	0.65
1:E:77:ASP:OD1	1:E:77:ASP:C	2.40	0.64
1:A:152:VAL:O	1:A:153:PRO:O	2.15	0.64
1:C:196:GLU:C	1:C:198:GLN:H	2.05	0.63
1:C:38:ARG:HD3	1:C:38:ARG:H	1.58	0.63
1:C:142:ILE:HG23	1:C:145:ARG:NH1	2.13	0.62
1:A:168:LEU:O	1:A:172:VAL:HG22	2.00	0.62
1:C:38:ARG:H	1:C:38:ARG:CD	2.13	0.61
1:B:119:GLU:N	1:B:119:GLU:OE1	2.33	0.61
1:D:187:ILE:O	1:D:187:ILE:CG2	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:O	1:A:43:SER:HB2	2.01	0.61
1:C:38:ARG:N	1:C:38:ARG:CD	2.64	0.61
1:C:187:ILE:HD12	1:C:202:LEU:HG	1.83	0.61
1:C:198:GLN:HB3	1:C:200:GLU:OE1	2.01	0.60
1:C:198:GLN:O	1:C:199:ALA:HB3	2.00	0.60
1:D:62:LEU:O	1:D:74:CYS:HB2	2.02	0.60
1:C:84:LYS:HE3	1:C:90:TYR:CE1	2.36	0.60
1:E:165:GLU:CG	1:E:166:GLU:N	2.64	0.59
1:D:194:GLY:C	1:D:196:GLU:H	2.08	0.59
1:B:159:ARG:HB2	1:B:205:VAL:HG12	1.84	0.59
1:A:169:THR:HG22	1:A:170:GLN:N	2.17	0.58
1:A:165:GLU:HG3	1:A:166:GLU:N	2.18	0.58
1:A:159:ARG:HG2	1:A:205:VAL:HG12	1.85	0.58
1:C:168:LEU:O	1:C:168:LEU:HD22	2.02	0.58
1:A:159:ARG:HD3	1:A:179:TRP:CH2	2.39	0.57
1:D:176:SER:HB3	1:D:179:TRP:CD1	2.40	0.56
1:C:192:ASN:HB3	1:C:198:GLN:OE1	2.05	0.56
1:E:159:ARG:CD	1:E:179:TRP:CH2	2.87	0.56
1:A:91:LEU:HD22	1:E:56:LEU:HD21	1.87	0.56
1:C:165:GLU:HG3	1:C:193:TYR:CE2	2.40	0.56
1:B:173:SER:HB3	1:C:159:ARG:NH2	2.20	0.56
1:D:194:GLY:C	1:D:196:GLU:N	2.64	0.56
1:A:47:ARG:NH2	1:A:87:THR:HB	2.21	0.55
1:B:119:GLU:H	1:B:119:GLU:CD	2.14	0.55
1:E:154:VAL:O	1:E:154:VAL:CG2	2.43	0.55
1:A:95:ASP:OD1	1:A:96:PRO:HD2	2.07	0.55
1:A:172:VAL:HG21	1:B:160:VAL:CG2	2.37	0.55
1:B:152:VAL:HG12	1:B:153:PRO:HD2	1.88	0.55
1:B:186:SER:C	1:B:187:ILE:HD13	2.32	0.55
1:E:187:ILE:HD11	1:E:202:LEU:HG	1.90	0.54
1:C:93:ASP:O	1:C:94:ARG:HD2	2.07	0.54
1:C:165:GLU:OE2	1:C:194:GLY:HA2	2.07	0.54
1:A:168:LEU:C	1:A:168:LEU:HD13	2.32	0.54
1:B:80:LEU:O	1:B:81:ASP:C	2.50	0.54
1:B:152:VAL:O	1:B:153:PRO:O	2.25	0.54
1:C:198:GLN:CB	1:C:200:GLU:OE1	2.56	0.54
1:D:156:HIS:CE1	1:D:208:GLU:HG2	2.43	0.54
1:B:85:ASP:C	1:B:85:ASP:OD1	2.50	0.54
1:C:183:GLN:HG2	1:C:184:LEU:N	2.23	0.54
1:E:182:GLU:HG3	1:E:206:SER:HB3	1.88	0.54
1:E:172:VAL:O	1:E:175:MET:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:GLU:HG3	1:D:166:GLU:H	1.72	0.54
1:A:156:HIS:NE2	1:A:208:GLU:HG2	2.22	0.53
1:D:66:PRO:HA	1:D:71:TYR:CD1	2.44	0.53
1:D:165:GLU:HG3	1:D:166:GLU:N	2.23	0.53
1:E:165:GLU:CG	1:E:166:GLU:H	2.20	0.53
1:B:66:PRO:HA	1:B:71:TYR:CG	2.43	0.53
1:C:134:LEU:O	1:C:138:VAL:HG23	2.07	0.53
1:B:69:PHE:CD1	1:B:69:PHE:C	2.87	0.53
1:E:119:GLU:N	1:E:119:GLU:OE1	2.41	0.53
1:A:49:ASN:HB3	1:A:91:LEU:HD23	1.90	0.53
1:C:176:SER:OG	1:C:177:ASP:N	2.39	0.53
1:C:35:LEU:C	1:C:37:GLN:H	2.16	0.52
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.90	0.52
1:A:158:TYR:CE1	1:E:181:PHE:HB3	2.44	0.52
1:C:195:ASN:HD22	1:C:198:GLN:HG2	1.74	0.52
1:D:95:ASP:OD1	1:D:96:PRO:HD2	2.09	0.52
1:D:162:GLN:HB3	1:D:202:LEU:HD23	1.92	0.52
1:E:95:ASP:OD1	1:E:96:PRO:HD2	2.09	0.52
1:C:165:GLU:HA	1:C:201:PHE:HE1	1.75	0.52
1:C:189:SER:O	1:C:190:SER:C	2.51	0.52
1:B:165:GLU:H	1:B:200:GLU:HG3	1.73	0.52
1:C:66:PRO:HA	1:C:71:TYR:CD1	2.44	0.52
1:C:37:GLN:HA	1:C:38:ARG:NH1	2.24	0.52
1:E:85:ASP:HB3	1:E:91:LEU:HD21	1.92	0.52
1:E:165:GLU:H	1:E:200:GLU:HG3	1.74	0.52
1:D:172:VAL:HA	1:D:175:MET:HE2	1.88	0.52
1:A:94:ARG:NH2	1:A:125:GLU:OE2	2.41	0.52
1:C:99:PHE:O	1:C:100:GLY:C	2.52	0.52
1:D:71:TYR:O	1:D:74:CYS:HB3	2.10	0.52
1:B:66:PRO:HA	1:B:71:TYR:CD1	2.45	0.52
1:C:171:MET:HE1	1:C:203:CYS:SG	2.50	0.51
1:B:152:VAL:O	1:B:153:PRO:C	2.52	0.51
1:C:181:PHE:C	1:C:181:PHE:CD2	2.89	0.51
1:E:166:GLU:C	1:E:168:LEU:N	2.69	0.51
1:A:66:PRO:HA	1:A:71:TYR:CE1	2.45	0.51
1:E:40:GLY:C	1:E:42:VAL:H	2.17	0.51
1:A:36:ALA:HB2	1:B:69:PHE:CZ	2.46	0.50
1:B:172:VAL:CG2	1:B:173:SER:N	2.75	0.50
1:C:35:LEU:C	1:C:37:GLN:N	2.69	0.50
1:D:165:GLU:HG3	1:D:166:GLU:HG3	1.93	0.50
1:C:65:ASP:OD1	1:C:67:LYS:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LEU:N	1:D:73:LEU:HD12	2.26	0.50
1:E:43:SER:O	1:E:59:ARG:NE	2.42	0.50
1:C:165:GLU:CA	1:C:200:GLU:HG3	2.41	0.49
1:A:47:ARG:NH2	1:A:87:THR:OG1	2.45	0.49
1:E:166:GLU:O	1:E:168:LEU:N	2.44	0.49
1:A:47:ARG:NH2	1:A:87:THR:CB	2.75	0.49
1:A:145:ARG:NH1	1:A:146:ASP:OD2	2.45	0.49
1:E:172:VAL:O	1:E:173:SER:C	2.56	0.49
1:B:173:SER:CB	1:C:159:ARG:HH21	2.26	0.49
1:E:152:VAL:O	1:E:153:PRO:C	2.55	0.49
1:B:172:VAL:HG23	1:B:173:SER:N	2.28	0.49
1:C:66:PRO:HA	1:C:71:TYR:CG	2.48	0.49
1:E:134:LEU:O	1:E:135:ILE:C	2.56	0.49
1:E:38:ARG:NH1	1:E:38:ARG:CG	2.61	0.48
1:B:47:ARG:HH21	1:B:87:THR:HB	1.76	0.48
1:A:47:ARG:HH21	1:A:87:THR:CB	2.27	0.48
1:A:172:VAL:HG21	1:B:160:VAL:HG23	1.95	0.48
1:C:181:PHE:HB3	1:D:158:TYR:CE1	2.48	0.48
1:C:119:GLU:CD	1:C:119:GLU:H	2.20	0.48
1:C:114:ASN:OD1	1:C:114:ASN:N	2.46	0.48
1:B:69:PHE:O	1:B:72:ARG:HD3	2.14	0.48
1:A:187:ILE:HD12	1:A:187:ILE:HA	1.72	0.48
1:C:65:ASP:C	1:C:67:LYS:H	2.22	0.48
1:C:165:GLU:HG3	1:C:193:TYR:CZ	2.49	0.48
1:C:161:LEU:CD1	1:C:161:LEU:N	2.77	0.47
1:D:64:ARG:HH12	1:D:109:GLY:CA	2.24	0.47
1:D:172:VAL:HG23	1:D:173:SER:N	2.29	0.47
1:A:166:GLU:HG2	1:A:167:GLU:N	2.29	0.47
1:D:175:MET:HE3	1:D:175:MET:HB2	1.78	0.47
1:A:49:ASN:C	1:A:49:ASN:OD1	2.57	0.47
1:A:179:TRP:CE3	1:A:205:VAL:HG13	2.50	0.47
1:A:166:GLU:C	1:A:168:LEU:H	2.23	0.47
1:A:59:ARG:HD3	1:A:74:CYS:O	2.15	0.47
1:D:75:GLN:HG2	1:D:76:ALA:N	2.30	0.47
1:D:162:GLN:HB3	1:D:202:LEU:CD2	2.45	0.47
1:E:113:ILE:HG23	1:E:117:LEU:HB3	1.97	0.47
1:E:165:GLU:HG3	1:E:166:GLU:H	1.79	0.47
1:A:57:THR:OG1	1:A:58:THR:N	2.46	0.46
1:E:179:TRP:CE3	1:E:205:VAL:HG13	2.50	0.46
1:C:82:SER:O	1:C:84:LYS:HG3	2.15	0.46
1:E:171:MET:CE	1:E:203:CYS:SG	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:VAL:HG23	1:A:173:SER:N	2.31	0.46
1:D:187:ILE:O	1:D:187:ILE:HG23	2.16	0.46
1:C:35:LEU:HD12	1:D:90:TYR:HB3	1.97	0.46
1:D:145:ARG:NH1	1:D:146:ASP:OD2	2.49	0.46
1:A:73:LEU:HD13	1:A:73:LEU:N	2.31	0.46
1:A:69:PHE:C	1:A:69:PHE:CD2	2.94	0.46
1:C:165:GLU:CB	1:C:200:GLU:HG3	2.46	0.46
1:E:181:PHE:C	1:E:181:PHE:CD2	2.93	0.46
1:D:161:LEU:CD1	1:D:161:LEU:N	2.80	0.45
1:A:169:THR:O	1:A:173:SER:HB3	2.17	0.45
1:B:73:LEU:O	1:B:74:CYS:C	2.59	0.45
1:E:48:LEU:O	1:E:54:TYR:HA	2.16	0.45
1:A:131:ILE:O	1:A:132:THR:C	2.59	0.45
1:A:169:THR:O	1:A:170:GLN:C	2.60	0.45
1:D:37:GLN:O	1:D:37:GLN:HG3	2.17	0.45
1:E:98:TYR:CE2	1:E:121:GLY:HA3	2.51	0.45
1:E:77:ASP:OD1	1:E:79:ASP:N	2.48	0.45
1:C:85:ASP:O	1:C:86:GLU:C	2.60	0.45
1:A:134:LEU:O	1:A:135:ILE:C	2.60	0.45
1:A:98:TYR:CE2	1:A:121:GLY:HA3	2.52	0.45
1:A:85:ASP:C	1:A:87:THR:H	2.25	0.44
1:A:165:GLU:O	1:A:168:LEU:HB2	2.17	0.44
1:D:79:ASP:OD1	1:D:79:ASP:N	2.44	0.44
1:D:180:LYS:HD2	1:E:156:HIS:ND1	2.32	0.44
1:B:125:GLU:O	1:B:129:TYR:HD1	1.99	0.44
1:D:66:PRO:HA	1:D:71:TYR:CG	2.52	0.44
1:B:168:LEU:HA	1:B:168:LEU:HD23	1.71	0.44
1:C:105:TYR:OH	1:C:133:SER:HB2	2.17	0.44
1:D:176:SER:HB3	1:D:179:TRP:HD1	1.81	0.44
1:E:69:PHE:CE2	1:E:129:TYR:HD2	2.36	0.44
1:B:70:LEU:C	1:B:72:ARG:N	2.75	0.44
1:C:165:GLU:N	1:C:200:GLU:CG	2.67	0.44
1:C:188:GLY:O	1:C:189:SER:HB3	2.18	0.44
1:A:65:ASP:HA	1:A:66:PRO:HD2	1.79	0.44
1:D:65:ASP:HA	1:D:66:PRO:HD2	1.86	0.44
1:B:64:ARG:HG3	1:B:106:LEU:O	2.18	0.44
1:D:49:ASN:OD1	1:D:49:ASN:C	2.61	0.44
1:E:185:VAL:HG12	1:E:186:SER:N	2.33	0.44
1:A:99:PHE:O	1:A:100:GLY:C	2.61	0.43
1:B:108:HIS:ND1	1:B:110:LYS:HB2	2.33	0.43
1:D:165:GLU:O	1:D:168:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HG3	1:A:73:LEU:N	2.33	0.43
1:A:137:LEU:O	1:A:140:ASP:HB2	2.18	0.43
1:A:202:LEU:HD23	1:A:202:LEU:HA	1.86	0.43
1:A:68:SER:HA	1:A:129:TYR:O	2.19	0.43
1:A:171:MET:HE2	1:A:171:MET:HB3	1.91	0.43
1:A:71:TYR:O	1:A:74:CYS:CB	2.63	0.43
1:B:61:THR:O	1:B:61:THR:HG22	2.19	0.43
1:A:156:HIS:HE2	1:A:208:GLU:HG2	1.84	0.43
1:C:49:ASN:C	1:C:49:ASN:OD1	2.61	0.43
1:C:155:LYS:HE2	1:C:155:LYS:HB3	1.94	0.43
1:C:157:VAL:HG23	1:C:209:LEU:HD11	2.01	0.43
1:E:60:GLN:O	1:E:61:THR:C	2.60	0.42
1:E:67:LYS:HB2	1:E:67:LYS:HE3	1.73	0.42
1:A:115:LYS:C	1:A:117:LEU:H	2.27	0.42
1:C:179:TRP:CE3	1:C:205:VAL:HG13	2.54	0.42
1:C:162:GLN:O	1:C:162:GLN:HG3	2.19	0.42
1:C:169:THR:O	1:C:173:SER:HB2	2.19	0.42
1:E:176:SER:HB3	1:E:179:TRP:CD1	2.55	0.42
1:C:71:TYR:C	1:C:73:LEU:H	2.26	0.42
1:D:180:LYS:N	1:D:180:LYS:HD3	2.33	0.42
1:A:42:VAL:O	1:A:43:SER:CB	2.65	0.42
1:D:166:GLU:C	1:D:168:LEU:H	2.27	0.42
1:E:175:MET:HB2	1:E:175:MET:HE3	1.88	0.42
1:B:51:GLY:HA3	1:B:94:ARG:O	2.20	0.42
1:A:152:VAL:O	1:A:153:PRO:C	2.63	0.42
1:C:165:GLU:HA	1:C:201:PHE:CE1	2.54	0.42
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.81	0.41
1:B:83:ASP:OD1	1:B:83:ASP:N	2.53	0.41
1:C:95:ASP:OD1	1:C:96:PRO:HD2	2.19	0.41
1:A:175:MET:HE3	1:A:175:MET:HB2	1.65	0.41
1:B:186:SER:O	1:B:187:ILE:HD13	2.20	0.41
1:D:159:ARG:HB3	1:D:205:VAL:HG12	2.02	0.41
1:D:77:ASP:HA	1:D:78:PRO:HD2	1.93	0.41
1:D:98:TYR:CE2	1:D:121:GLY:HA3	2.56	0.41
1:A:86:GLU:OE2	1:A:87:THR:CG2	2.68	0.41
1:C:69:PHE:CD1	1:C:69:PHE:C	2.98	0.41
1:E:44:LYS:HE2	1:E:45:TRP:NE1	2.35	0.41
1:E:94:ARG:HH21	1:E:125:GLU:CD	2.28	0.41
1:E:172:VAL:HG23	1:E:173:SER:H	1.85	0.41
1:A:73:LEU:O	1:A:74:CYS:C	2.62	0.41
1:A:49:ASN:OD1	1:A:52:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ASP:HB3	1:C:80:LEU:HB2	2.01	0.41
1:E:185:VAL:O	1:E:201:PHE:HA	2.21	0.41
1:B:84:LYS:HE2	1:B:90:TYR:CZ	2.56	0.41
1:B:152:VAL:HG12	1:B:153:PRO:CD	2.50	0.41
1:E:159:ARG:NH2	1:E:161:LEU:HD11	2.36	0.41
1:B:53:THR:HG22	1:B:55:PHE:CE2	2.56	0.41
1:B:179:TRP:CE2	1:B:207:LYS:HD3	2.56	0.41
1:C:130:ASN:O	1:C:130:ASN:CG	2.64	0.41
1:C:131:ILE:O	1:C:132:THR:C	2.64	0.41
1:E:71:TYR:O	1:E:74:CYS:HB3	2.20	0.41
1:E:152:VAL:HG12	1:E:153:PRO:CG	2.49	0.41
1:B:208:GLU:OE1	1:B:210:HIS:NE2	2.54	0.41
1:A:105:TYR:CG	1:A:134:LEU:HD13	2.56	0.40
1:D:60:GLN:C	1:D:62:LEU:N	2.78	0.40
1:D:119:GLU:OE1	1:D:119:GLU:N	2.53	0.40
1:A:111:LEU:HD11	1:A:113:ILE:HD11	2.03	0.40
1:B:63:CYS:O	1:B:64:ARG:C	2.64	0.40
1:E:69:PHE:HE2	1:E:129:TYR:CD2	2.39	0.40
1:D:163:CYS:SG	1:D:171:MET:CE	3.04	0.40
1:E:42:VAL:O	1:E:42:VAL:CG1	2.69	0.40
1:E:85:ASP:OD2	1:E:87:THR:N	2.55	0.40
1:E:186:SER:C	1:E:187:ILE:CG1	2.90	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	155/202 (77%)	128 (83%)	22 (14%)	5 (3%)	3	16
1	B	168/202 (83%)	152 (90%)	12 (7%)	4 (2%)	4	21
1	C	175/202 (87%)	146 (83%)	23 (13%)	6 (3%)	3	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	173/202 (86%)	148 (86%)	20 (12%)	5 (3%)	3	18
1	E	165/202 (82%)	144 (87%)	17 (10%)	4 (2%)	4	21
All	All	836/1010 (83%)	718 (86%)	94 (11%)	24 (3%)	3	18

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	74	CYS
1	A	153	PRO
1	B	81	ASP
1	C	198	GLN
1	D	195	ASN
1	D	199	ALA
1	B	153	PRO
1	C	153	PRO
1	C	189	SER
1	C	199	ALA
1	D	78	PRO
1	D	153	PRO
1	E	85	ASP
1	E	153	PRO
1	B	187	ILE
1	E	167	GLU
1	A	64	ARG
1	C	39	PRO
1	D	76	ALA
1	E	166	GLU
1	A	154	VAL
1	B	78	PRO
1	C	100	GLY

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	147/181 (81%)	130 (88%)	17 (12%)	5	21
1	B	156/181 (86%)	134 (86%)	22 (14%)	3	14
1	C	161/181 (89%)	140 (87%)	21 (13%)	4	17
1	D	160/181 (88%)	152 (95%)	8 (5%)	22	50
1	E	153/181 (84%)	138 (90%)	15 (10%)	7	28
All	All	777/905 (86%)	694 (89%)	83 (11%)	6	24

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	ARG
1	A	61	THR
1	A	64	ARG
1	A	69	PHE
1	A	73	LEU
1	A	75	GLN
1	A	84	LYS
1	A	86	GLU
1	A	119	GLU
1	A	141	LYS
1	A	159	ARG
1	A	161	LEU
1	A	169	THR
1	A	173	SER
1	A	187	ILE
1	A	205	VAL
1	B	35	LEU
1	B	38	ARG
1	B	53	THR
1	B	60	GLN
1	B	67	LYS
1	B	73	LEU
1	B	75	GLN
1	B	79	ASP
1	B	80	LEU
1	B	119	GLU
1	B	133	SER
1	B	154	VAL
1	B	155	LYS
1	B	159	ARG

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Mol	Chain	Res	Type
1	B	161	LEU
1	B	166	GLU
1	B	168	LEU
1	B	172	VAL
1	B	197	ASP
1	B	205	VAL
1	B	207	LYS
1	B	211	ASN
1	C	35	LEU
1	C	42	VAL
1	C	44	LYS
1	C	46	VAL
1	C	61	THR
1	C	67	LYS
1	C	114	ASN
1	C	119	GLU
1	C	155	LYS
1	C	159	ARG
1	C	161	LEU
1	C	165	GLU
1	C	166	GLU
1	C	168	LEU
1	C	169	THR
1	C	172	VAL
1	C	187	ILE
1	C	192	ASN
1	C	195	ASN
1	C	200	GLU
1	C	205	VAL
1	D	46	VAL
1	D	86	GLU
1	D	112	VAL
1	D	119	GLU
1	D	157	VAL
1	D	166	GLU
1	D	173	SER
1	D	187	ILE
1	E	35	LEU
1	E	38	ARG
1	E	42	VAL
1	E	67	LYS
1	E	69	PHE

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Mol	Chain	Res	Type
1	E	82	SER
1	E	87	THR
1	E	119	GLU
1	E	145	ARG
1	E	161	LEU
1	E	168	LEU
1	E	169	THR
1	E	172	VAL
1	E	186	SER
1	E	205	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	164	GLN
1	B	75	GLN
1	B	130	ASN
1	B	164	GLN
1	B	198	GLN
1	C	75	GLN
1	C	130	ASN
1	C	195	ASN
1	C	211	ASN
1	D	130	ASN
1	D	156	HIS
1	D	192	ASN
1	E	130	ASN
1	E	151	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 [i](#)

There are no oligosaccharides 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	161/202 (79%)	1.06	21 (13%) 7 4	40, 66, 82, 85	2 (1%)
1	B	172/202 (85%)	0.98	28 (16%) 4 2	33, 65, 85, 96	1 (0%)
1	C	177/202 (87%)	0.65	9 (5%) 33 18	52, 66, 83, 85	0
1	D	177/202 (87%)	0.83	21 (11%) 9 5	53, 68, 84, 106	0
1	E	169/202 (83%)	0.63	10 (5%) 28 15	42, 64, 79, 84	0
All	All	856/1010 (84%)	0.82	89 (10%) 11 6	33, 66, 83, 106	3 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	PRO	13.1
1	B	189	SER	9.7
1	A	77	ASP	8.5
1	D	190	SER	5.7
1	D	191	TYR	4.5
1	D	35	LEU	3.8
1	E	172	VAL	3.7
1	B	131	ILE	3.5
1	D	189	SER	3.5
1	D	39	PRO	3.4
1	D	198	GLN	3.1
1	B	99	PHE	3.1
1	D	149	THR	3.0
1	A	152	VAL	3.0
1	B	78	PRO	3.0
1	D	193	TYR	3.0
1	B	199	ALA	3.0
1	A	104	ASN	3.0
1	B	127	GLU	3.0
1	D	150	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	199	ALA	3.0
1	D	34	ALA	2.9
1	B	210	HIS	2.9
1	B	96	PRO	2.9
1	A	90	TYR	2.8
1	E	177	ASP	2.8
1	B	211	ASN	2.8
1	B	129	TYR	2.8
1	E	33	SER	2.8
1	D	134	LEU	2.8
1	B	106	LEU	2.7
1	E	34	ALA	2.7
1	A	101	PRO	2.7
1	B	128	PHE	2.7
1	A	96	PRO	2.7
1	B	153	PRO	2.6
1	A	177	ASP	2.6
1	D	195	ASN	2.6
1	E	170	GLN	2.6
1	B	132	THR	2.6
1	E	152	VAL	2.6
1	A	129	TYR	2.6
1	C	190	SER	2.6
1	A	99	PHE	2.6
1	B	80	LEU	2.6
1	C	35	LEU	2.6
1	B	154	VAL	2.6
1	D	192	ASN	2.5
1	A	34	ALA	2.5
1	E	199	ALA	2.5
1	B	109	GLY	2.5
1	B	126	ALA	2.5
1	D	36	ALA	2.5
1	A	97	THR	2.5
1	A	103	LEU	2.5
1	C	211	ASN	2.4
1	B	198	GLN	2.4
1	D	42	VAL	2.4
1	B	108	HIS	2.4
1	A	208	GLU	2.4
1	D	196	GLU	2.4
1	A	150	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	96	PRO	2.3
1	E	175	MET	2.3
1	B	105	TYR	2.3
1	A	111	LEU	2.3
1	D	43	SER	2.3
1	A	156	HIS	2.3
1	B	135	ILE	2.2
1	A	108	HIS	2.2
1	D	40	GLY	2.2
1	A	102	VAL	2.2
1	E	107	ARG	2.2
1	B	149	THR	2.2
1	A	153	PRO	2.2
1	A	128	PHE	2.2
1	C	144	GLU	2.1
1	D	146	ASP	2.1
1	B	123	LEU	2.1
1	D	194	GLY	2.1
1	C	150	SER	2.1
1	B	122	VAL	2.1
1	C	99	PHE	2.1
1	B	134	LEU	2.0
1	C	152	VAL	2.0
1	B	130	ASN	2.0
1	C	76	ALA	2.0
1	E	90	TYR	2.0
1	B	103	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.