Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:37 pm BST

PDB ID	:	3DRX
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 following versions of software and data (see references ①) were used in the production of this report:

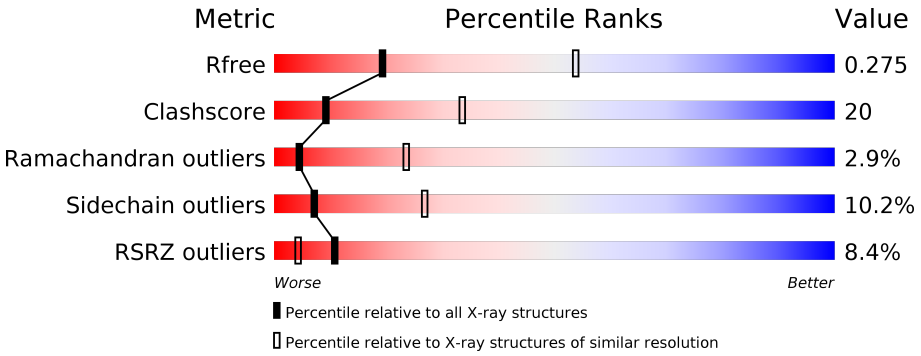
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (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 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 <=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	4% 47% 26% 7% 20%
1	B	202	5% 54% 25% 6% 15%
1	C	202	8% 52% 26% 8% 12%
1	D	202	13% 62% 22% • 12%
1	E	202	5% 53% 24% 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:

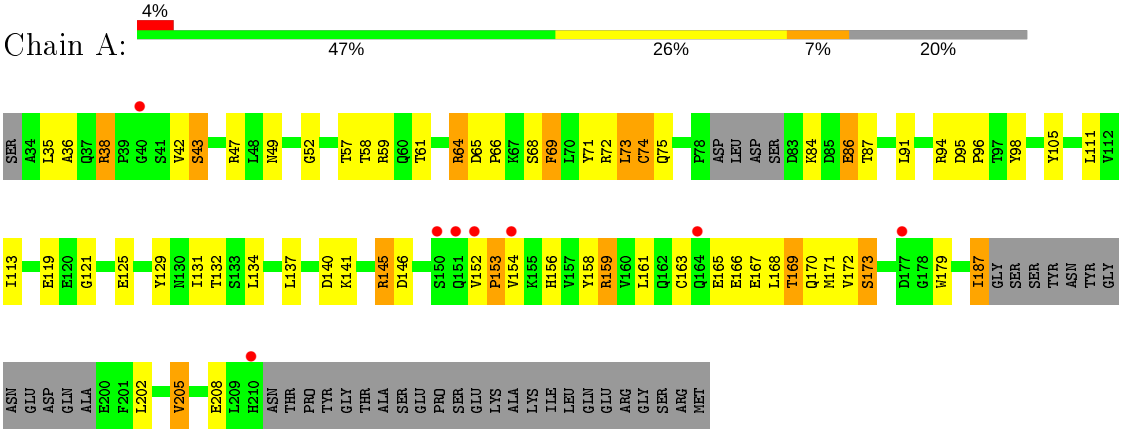
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	SER	-	EXPRESSION TAG	UNP Q9NXV2
B	33	SER	-	EXPRESSION TAG	UNP Q9NXV2
C	33	SER	-	EXPRESSION TAG	UNP Q9NXV2
D	33	SER	-	EXPRESSION TAG	UNP Q9NXV2
E	33	SER	-	EXPRESSION TAG	UNP Q9NXV2

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

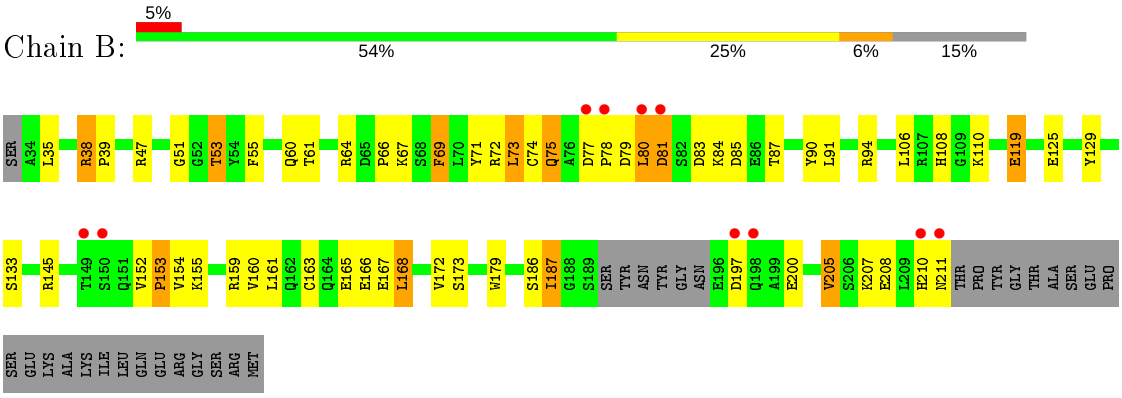
• Molecule 1: BTB/POZ domain-containing protein KCTD5

Chain A:



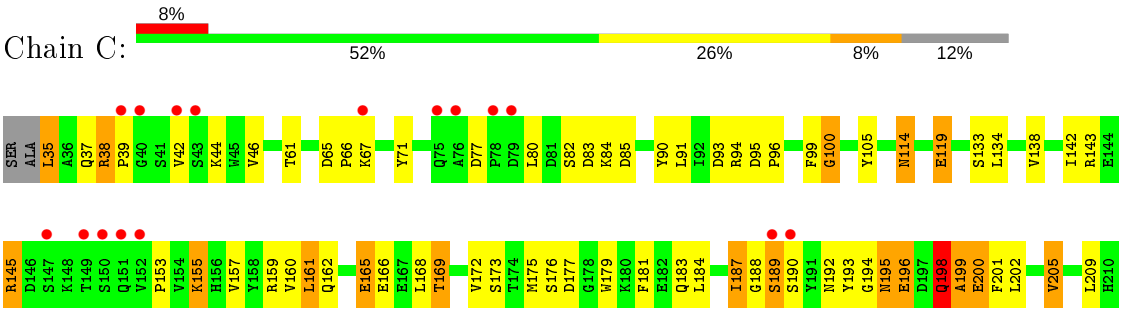
• Molecule 1: BTB/POZ domain-containing protein KCTD5

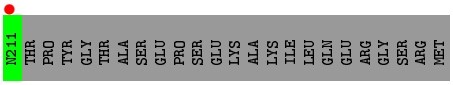
Chain B:



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

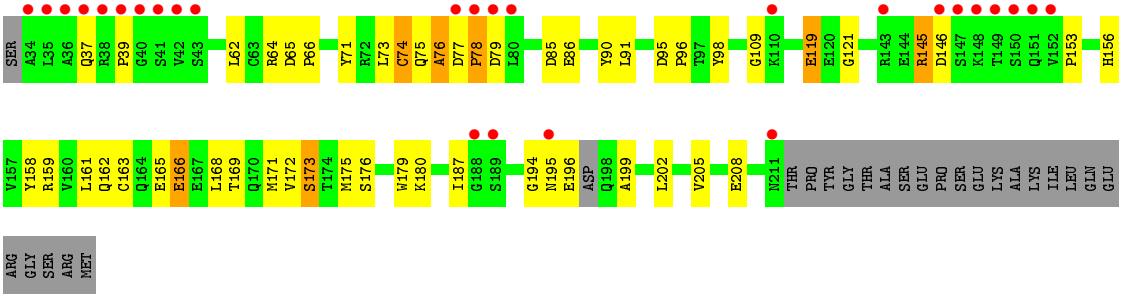
Chain C:





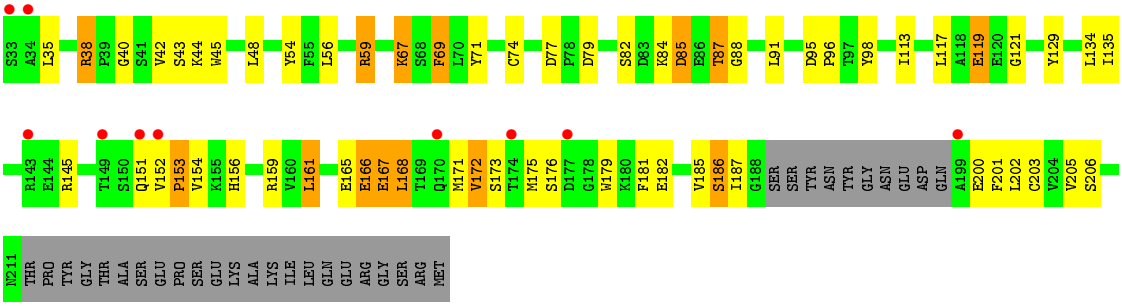
• Molecule 1: BTB/POZ domain-containing protein KCTD5

Chain D:



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

Chain E:



4 Data and refinement statistics (i)

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 19.94 – 3.11	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.11) 99.0 (19.94-3.11)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.227 , 0.275 0.225 , 0.275	Depositor DCC
R_{free} test set	1321 reflections (5.08%)	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 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[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	0.39	0/1329	0.52	0/1793
1	B	0.44	0/1409	0.53	0/1903
1	C	0.45	0/1457	0.61	1/1970 (0.1%)
1	D	0.42	0/1453	0.53	0/1963
1	E	0.43	0/1383	0.56	0/1868
All	All	0.42	0/7031	0.55	1/9497 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	143	ARG	NE-CZ-NH2	5.36	122.98	120.30

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	1306	0	1309	62	0
1	B	1385	0	1371	46	0
1	C	1430	0	1405	67	0
1	D	1427	0	1405	46	0
1	E	1359	0	1353	65	0
All	All	6907	0	6843	274	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 20.

All (274) 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:HH11	1:A:38:ARG:H	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:152:VAL:HG13	1:E:153:PRO:HD2	1.59	0.84
1:E:38:ARG:NH1	1:E:38:ARG:HG2	1.85	0.84
1:C:38:ARG:HD3	1:C:38:ARG:N	1.93	0.84
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
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: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:A:71:TYR:O	1:A:74:CYS:HB3	1.90	0.71
1:E:186:SER:C	1:E:187:ILE:HG13	2.12	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:172:VAL:HA	1:D:175:MET:HE2	1.73	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:E:85:ASP:OD2	1:E:85:ASP:C	2.32	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: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:172:VAL:HA	1:C:175:MET:HE2	1.77	0.65
1:C:85:ASP:HB3	1:C:91:LEU:HD21	1.79	0.65
1:A:152:VAL:O	1:A:153:PRO:O	2.15	0.64
1:C:38:ARG:HD3	1:C:38:ARG:H	1.58	0.63
1:E:166:GLU:C	1:E:168:LEU:H	2.02	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:CD	1:C:38:ARG:H	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
1:A:42:VAL:O	1:A:43:SER:HB2	2.01	0.61
1:C:187:ILE:HD12	1:C:202:LEU:HG	1.83	0.61
1:C:38:ARG:CD	1:C:38:ARG:N	2.64	0.61
1:C:192:ASN:HB3	1:C:198:GLN:CD	2.20	0.60
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:77:ASP:OD1	1:E:77:ASP:C	2.40	0.60
1:E:165:GLU:CG	1:E:166:GLU:N	2.64	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:HD22	1:C:168:LEU:O	2.02	0.58
1:C:196:GLU:C	1:C:198:GLN:H	2.05	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:165:GLU:HG3	1:C:193:TYR:CE2	2.40	0.56
1:A:91:LEU:HD22	1:E:56:LEU:HD21	1.87	0.56
1:B:173:SER:HB3	1:C:159:ARG:NH2	2.20	0.56
1:C:176:SER:OG	1:C:177:ASP:N	2.39	0.56
1:A:47:ARG:NH2	1:A:87:THR:HB	2.21	0.55
1:E:154:VAL:O	1:E:154:VAL:CG2	2.43	0.55
1:A:172:VAL:HG21	1:B:160:VAL:CG2	2.37	0.55
1:A:95:ASP:OD1	1:A:96:PRO:HD2	2.07	0.55
1:B:152:VAL:HG12	1:B:153:PRO:HD2	1.88	0.55
1:D:194:GLY:C	1:D:196:GLU:H	2.08	0.55
1:E:187:ILE:HD11	1:E:202:LEU:HG	1.90	0.54
1:C:165:GLU:OE2	1:C:194:GLY:HA2	2.07	0.54
1:C:93:ASP:O	1:C:94:ARG:HD2	2.07	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: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
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:165:GLU:HG3	1:D:166:GLU:N	2.23	0.53
1:D:66:PRO:HA	1:D:71:TYR:CD1	2.44	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:E:119:GLU:N	1:E:119:GLU:OE1	2.41	0.53
1:E:171:MET:HE1	1:E:203:CYS:SG	2.48	0.53
1:A:49:ASN:HB3	1:A:91:LEU:HD23	1.90	0.53
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:B:165:GLU:H	1:B:200:GLU:HG3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:165:GLU:H	1:E:200:GLU:HG3	1.74	0.52
1:E:85:ASP:HB3	1:E:91:LEU:HD21	1.92	0.52
1:A:94:ARG:NH2	1:A:125:GLU:OE2	2.41	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:D:194:GLY:C	1:D:196:GLU:N	2.64	0.51
1:A:66:PRO:HA	1:A:71:TYR:CE1	2.45	0.51
1:E:171:MET:CE	1:E:203:CYS:SG	2.99	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:D:165:GLU:HG3	1:D:166:GLU:HG3	1.93	0.50
1:B:186:SER:C	1:B:187:ILE:HD13	2.32	0.50
1:B:85:ASP:OD1	1:B:85:ASP:C	2.50	0.50
1:C:65:ASP:OD1	1:C:67:LYS:HD3	2.12	0.50
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:168:LEU:C	1:A:168:LEU:HD13	2.32	0.49
1:A:47:ARG:NH2	1:A:87:THR:OG1	2.45	0.49
1:B:80:LEU:O	1:B:81:ASP:C	2.50	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:B:173:SER:CB	1:C:159:ARG:HH21	2.26	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: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:B:69:PHE:CD1	1:B:69:PHE:C	2.87	0.48
1:A:47:ARG:HH21	1:A:87:THR:CB	2.27	0.48
1:C:35:LEU:C	1:C:37:GLN:H	2.16	0.48
1:A:172:VAL:HG21	1:B:160:VAL:HG23	1.95	0.48
1:C:114:ASN:N	1:C:114:ASN:OD1	2.46	0.48
1:C:181:PHE:HB3	1:D:158:TYR:CE1	2.48	0.48
1:E:171:MET:HE1	1:E:172:VAL:HG13	1.96	0.48
1:B:119:GLU:H	1:B:119:GLU:CD	2.14	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:165:GLU:HG3	1:C:193:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:LEU:CD1	1:C:161:LEU:N	2.77	0.47
1:C:189:SER:O	1:C:190:SER:C	2.51	0.47
1:D:172:VAL:HG23	1:D:173:SER:N	2.29	0.47
1:D:64:ARG:HH12	1:D:109:GLY:CA	2.24	0.47
1:A:166:GLU:HG2	1:A:167:GLU:N	2.29	0.47
1:A:179:TRP:CE3	1:A:205:VAL:HG13	2.50	0.47
1:C:99:PHE:O	1:C:100:GLY:C	2.52	0.47
1:A:59:ARG:HD3	1:A:74:CYS:O	2.15	0.47
1:D:162:GLN:HB3	1:D:202:LEU:CD2	2.45	0.47
1:D:75:GLN:HG2	1:D:76:ALA:N	2.30	0.47
1:A:57:THR:OG1	1:A:58:THR:N	2.46	0.47
1:B:152:VAL:O	1:B:153:PRO:C	2.52	0.47
1:E:113:ILE:HG23	1:E:117:LEU:HB3	1.97	0.47
1:C:181:PHE:C	1:C:181:PHE:CD2	2.89	0.47
1:E:165:GLU:HG3	1:E:166:GLU:H	1.79	0.47
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:166:GLU:C	1:E:168:LEU:N	2.69	0.46
1:A:172:VAL:HG23	1:A:173:SER:N	2.31	0.46
1:D:187:ILE:HG23	1:D:187:ILE:O	2.16	0.46
1:D:145:ARG:NH1	1:D:146:ASP:OD2	2.49	0.46
1:C:35:LEU:HD12	1:D:90:TYR:HB3	1.97	0.46
1:E:40:GLY:C	1:E:42:VAL:H	2.17	0.46
1:A:73:LEU:HD13	1:A:73:LEU:N	2.31	0.46
1:D:163:CYS:SG	1:D:171:MET:CE	3.04	0.46
1:C:165:GLU:CB	1:C:200:GLU:HG3	2.46	0.46
1:D:161:LEU:N	1:D:161:LEU:CD1	2.80	0.45
1:A:169:THR:O	1:A:173:SER:HB3	2.17	0.45
1:C:35:LEU:C	1:C:37:GLN:N	2.69	0.45
1:D:172:VAL:HA	1:D:175:MET:HE3	1.93	0.45
1:E:48:LEU:O	1:E:54:TYR:HA	2.16	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:A:98:TYR:CE2	1:A:121:GLY:HA3	2.52	0.45
1:A:165:GLU:O	1:A:168:LEU:HB2	2.17	0.44
1:D:180:LYS:HD2	1:E:156:HIS:ND1	2.32	0.44
1:D:79:ASP:OD1	1:D:79:ASP:N	2.44	0.44
1:E:172:VAL:O	1:E:173:SER:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:HA	1:B:168:LEU:HD23	1.71	0.44
1:E:152:VAL:O	1:E:153:PRO:C	2.55	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: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:E:134:LEU:O	1:E:135:ILE:C	2.56	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:C:119:GLU:H	1:C:119:GLU:CD	2.20	0.44
1:E:185:VAL:HG12	1:E:186:SER:N	2.33	0.44
1:D:163:CYS:SG	1:D:171:MET:HE2	2.58	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
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:72:ARG:HG3	1:A:73:LEU:N	2.33	0.43
1:A:68:SER:HA	1:A:129:TYR:O	2.19	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:C:65:ASP:C	1:C:67:LYS:H	2.22	0.43
1:A:156:HIS:HE2	1:A:208:GLU:HG2	1.84	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:67:LYS:HE3	1:E:67:LYS:HB2	1.73	0.42
1:A:49:ASN:C	1:A:49:ASN:OD1	2.57	0.42
1:C:179:TRP:CE3	1:C:205:VAL:HG13	2.54	0.42
1:C:162:GLN:HG3	1:C:162:GLN:O	2.19	0.42
1:C:169:THR:O	1:C:173:SER:HB2	2.19	0.42
1:A:166:GLU:C	1:A:168:LEU:H	2.23	0.42
1:E:176:SER:HB3	1:E:179:TRP:CD1	2.55	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:B:51:GLY:HA3	1:B:94:ARG:O	2.20	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:N	1:B:83:ASP:OD1	2.53	0.41
1:C:95:ASP:OD1	1:C:96:PRO:HD2	2.19	0.41
1:B:186:SER:O	1:B:187:ILE:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ARG:HB3	1:D:205:VAL:HG12	2.02	0.41
1:E:172:VAL:HA	1:E:175:MET:HE2	2.01	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:E:172:VAL:HG23	1:E:173:SER:H	1.85	0.41
1:E:44:LYS:HE2	1:E:45:TRP:NE1	2.35	0.41
1:A:171:MET:HB3	1:A:171:MET:HE2	1.80	0.41
1:A:49:ASN:OD1	1:A:52:GLY:N	2.53	0.41
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:A:69:PHE:C	1:A:69:PHE:CD2	2.94	0.41
1:B:84:LYS:HE2	1:B:90:TYR:CZ	2.56	0.41
1:A:131:ILE:O	1:A:132:THR:C	2.59	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:E:181:PHE:CD2	1:E:181:PHE:C	2.93	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:E:152:VAL:HG12	1:E:153:PRO:CG	2.49	0.41
1:E:71:TYR:O	1:E:74:CYS:HB3	2.20	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:119:GLU:N	1:D:119:GLU:OE1	2.53	0.40
1:B:73:LEU:O	1:B:74:CYS:C	2.59	0.40
1:C:196:GLU:C	1:C:198:GLN:N	2.72	0.40
1:A:111:LEU:HD11	1:A:113:ILE:HD11	2.03	0.40
1:A:169:THR:O	1:A:170:GLN:C	2.60	0.40
1:E:69:PHE:HE2	1:E:129:TYR:CD2	2.39	0.40
1:C:83:ASP:OD1	1:C:83:ASP:N	2.54	0.40
1:E:42:VAL:CG1	1:E:42:VAL:O	2.69	0.40
1:E:85:ASP:OD2	1:E:87:THR:N	2.55	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%)	4	21
1	B	168/202 (83%)	152 (90%)	12 (7%)	4 (2%)	6	26
1	C	175/202 (87%)	146 (83%)	23 (13%)	6 (3%)	3	19
1	D	173/202 (86%)	148 (86%)	20 (12%)	5 (3%)	4	23
1	E	165/202 (82%)	144 (87%)	17 (10%)	4 (2%)	6	26
All	All	836/1010 (83%)	718 (86%)	94 (11%)	24 (3%)	4	23

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 (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	147/181 (81%)	129 (88%)	18 (12%)	5 20
1	B	156/181 (86%)	134 (86%)	22 (14%)	3 15
1	C	161/181 (89%)	141 (88%)	20 (12%)	4 19
1	D	160/181 (88%)	154 (96%)	6 (4%)	33 65
1	E	153/181 (84%)	140 (92%)	13 (8%)	10 36
All	All	777/905 (86%)	698 (90%)	79 (10%)	7 27

All (79) 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	145	ARG
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

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Mol	Chain	Res	Type
1	B	69	PHE
1	B	73	LEU
1	B	75	GLN
1	B	77	ASP
1	B	79	ASP
1	B	80	LEU
1	B	119	GLU
1	B	133	SER
1	B	145	ARG
1	B	154	VAL
1	B	155	LYS
1	B	161	LEU
1	B	166	GLU
1	B	168	LEU
1	B	197	ASP
1	B	205	VAL
1	B	211	ASN
1	C	35	LEU
1	C	38	ARG
1	C	42	VAL
1	C	44	LYS
1	C	46	VAL
1	C	61	THR
1	C	114	ASN
1	C	119	GLU
1	C	145	ARG
1	C	155	LYS
1	C	161	LEU
1	C	165	GLU
1	C	166	GLU
1	C	169	THR
1	C	187	ILE
1	C	195	ASN
1	C	196	GLU
1	C	198	GLN
1	C	200	GLU
1	C	205	VAL
1	D	74	CYS
1	D	86	GLU
1	D	119	GLU
1	D	145	ARG
1	D	166	GLU

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Mol	Chain	Res	Type
1	D	173	SER
1	E	35	LEU
1	E	38	ARG
1	E	59	ARG
1	E	67	LYS
1	E	69	PHE
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	172	VAL
1	E	186	SER

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	164	GLN
1	B	75	GLN
1	C	75	GLN
1	C	164	GLN
1	C	195	ASN
1	D	156	HIS
1	D	192	ASN
1	E	151	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 carbohydrates 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, 95^{th} 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%)	0.12	8 (4%) 28 13	53, 66, 82, 85	2 (1%)
1	B	172/202 (85%)	0.14	10 (5%) 23 10	52, 65, 85, 96	1 (0%)
1	C	177/202 (87%)	0.23	17 (9%) 8 3	52, 66, 83, 85	0
1	D	177/202 (87%)	0.58	27 (15%) 2 1	53, 68, 84, 106	0
1	E	169/202 (83%)	0.09	10 (5%) 22 10	42, 64, 79, 84	0
All	All	856/1010 (84%)	0.24	72 (8%) 11 4	42, 66, 83, 106	3 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	36	ALA	8.8
1	D	78	PRO	5.8
1	D	35	LEU	5.8
1	D	41	SER	4.9
1	D	79	ASP	4.8
1	D	39	PRO	4.7
1	D	37	GLN	4.7
1	A	177	ASP	4.6
1	D	40	GLY	4.5
1	D	43	SER	4.2
1	B	78	PRO	3.9
1	D	146	ASP	3.9
1	D	77	ASP	3.9
1	D	152	VAL	3.8
1	E	177	ASP	3.8
1	E	33	SER	3.6
1	E	170	GLN	3.5
1	D	34	ALA	3.5
1	C	211	ASN	3.5
1	C	42	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	197	ASP	3.5
1	B	211	ASN	3.4
1	B	210	HIS	3.4
1	C	79	ASP	3.4
1	D	189	SER	3.3
1	B	198	GLN	3.3
1	D	38	ARG	3.2
1	D	151	GLN	3.2
1	C	67	LYS	3.1
1	D	149	THR	3.1
1	C	151	GLN	3.1
1	A	210	HIS	3.1
1	D	147	SER	3.0
1	D	211	ASN	3.0
1	A	151	GLN	2.9
1	E	151	GLN	2.9
1	C	147	SER	2.8
1	B	149	THR	2.8
1	C	39	PRO	2.8
1	C	78	PRO	2.6
1	C	43	SER	2.6
1	D	42	VAL	2.6
1	D	195	ASN	2.6
1	A	150	SER	2.5
1	D	143	ARG	2.5
1	E	174	THR	2.5
1	B	150	SER	2.5
1	C	152	VAL	2.4
1	D	188	GLY	2.4
1	E	143	ARG	2.4
1	E	199	ALA	2.4
1	C	75	GLN	2.4
1	E	34	ALA	2.4
1	D	110	LYS	2.4
1	B	80	LEU	2.3
1	E	149	THR	2.3
1	A	154	VAL	2.3
1	C	149	THR	2.3
1	E	152	VAL	2.3
1	A	152	VAL	2.2
1	D	150	SER	2.2
1	A	164	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	150	SER	2.2
1	B	81	ASP	2.2
1	C	40	GLY	2.2
1	D	148	LYS	2.2
1	D	80	LEU	2.1
1	B	77	ASP	2.1
1	C	189	SER	2.1
1	C	76	ALA	2.1
1	C	190	SER	2.0
1	A	40	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 carbohydrates 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.