Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 08:47 PM EST

PDB ID	:	2OCY
Title	:	Complex of the guanine exchange factor Sec2p and the Rab GTPase Sec4p
Authors	:	Reinisch, K.M.; Dong, G.
Deposited on	:	2006-12-21
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

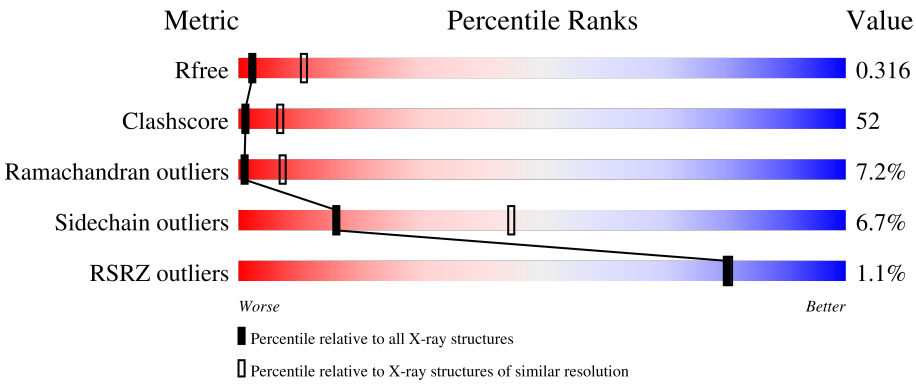
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	154	23% 61% 12% •
1	B	154	43% 45% 9% •
2	C	170	3% 33% 46% 7% • 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3592 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 Rab guanine nucleotide exchange factor SEC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	149	1212	744	212	253	3	27	0	0
1	B	149	1212	744	212	253	3	9	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SER	-	cloning artifact	UNP P17065
A	15	MSE	-	cloning artifact	UNP P17065
A	16	ALA	-	cloning artifact	UNP P17065
A	115	MSE	MET	modified residue	UNP P17065
A	158	MSE	MET	modified residue	UNP P17065
B	14	SER	-	cloning artifact	UNP P17065
B	15	MSE	-	cloning artifact	UNP P17065
B	16	ALA	-	cloning artifact	UNP P17065
B	115	MSE	MET	modified residue	UNP P17065
B	158	MSE	MET	modified residue	UNP P17065

- Molecule 2 is a protein called Ras-related protein SEC4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	C	147	1168	753	189	223	1	2	79	0	0

There are 3 discrepancies between the modelled and reference sequences:

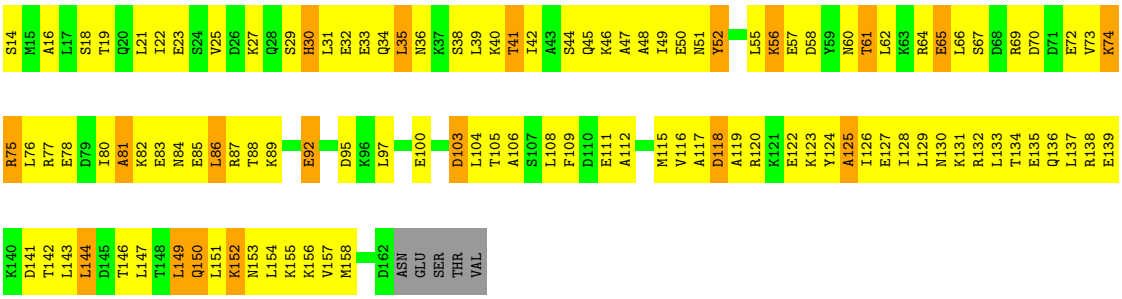
Chain	Residue	Modelled	Actual	Comment	Reference
C	21	MSE	MET	modified residue	UNP P07560
C	94	MSE	MET	modified residue	UNP P07560
C	137	MSE	MET	modified residue	UNP P07560

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.

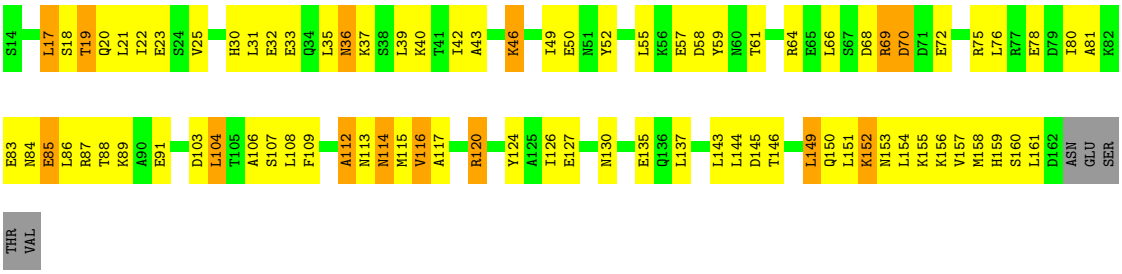
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain A: 23% 61% 12%



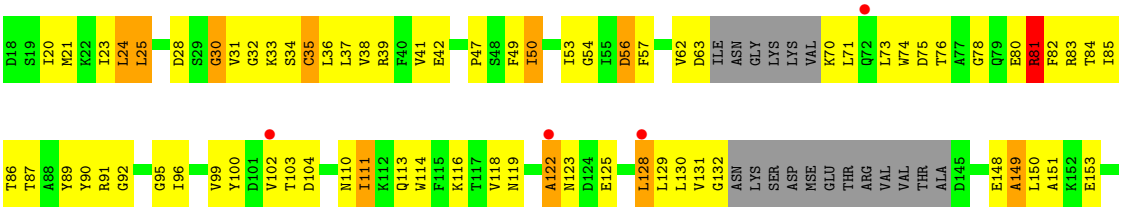
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

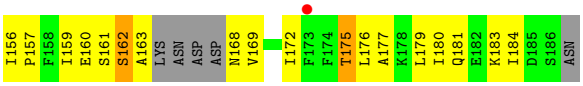
Chain B: 43% 45% 9%



• Molecule 2: Ras-related protein SEC4

Chain C: 3% 33% 46% 7% 14%




I156
P157
F158
I159
E160
S161
S162
A163
LYS
ASN
ASP
ASP
N168
V169
I172
F173
F174
T175
L176
A177
K178
L179
I180
Q181
E182
K183
I184
D185
S186
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.00Å 93.00Å 295.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30 46.50 – 3.31	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-3.30) 98.3 (46.50-3.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 3.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.325 0.246 , 0.316	Depositor DCC
R_{free} test set	1124 reflections (9.46%)	wwPDB-VP
Wilson B-factor (Å^2)	101.8	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 141.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3592	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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 (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	0.38	0/1214	0.62	0/1620
1	B	0.39	0/1214	0.61	0/1620
2	C	0.37	0/1182	0.61	0/1588
All	All	0.38	0/3610	0.62	0/4828

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	1212	0	1234	166	0
1	B	1212	0	1234	114	0
2	C	1168	0	1178	138	0
All	All	3592	0	3646	363	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 52.

All (363) 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:A:55:LEU:HD23	1:B:55:LEU:HD23	1.25	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:TYR:HB3	2:C:111:ILE:HD11	1.33	1.08
2:C:76:THR:HG22	2:C:78:GLY:H	1.25	0.99
1:A:149:LEU:HD23	1:A:150:GLN:N	1.87	0.89
2:C:159:ILE:HG22	2:C:160:GLU:H	1.35	0.89
2:C:23:ILE:HB	2:C:73:LEU:CD2	2.04	0.88
1:A:92:GLU:O	1:A:92:GLU:HG2	1.73	0.87
2:C:25:LEU:HD12	2:C:25:LEU:H	1.43	0.84
2:C:37:LEU:HD22	2:C:37:LEU:N	1.91	0.83
1:B:146:THR:HG22	1:B:150:GLN:HE21	1.45	0.79
1:A:100:GLU:OE1	2:C:85:ILE:HG13	1.82	0.79
1:A:143:LEU:HD23	1:A:143:LEU:O	1.83	0.79
1:A:108:LEU:CD2	1:B:108:LEU:HG	2.13	0.78
2:C:129:LEU:HD23	2:C:130:LEU:N	1.99	0.78
1:A:131:LYS:HA	1:A:134:THR:HG22	1.67	0.77
2:C:34:SER:C	2:C:36:LEU:H	1.89	0.77
2:C:162:SER:HB3	2:C:168:ASN:HD21	1.49	0.76
1:A:108:LEU:HD22	1:B:108:LEU:HG	1.67	0.76
2:C:80:GLU:OE2	2:C:81:ARG:HG2	1.85	0.75
2:C:23:ILE:HG22	2:C:24:LEU:N	2.02	0.75
2:C:57:PHE:HB2	2:C:74:TRP:CZ3	2.22	0.75
2:C:177:ALA:HA	2:C:180:ILE:HD12	1.69	0.75
2:C:176:LEU:O	2:C:180:ILE:HG13	1.88	0.74
1:B:17:LEU:HD23	1:B:17:LEU:H	1.52	0.73
1:A:100:GLU:CD	2:C:82:PHE:HA	2.09	0.72
2:C:23:ILE:HG22	2:C:24:LEU:H	1.55	0.71
1:B:46:LYS:O	1:B:49:ILE:HG22	1.91	0.71
1:A:126:ILE:HD13	1:B:126:ILE:HG22	1.72	0.71
1:B:112:ALA:O	1:B:115:MSE:HB3	1.91	0.70
1:A:35:LEU:HB2	1:B:35:LEU:HD12	1.74	0.69
2:C:70:LYS:C	2:C:71:LEU:HD12	2.13	0.69
1:A:123:LYS:CG	1:B:126:ILE:HD12	2.23	0.69
1:A:111:GLU:O	1:A:115:MSE:HG3	1.92	0.69
2:C:20:ILE:HG12	2:C:70:LYS:HB3	1.75	0.68
1:A:76:LEU:HD23	1:B:76:LEU:CB	2.23	0.68
1:A:78:GLU:O	1:A:82:LYS:HG2	1.94	0.68
2:C:100:TYR:HB3	2:C:111:ILE:CD1	2.16	0.68
2:C:21:MSE:HE1	2:C:177:ALA:HB1	1.76	0.67
1:A:39:LEU:O	1:A:42:ILE:HG13	1.93	0.67
1:A:87:ARG:HG3	1:B:87:ARG:HA	1.75	0.67
1:A:130:ASN:HD21	1:B:130:ASN:N	1.92	0.67
2:C:129:LEU:HA	2:C:156:ILE:CG2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:ILE:HB	2:C:73:LEU:HD23	1.77	0.67
2:C:128:LEU:CD2	2:C:129:LEU:H	2.07	0.67
1:A:67:SER:HA	1:A:70:ASP:OD2	1.95	0.66
2:C:33:LYS:NZ	2:C:161:SER:HB3	2.10	0.66
1:A:55:LEU:CD2	1:B:55:LEU:HD23	2.17	0.66
2:C:49:PHE:HB3	2:C:53:ILE:HD12	1.78	0.66
1:A:84:ASN:HA	1:B:83:GLU:OE2	1.96	0.66
1:A:38:SER:O	1:A:42:ILE:HG23	1.96	0.65
2:C:179:LEU:O	2:C:183:LYS:HG2	1.97	0.65
1:A:35:LEU:HD12	1:B:35:LEU:CA	2.27	0.64
1:A:133:LEU:C	1:A:135:GLU:H	2.01	0.64
2:C:37:LEU:N	2:C:37:LEU:CD2	2.59	0.64
1:A:158:MSE:SE	1:B:158:MSE:HE1	2.47	0.64
2:C:148:GLU:O	2:C:151:ALA:HB3	1.96	0.64
2:C:156:ILE:HG23	2:C:157:PRO:HD2	1.79	0.64
1:B:158:MSE:HE2	1:B:158:MSE:HA	1.80	0.64
1:A:51:ASN:O	1:A:55:LEU:HB2	1.98	0.64
1:A:123:LYS:HG3	1:B:126:ILE:HD12	1.79	0.64
2:C:130:LEU:HD23	2:C:131:VAL:N	2.13	0.64
1:A:75:ARG:HH11	1:A:75:ARG:CB	2.10	0.63
1:B:154:LEU:C	1:B:156:LYS:H	2.02	0.63
2:C:176:LEU:HG	2:C:180:ILE:HD11	1.81	0.62
2:C:129:LEU:HG	2:C:157:PRO:HG2	1.81	0.62
2:C:81:ARG:HH11	2:C:82:PHE:HZ	1.46	0.62
2:C:37:LEU:O	2:C:41:VAL:HG23	1.99	0.62
1:A:47:ALA:O	1:A:50:GLU:HB2	2.00	0.61
1:A:58:ASP:HA	1:A:61:THR:HG22	1.82	0.61
1:A:157:VAL:HG12	1:A:157:VAL:O	1.99	0.61
1:A:76:LEU:HD23	1:B:76:LEU:HB2	1.82	0.61
1:A:35:LEU:HD12	1:B:35:LEU:HA	1.83	0.60
1:A:151:LEU:HD23	1:B:151:LEU:CD2	2.31	0.60
2:C:181:GLN:C	2:C:183:LYS:H	2.04	0.60
1:A:58:ASP:HA	1:A:61:THR:CG2	2.31	0.60
1:A:133:LEU:C	1:A:135:GLU:N	2.51	0.60
1:A:141:ASP:O	1:A:144:LEU:HB2	2.02	0.60
1:A:69:ARG:O	1:A:73:VAL:HG23	2.02	0.60
1:A:32:GLU:O	1:A:36:ASN:HB2	2.01	0.60
2:C:34:SER:C	2:C:36:LEU:N	2.54	0.60
1:A:76:LEU:HD23	1:B:76:LEU:HB3	1.85	0.59
1:A:126:ILE:HG23	1:B:126:ILE:HG21	1.83	0.59
1:A:19:THR:O	1:A:23:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:HG3	1:A:77:ARG:HH21	1.68	0.58
2:C:24:LEU:C	2:C:24:LEU:HD12	2.24	0.58
2:C:23:ILE:CG2	2:C:24:LEU:H	2.15	0.58
2:C:159:ILE:HG22	2:C:160:GLU:N	2.13	0.58
1:A:156:LYS:C	1:A:158:MSE:H	2.05	0.58
2:C:34:SER:HB2	2:C:50:ILE:HD12	1.85	0.58
1:B:151:LEU:O	1:B:153:ASN:N	2.37	0.58
2:C:23:ILE:HB	2:C:73:LEU:HD22	1.84	0.58
2:C:129:LEU:HD23	2:C:130:LEU:H	1.69	0.58
1:B:103:ASP:O	1:B:106:ALA:N	2.36	0.57
1:A:151:LEU:HD23	1:B:151:LEU:HD21	1.85	0.57
1:A:75:ARG:HB3	1:A:75:ARG:NH1	2.20	0.57
2:C:23:ILE:CG2	2:C:24:LEU:N	2.68	0.57
2:C:62:VAL:HG12	2:C:63:ASP:N	2.19	0.57
2:C:128:LEU:HD22	2:C:129:LEU:H	1.68	0.57
1:B:61:THR:HG22	1:B:64:ARG:HH21	1.69	0.57
1:B:80:ILE:HG12	1:B:80:ILE:O	2.04	0.57
1:A:124:TYR:O	1:A:127:GLU:HB3	2.05	0.56
1:A:143:LEU:HD22	1:B:144:LEU:HD11	1.87	0.56
1:A:75:ARG:HH11	1:A:75:ARG:HB2	1.71	0.56
1:A:116:VAL:O	1:A:120:ARG:HG3	2.06	0.56
1:A:158:MSE:HE1	1:B:158:MSE:HE3	1.87	0.56
2:C:35:CYS:HA	2:C:38:VAL:HG23	1.87	0.56
2:C:80:GLU:OE2	2:C:81:ARG:NE	2.39	0.56
1:B:158:MSE:HE2	1:B:158:MSE:CA	2.36	0.56
1:A:100:GLU:OE2	2:C:81:ARG:O	2.23	0.55
1:A:118:ASP:O	1:A:122:GLU:HG3	2.06	0.55
1:A:67:SER:O	1:A:70:ASP:HB2	2.06	0.55
2:C:95:GLY:O	2:C:96:ILE:HG13	2.06	0.55
2:C:20:ILE:HD13	2:C:70:LYS:HD2	1.88	0.55
2:C:35:CYS:O	2:C:39:ARG:N	2.37	0.55
2:C:129:LEU:CD2	2:C:131:VAL:HG23	2.37	0.55
2:C:37:LEU:HD21	2:C:75:ASP:OD2	2.07	0.55
1:A:41:THR:O	1:A:41:THR:HG22	2.06	0.55
1:A:108:LEU:HD23	1:B:108:LEU:HG	1.87	0.55
1:B:17:LEU:HD23	1:B:17:LEU:N	2.21	0.55
1:A:149:LEU:C	1:A:151:LEU:H	2.10	0.55
1:A:88:THR:HG22	1:A:89:LYS:N	2.22	0.55
2:C:150:LEU:HD23	2:C:153:GLU:CD	2.28	0.55
2:C:162:SER:O	2:C:163:ALA:HB3	2.05	0.55
2:C:99:VAL:HG12	2:C:100:TYR:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:CD1	1:B:126:ILE:HG22	2.37	0.54
1:A:40:LYS:O	1:A:42:ILE:N	2.39	0.54
1:A:158:MSE:HE1	1:B:158:MSE:CE	2.37	0.54
1:B:17:LEU:H	1:B:17:LEU:CD2	2.18	0.54
1:A:103:ASP:O	1:A:104:LEU:C	2.46	0.54
2:C:87:THR:HA	2:C:90:TYR:CD2	2.43	0.54
1:A:77:ARG:O	1:A:78:GLU:C	2.45	0.54
2:C:33:LYS:HZ1	2:C:161:SER:HB3	1.72	0.54
2:C:82:PHE:O	2:C:86:THR:HG23	2.07	0.54
1:A:126:ILE:CD1	1:B:127:GLU:HA	2.38	0.53
1:B:103:ASP:O	1:B:104:LEU:C	2.46	0.53
2:C:102:VAL:C	2:C:104:ASP:H	2.12	0.53
1:A:35:LEU:HD23	1:A:36:ASN:N	2.22	0.53
1:B:158:MSE:C	1:B:160:SER:H	2.12	0.53
2:C:114:TRP:O	2:C:118:VAL:HG23	2.08	0.53
2:C:122:ALA:C	2:C:123:ASN:HD22	2.12	0.53
1:A:75:ARG:CB	1:A:75:ARG:NH1	2.72	0.53
2:C:86:THR:O	2:C:89:TYR:HB2	2.09	0.53
1:A:40:LYS:C	1:A:42:ILE:H	2.11	0.53
1:A:131:LYS:HA	1:A:134:THR:CG2	2.39	0.53
2:C:33:LYS:O	2:C:36:LEU:HB2	2.09	0.53
1:A:48:ALA:C	1:A:50:GLU:H	2.13	0.52
1:A:81:ALA:O	1:A:84:ASN:N	2.41	0.52
1:A:97:LEU:C	1:A:97:LEU:HD23	2.30	0.52
1:B:116:VAL:HG11	2:C:47:PRO:HB3	1.90	0.52
2:C:54:GLY:HA3	2:C:80:GLU:HG2	1.92	0.52
2:C:123:ASN:HB3	2:C:125:GLU:CD	2.29	0.52
1:A:116:VAL:HG23	1:B:116:VAL:HA	1.92	0.52
1:A:22:ILE:HG22	1:A:23:GLU:N	2.24	0.52
1:A:80:ILE:HG12	1:B:80:ILE:HB	1.92	0.52
1:A:83:GLU:OE1	1:A:83:GLU:HA	2.10	0.52
1:A:149:LEU:C	1:A:151:LEU:N	2.63	0.52
1:B:114:ASN:O	1:B:115:MSE:C	2.48	0.52
1:B:124:TYR:O	1:B:127:GLU:HB2	2.09	0.52
1:A:105:THR:HA	1:B:108:LEU:HD21	1.92	0.52
1:A:19:THR:HG22	1:A:23:GLU:OE1	2.10	0.51
1:A:48:ALA:O	1:A:50:GLU:N	2.42	0.51
1:A:126:ILE:HD11	1:B:130:ASN:HB2	1.92	0.51
2:C:87:THR:HA	2:C:90:TYR:HD2	1.75	0.51
1:A:149:LEU:O	1:A:151:LEU:N	2.43	0.51
1:A:117:ALA:O	1:A:119:ALA:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:O	1:A:67:SER:N	2.43	0.51
1:A:123:LYS:HG2	1:B:126:ILE:HD12	1.93	0.51
1:B:30:HIS:O	1:B:33:GLU:HB3	2.11	0.51
2:C:99:VAL:HG13	2:C:131:VAL:O	2.11	0.51
2:C:156:ILE:CG2	2:C:157:PRO:HD2	2.40	0.51
1:B:135:GLU:C	1:B:137:LEU:N	2.62	0.51
1:A:100:GLU:CG	2:C:82:PHE:HA	2.41	0.51
2:C:118:VAL:O	2:C:122:ALA:HB3	2.11	0.51
1:A:64:ARG:O	1:A:66:LEU:N	2.43	0.50
2:C:83:ARG:O	2:C:87:THR:HG23	2.11	0.50
2:C:128:LEU:HD23	2:C:129:LEU:H	1.76	0.50
2:C:31:VAL:HG12	2:C:31:VAL:O	2.11	0.50
1:A:151:LEU:O	1:A:154:LEU:N	2.45	0.50
2:C:111:ILE:HD13	2:C:114:TRP:HD1	1.75	0.50
1:B:154:LEU:C	1:B:156:LYS:N	2.64	0.50
2:C:25:LEU:HD12	2:C:25:LEU:N	2.21	0.50
1:B:42:ILE:HG13	1:B:43:ALA:N	2.27	0.50
1:A:139:GLU:O	1:A:142:THR:HG22	2.11	0.50
2:C:100:TYR:CZ	2:C:132:GLY:HA3	2.47	0.50
1:B:109:PHE:O	1:B:113:ASN:ND2	2.45	0.50
1:B:158:MSE:HE2	1:B:158:MSE:N	2.26	0.50
2:C:114:TRP:CE3	2:C:114:TRP:HA	2.47	0.50
1:A:132:ARG:C	1:A:133:LEU:HD12	2.32	0.49
1:A:135:GLU:O	1:A:137:LEU:N	2.45	0.49
1:A:88:THR:O	1:A:89:LYS:C	2.49	0.49
1:B:61:THR:HG22	1:B:64:ARG:NH2	2.27	0.49
1:B:135:GLU:C	1:B:137:LEU:H	2.14	0.49
2:C:111:ILE:HA	2:C:114:TRP:CD1	2.47	0.49
2:C:184:ILE:O	2:C:184:ILE:HG22	2.12	0.49
1:A:60:ASN:C	1:A:62:LEU:H	2.15	0.49
2:C:33:LYS:O	2:C:36:LEU:N	2.46	0.49
2:C:99:VAL:HA	2:C:131:VAL:O	2.12	0.49
2:C:81:ARG:NH1	2:C:82:PHE:HZ	2.10	0.49
2:C:114:TRP:HA	2:C:114:TRP:HE3	1.78	0.49
2:C:33:LYS:HZ2	2:C:161:SER:HB3	1.77	0.49
1:B:157:VAL:C	1:B:158:MSE:HE2	2.33	0.48
2:C:177:ALA:HA	2:C:180:ILE:CD1	2.41	0.48
2:C:150:LEU:HD23	2:C:153:GLU:OE2	2.12	0.48
1:A:30:HIS:O	1:A:34:GLN:HB2	2.13	0.48
1:B:57:GLU:O	1:B:61:THR:HG23	2.13	0.48
2:C:35:CYS:HA	2:C:38:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLU:O	1:A:34:GLN:C	2.52	0.48
2:C:54:GLY:H	2:C:80:GLU:HG2	1.78	0.48
2:C:168:ASN:O	2:C:172:ILE:HG13	2.14	0.48
1:B:17:LEU:O	1:B:18:SER:C	2.51	0.48
2:C:62:VAL:HG12	2:C:63:ASP:H	1.78	0.48
2:C:84:THR:HG22	2:C:84:THR:O	2.13	0.48
2:C:81:ARG:HG3	2:C:82:PHE:CE1	2.47	0.48
1:B:109:PHE:CG	2:C:57:PHE:HB3	2.47	0.48
1:A:103:ASP:HB3	2:C:82:PHE:HE1	1.79	0.48
1:A:81:ALA:O	1:A:82:LYS:C	2.52	0.47
1:A:44:SER:OG	1:A:45:GLN:N	2.47	0.47
1:B:84:ASN:C	1:B:86:LEU:H	2.18	0.47
1:A:64:ARG:O	1:A:65:GLU:C	2.53	0.47
1:A:69:ARG:O	1:A:70:ASP:C	2.53	0.47
1:B:151:LEU:O	1:B:152:LYS:C	2.52	0.47
1:B:154:LEU:O	1:B:156:LYS:N	2.47	0.47
2:C:100:TYR:CD1	2:C:100:TYR:C	2.87	0.47
2:C:110:ASN:O	2:C:113:GLN:N	2.47	0.47
1:B:39:LEU:O	1:B:42:ILE:HG12	2.14	0.47
1:A:66:LEU:HB2	1:B:66:LEU:HD12	1.97	0.47
1:B:69:ARG:HA	1:B:72:GLU:OE1	2.14	0.47
2:C:20:ILE:HG23	2:C:70:LYS:HB3	1.95	0.47
2:C:90:TYR:O	2:C:92:GLY:N	2.41	0.47
2:C:123:ASN:HB3	2:C:125:GLU:OE1	2.15	0.47
2:C:37:LEU:CD2	2:C:75:ASP:OD2	2.63	0.47
1:A:137:LEU:HD12	1:B:137:LEU:HD12	1.96	0.47
1:A:149:LEU:HD23	1:A:149:LEU:C	2.34	0.47
1:A:61:THR:HG23	1:A:61:THR:O	2.14	0.46
1:A:151:LEU:O	1:A:153:ASN:N	2.48	0.46
2:C:37:LEU:CD2	2:C:37:LEU:H	2.28	0.46
1:A:58:ASP:CA	1:A:61:THR:HG22	2.46	0.46
1:A:72:GLU:O	1:A:75:ARG:HG3	2.16	0.46
1:A:80:ILE:CD1	1:B:76:LEU:HD22	2.44	0.46
1:A:128:ILE:HG22	1:A:129:LEU:N	2.29	0.46
1:B:109:PHE:CB	2:C:57:PHE:HB3	2.45	0.46
1:A:129:LEU:C	1:A:131:LYS:H	2.18	0.46
1:B:88:THR:HG23	1:B:89:LYS:N	2.30	0.46
1:B:107:SER:O	1:B:108:LEU:C	2.52	0.46
1:A:74:LYS:O	1:A:77:ARG:N	2.48	0.46
1:A:125:ALA:O	1:A:128:ILE:HB	2.16	0.46
2:C:123:ASN:HD22	2:C:123:ASN:N	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ALA:O	1:A:122:GLU:N	2.49	0.45
1:B:37:LYS:O	1:B:40:LYS:HB3	2.16	0.45
1:B:87:ARG:O	1:B:87:ARG:HG2	2.16	0.45
1:B:87:ARG:O	1:B:91:GLU:HG3	2.16	0.45
1:A:27:LYS:O	1:A:31:LEU:HD13	2.16	0.45
1:A:36:ASN:O	1:A:39:LEU:HB2	2.16	0.45
1:A:48:ALA:C	1:A:50:GLU:N	2.69	0.45
1:A:142:THR:C	1:A:144:LEU:H	2.19	0.45
2:C:179:LEU:N	2:C:179:LEU:HD23	2.31	0.45
2:C:21:MSE:SE	2:C:180:ILE:HB	2.66	0.45
2:C:34:SER:O	2:C:36:LEU:N	2.49	0.45
1:A:86:LEU:HB3	1:B:87:ARG:HD2	1.98	0.45
1:A:156:LYS:C	1:A:158:MSE:N	2.70	0.45
1:A:58:ASP:C	1:A:61:THR:HG22	2.37	0.45
1:A:100:GLU:OE1	2:C:84:THR:HB	2.16	0.45
1:B:23:GLU:C	1:B:25:VAL:H	2.19	0.45
1:B:61:THR:HA	1:B:64:ARG:HH21	1.80	0.45
2:C:102:VAL:O	2:C:104:ASP:N	2.50	0.45
1:B:20:GLN:HA	1:B:20:GLN:OE1	2.18	0.44
2:C:21:MSE:CE	2:C:177:ALA:HB1	2.46	0.44
2:C:169:VAL:HA	2:C:172:ILE:HG13	2.00	0.44
1:A:109:PHE:O	1:A:112:ALA:N	2.51	0.44
1:B:143:LEU:O	1:B:146:THR:HB	2.18	0.44
1:B:25:VAL:O	1:B:25:VAL:HG12	2.17	0.44
1:A:142:THR:C	1:A:144:LEU:N	2.71	0.44
1:A:151:LEU:O	1:A:152:LYS:C	2.56	0.44
1:B:68:ASP:O	1:B:72:GLU:HG3	2.18	0.44
1:A:29:SER:O	1:A:31:LEU:N	2.51	0.44
1:B:52:TYR:CD2	1:B:52:TYR:C	2.91	0.44
1:B:112:ALA:O	1:B:113:ASN:C	2.56	0.44
1:B:144:LEU:C	1:B:144:LEU:HD23	2.38	0.44
2:C:113:GLN:O	2:C:116:LYS:HB2	2.17	0.44
1:B:158:MSE:O	1:B:160:SER:N	2.50	0.44
2:C:53:ILE:HG23	2:C:82:PHE:HE2	1.82	0.44
1:A:55:LEU:O	1:A:58:ASP:N	2.51	0.43
2:C:35:CYS:HB2	2:C:38:VAL:HB	2.00	0.43
1:B:49:ILE:CG2	1:B:50:GLU:N	2.82	0.43
1:B:39:LEU:O	1:B:39:LEU:HD23	2.18	0.43
2:C:175:THR:O	2:C:176:LEU:C	2.56	0.43
1:A:158:MSE:SE	1:B:158:MSE:CE	3.16	0.43
1:A:85:GLU:O	1:A:88:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HD11	1:B:130:ASN:CB	2.48	0.43
1:B:19:THR:O	1:B:22:ILE:HB	2.19	0.43
1:A:27:LYS:HD2	1:A:27:LYS:HA	1.89	0.43
1:A:57:GLU:O	1:A:61:THR:HB	2.18	0.43
1:A:55:LEU:O	1:A:56:LYS:C	2.55	0.43
1:A:29:SER:C	1:A:31:LEU:H	2.21	0.43
1:A:33:GLU:O	1:A:36:ASN:N	2.52	0.43
1:B:109:PHE:HB3	2:C:57:PHE:HB3	2.01	0.43
2:C:20:ILE:HG23	2:C:70:LYS:CG	2.48	0.43
1:A:35:LEU:HB2	1:B:35:LEU:HB2	2.01	0.43
2:C:39:ARG:NH1	2:C:163:ALA:HB2	2.33	0.42
2:C:81:ARG:NH1	2:C:82:PHE:CZ	2.87	0.42
1:A:80:ILE:O	1:A:81:ALA:C	2.57	0.42
1:B:149:LEU:HD22	1:B:153:ASN:ND2	2.33	0.42
1:A:55:LEU:O	1:A:57:GLU:N	2.53	0.42
1:A:155:LYS:O	1:A:158:MSE:HB3	2.20	0.42
1:A:31:LEU:HA	1:A:34:GLN:HB3	2.01	0.42
1:B:17:LEU:O	1:B:20:GLN:N	2.53	0.42
1:B:46:LYS:HD2	1:B:46:LYS:HA	1.81	0.42
2:C:34:SER:CB	2:C:50:ILE:HD12	2.48	0.42
1:B:116:VAL:O	1:B:117:ALA:C	2.58	0.42
2:C:110:ASN:O	2:C:111:ILE:C	2.56	0.42
2:C:130:LEU:HD23	2:C:130:LEU:C	2.39	0.42
1:A:157:VAL:O	1:A:157:VAL:CG1	2.67	0.42
2:C:20:ILE:HG23	2:C:70:LYS:HG2	2.02	0.42
2:C:80:GLU:O	2:C:82:PHE:N	2.52	0.42
1:A:137:LEU:CD1	1:B:137:LEU:HA	2.50	0.42
1:B:31:LEU:O	1:B:32:GLU:C	2.58	0.42
1:B:116:VAL:HG12	1:B:120:ARG:HG3	2.02	0.42
2:C:81:ARG:HG3	2:C:82:PHE:CZ	2.55	0.42
1:A:52:TYR:CD2	1:A:52:TYR:O	2.73	0.42
1:B:58:ASP:O	1:B:59:TYR:C	2.57	0.42
1:A:18:SER:OG	1:A:19:THR:N	2.53	0.41
1:A:137:LEU:HD12	1:B:137:LEU:CD1	2.50	0.41
1:B:157:VAL:HG12	1:B:158:MSE:CE	2.49	0.41
2:C:30:GLY:C	2:C:32:GLY:H	2.23	0.41
2:C:102:VAL:HG23	2:C:161:SER:OG	2.19	0.41
2:C:181:GLN:C	2:C:183:LYS:N	2.71	0.41
1:A:14:SER:C	1:A:16:ALA:H	2.23	0.41
1:A:60:ASN:C	1:A:62:LEU:N	2.74	0.41
2:C:129:LEU:HD21	2:C:131:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:57:PHE:HB2	2:C:74:TRP:HZ3	1.79	0.41
2:C:149:ALA:O	2:C:153:GLU:HG3	2.20	0.41
1:A:18:SER:O	1:A:21:LEU:N	2.54	0.41
1:A:29:SER:C	1:A:31:LEU:N	2.73	0.41
1:A:119:ALA:O	1:A:120:ARG:C	2.59	0.41
1:A:131:LYS:CA	1:A:134:THR:HG22	2.44	0.41
1:A:144:LEU:O	1:A:147:LEU:N	2.53	0.41
1:B:75:ARG:O	1:B:78:GLU:HB3	2.20	0.41
1:B:154:LEU:O	1:B:158:MSE:HG2	2.21	0.41
2:C:37:LEU:HD22	2:C:37:LEU:H	1.78	0.41
1:A:21:LEU:O	1:A:25:VAL:HG23	2.21	0.41
1:A:80:ILE:HG12	1:B:80:ILE:CB	2.50	0.41
2:C:49:PHE:N	2:C:56:ASP:OD1	2.41	0.41
1:A:46:LYS:O	1:A:47:ALA:C	2.59	0.41
1:A:151:LEU:C	1:A:153:ASN:N	2.74	0.41
1:A:74:LYS:O	1:A:75:ARG:C	2.57	0.41
1:A:151:LEU:HD23	1:B:151:LEU:HD23	2.02	0.41
1:A:21:LEU:HA	1:B:21:LEU:HD13	2.03	0.41
1:A:35:LEU:HD23	1:A:35:LEU:C	2.40	0.41
1:A:69:ARG:CZ	1:B:70:ASP:OD1	2.68	0.41
1:A:105:THR:HG22	1:A:106:ALA:N	2.36	0.41
1:B:36:ASN:HD22	1:B:36:ASN:HA	1.59	0.41
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.93	0.41
1:B:154:LEU:O	1:B:157:VAL:N	2.54	0.41
2:C:28:ASP:OD2	2:C:75:ASP:OD2	2.39	0.41
2:C:176:LEU:C	2:C:180:ILE:HG13	2.42	0.41
1:A:130:ASN:HD21	1:B:130:ASN:CA	2.34	0.40
2:C:129:LEU:HA	2:C:156:ILE:HG21	2.02	0.40
1:A:135:GLU:C	1:A:137:LEU:N	2.73	0.40
1:B:32:GLU:O	1:B:36:ASN:HB2	2.21	0.40
1:A:133:LEU:O	1:A:135:GLU:N	2.55	0.40
1:A:138:ARG:O	1:A:141:ASP:HB3	2.20	0.40
1:B:81:ALA:O	1:B:85:GLU:OE1	2.39	0.40
1:A:146:THR:O	1:A:150:GLN:HG3	2.21	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	147/154 (96%)	91 (62%)	44 (30%)	12 (8%)	1 5
1	B	147/154 (96%)	108 (74%)	31 (21%)	8 (5%)	2 12
2	C	139/170 (82%)	103 (74%)	25 (18%)	11 (8%)	1 6
All	All	433/478 (91%)	302 (70%)	100 (23%)	31 (7%)	1 7

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	152	LYS
2	C	81	ARG
2	C	162	SER
1	A	41	THR
1	A	118	ASP
1	A	136	GLN
1	B	46	LYS
1	B	161	LEU
2	C	103	THR
2	C	122	ALA
1	A	30	HIS
1	A	65	GLU
1	A	103	ASP
1	A	150	GLN
1	B	104	LEU
1	B	112	ALA
1	B	155	LYS
1	B	159	HIS
2	C	30	GLY
2	C	175	THR
1	A	49	ILE
1	A	81	ALA
1	A	125	ALA
1	A	152	LYS

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Mol	Chain	Res	Type
2	C	119	ASN
2	C	149	ALA
1	A	56	LYS
2	C	35	CYS
2	C	91	ARG
1	B	116	VAL
2	C	111	ILE

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	137/139 (99%)	127 (93%)	10 (7%)	14	41
1	B	137/139 (99%)	127 (93%)	10 (7%)	14	41
2	C	128/146 (88%)	121 (94%)	7 (6%)	21	52
All	All	402/424 (95%)	375 (93%)	27 (7%)	16	45

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	52	TYR
1	A	61	THR
1	A	74	LYS
1	A	75	ARG
1	A	86	LEU
1	A	92	GLU
1	A	95	ASP
1	A	144	LEU
1	A	149	LEU
1	B	17	LEU
1	B	19	THR
1	B	36	ASN
1	B	69	ARG
1	B	70	ASP

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Mol	Chain	Res	Type
1	B	85	GLU
1	B	114	ASN
1	B	120	ARG
1	B	145	ASP
1	B	149	LEU
2	C	24	LEU
2	C	25	LEU
2	C	42	GLU
2	C	50	ILE
2	C	56	ASP
2	C	81	ARG
2	C	128	LEU

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	45	GLN
1	A	60	ASN
1	B	36	ASN
1	B	113	ASN
1	B	150	GLN
1	B	153	ASN
2	C	119	ASN
2	C	123	ASN
2	C	181	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	146/154 (94%)	-0.28	0	100	100	26, 74, 126, 173	9 (6%)
1	B	146/154 (94%)	-0.32	0	100	100	23, 69, 117, 145	3 (2%)
2	C	145/170 (85%)	0.13	5 (3%)	45	43	46, 123, 171, 181	18 (12%)
All	All	437/478 (91%)	-0.16	5 (1%)	80	81	23, 81, 164, 181	30 (6%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	173	PHE	2.8
2	C	122	ALA	2.2
2	C	128	LEU	2.1
2	C	72	GLN	2.1
2	C	102	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.