Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:45 pm BST

PDB ID	:	3ZGX
Title	:	Crystal structure of the kleisin-N SMC interface in prokaryotic condensin
Authors	:	Burmann, F.; Shin, H.; Basquin, J.; Soh, Y.; Gimenez, V.; Kim, Y.; Oh, B.; Gruber, S.
Deposited on	:	2012-12-19
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

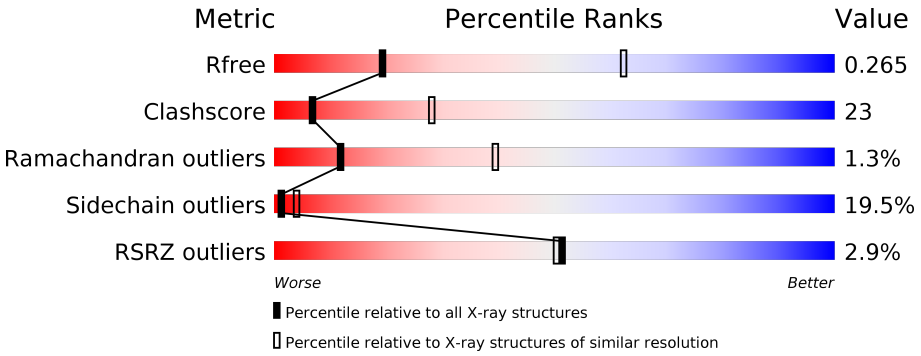
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	426	4% 37% 37% 7% 19%
1	B	426	2% 39% 36% 7% 18%
2	C	94	% 34% 30% • • 29%
2	Z	94	35% 29% 5% • 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6349 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 CHROMOSOME PARTITION PROTEIN SMC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2622	1656	449	509	8			
1	B	351	Total	C	N	O	S	0	0	0
			2655	1676	456	516	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLY	-	linker	UNP P51834
A	221	PRO	-	linker	UNP P51834
A	222	GLY	-	linker	UNP P51834
B	220	GLY	-	linker	UNP P51834
B	221	PRO	-	linker	UNP P51834
B	222	GLY	-	linker	UNP P51834

- Molecule 2 is a protein called SEGREGATION AND CONDENSATION PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	67	Total	C	N	O	S	0	0	0
			534	352	84	95	3			
2	Z	67	Total	C	N	O	S	0	0	0
			538	354	84	97	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	87	THR	-	expression tag	UNP P35154
C	88	SER	-	expression tag	UNP P35154
C	89	HIS	-	expression tag	UNP P35154
C	90	HIS	-	expression tag	UNP P35154
C	91	HIS	-	expression tag	UNP P35154
C	92	HIS	-	expression tag	UNP P35154

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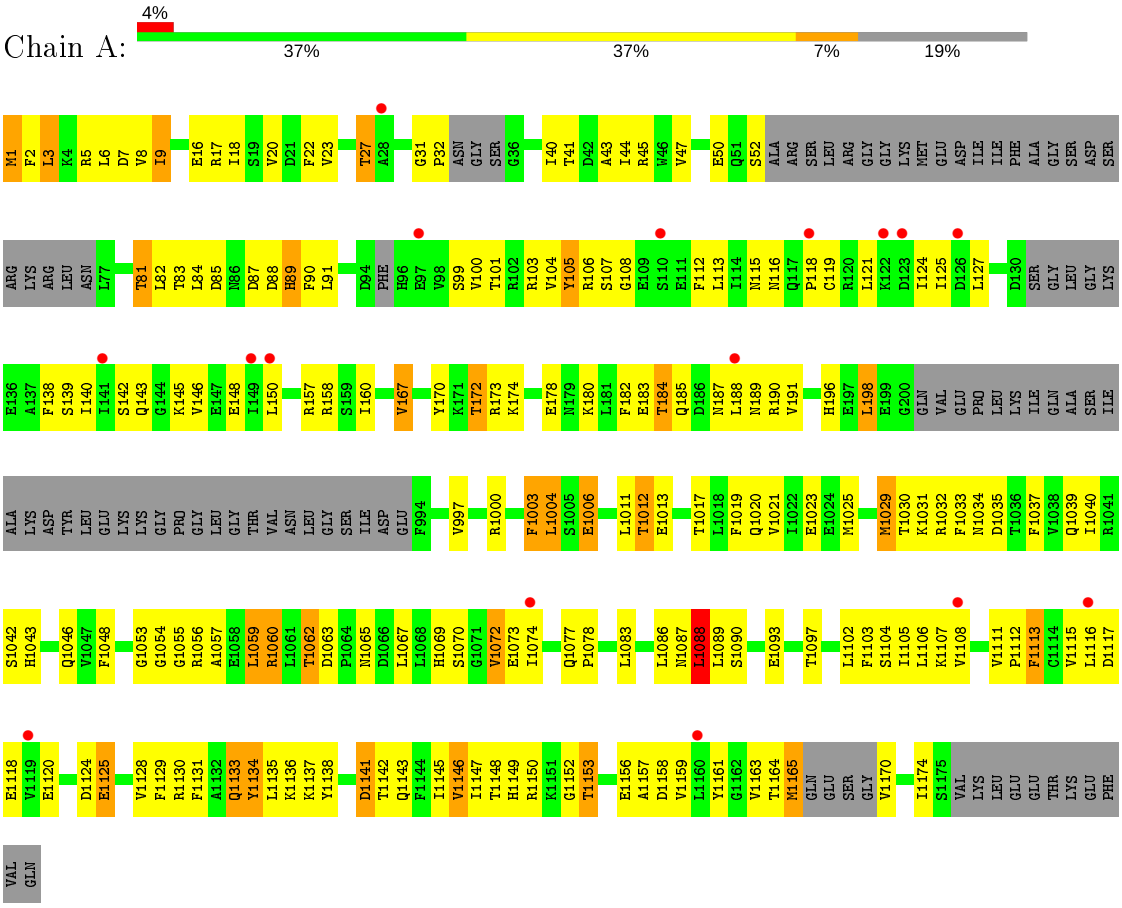
Chain	Residue	Modelled	Actual	Comment	Reference
C	93	HIS	-	expression tag	UNP P35154
C	94	HIS	-	expression tag	UNP P35154
Z	87	THR	-	expression tag	UNP P35154
Z	88	SER	-	expression tag	UNP P35154
Z	89	HIS	-	expression tag	UNP P35154
Z	90	HIS	-	expression tag	UNP P35154
Z	91	HIS	-	expression tag	UNP P35154
Z	92	HIS	-	expression tag	UNP P35154
Z	93	HIS	-	expression tag	UNP P35154
Z	94	HIS	-	expression tag	UNP P35154

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.

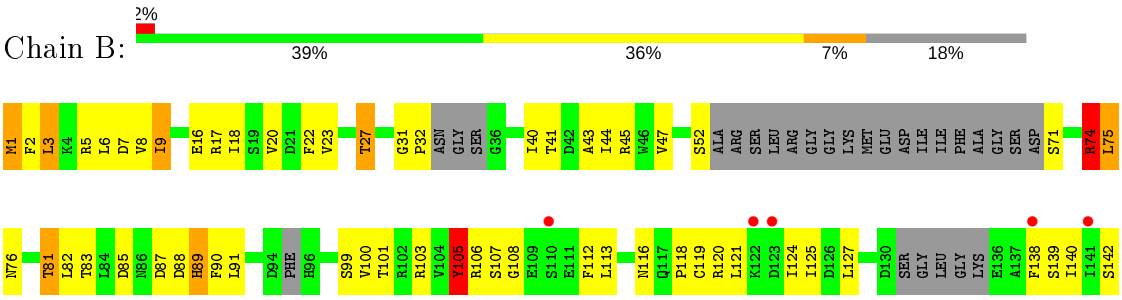
• Molecule 1: CHROMOSOME PARTITION PROTEIN SMC

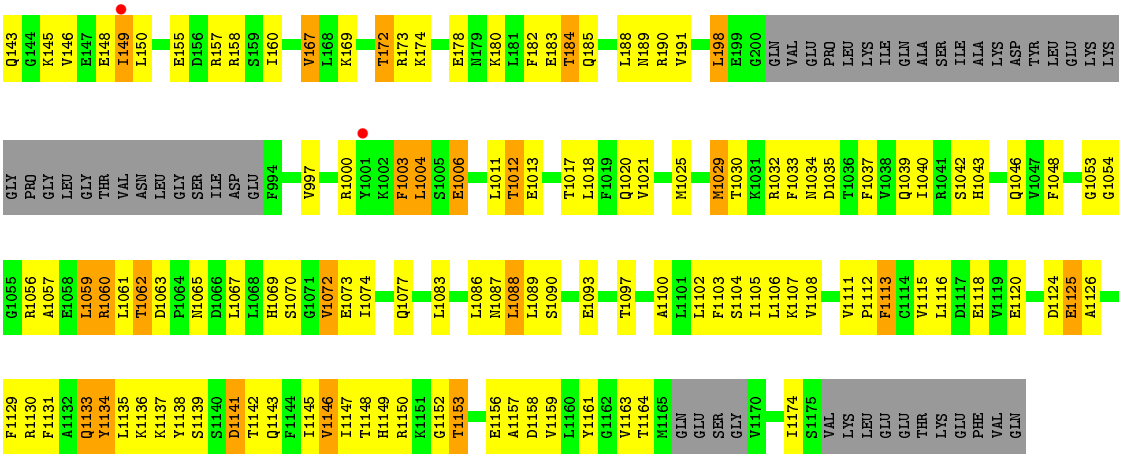
Chain A:



• Molecule 1: CHROMOSOME PARTITION PROTEIN SMC

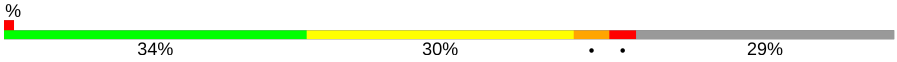
Chain B:

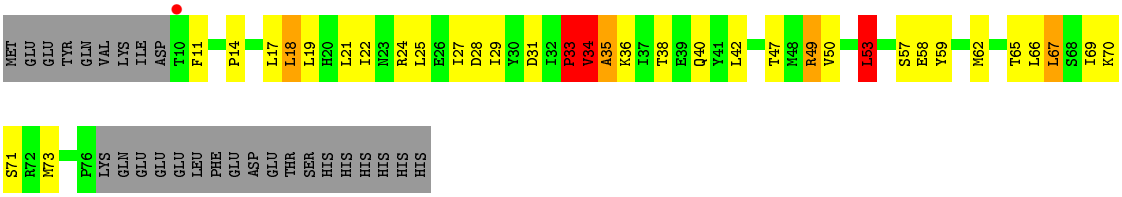




- Molecule 2: SEGREGATION AND CONDENSATION PROTEIN A

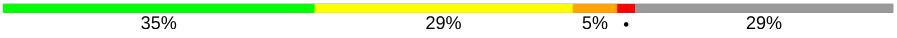
Chain C:

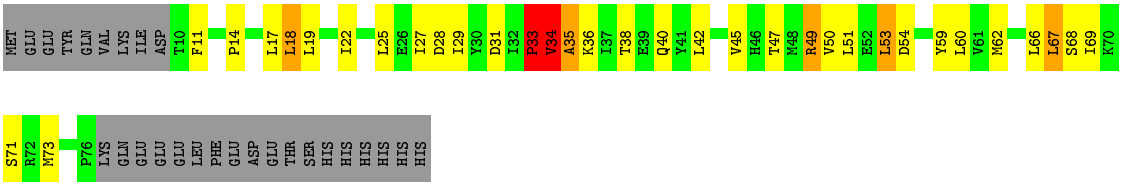




- Molecule 2: SEGREGATION AND CONDENSATION PROTEIN A

Chain Z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	107.44Å 107.44Å 102.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.97 – 3.40 75.97 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (75.97-3.40) 99.8 (75.97-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 3.41Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.243 , 0.277 0.241 , 0.265	Depositor DCC
R_{free} test set	808 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	100.8	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 105.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,-l,-k 0.004 for -h,l,k 0.009 for l,-k,h 0.014 for -l,-k,-h 0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.490 for h,-k,-l	Depositor
Outliers	0 of 16156 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6349	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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	0.49	0/2655	0.72	1/3584 (0.0%)
1	B	0.52	0/2687	0.75	1/3629 (0.0%)
2	C	0.53	0/543	0.82	3/739 (0.4%)
2	Z	0.53	0/547	0.82	3/744 (0.4%)
All	All	0.51	0/6432	0.75	8/8696 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
2	C	0	2
2	Z	0	2
All	All	0	9

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	18	LEU	CA-CB-CG	6.32	129.83	115.30
2	C	18	LEU	CA-CB-CG	6.08	129.28	115.30
2	Z	35	ALA	N-CA-C	-5.74	95.50	111.00
2	C	35	ALA	N-CA-C	-5.74	95.51	111.00
2	Z	53	LEU	CA-CB-CG	5.56	128.09	115.30
2	C	53	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	1102	LEU	CA-CB-CG	-5.35	102.99	115.30
1	B	1102	LEU	CA-CB-CG	-5.12	103.51	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	TYR	Peptide
1	A	1087	ASN	Peptide
1	A	1088	LEU	Peptide
1	B	105	TYR	Peptide
1	B	1087	ASN	Peptide
2	C	33	PRO	Peptide
2	C	34	VAL	Peptide
2	Z	33	PRO	Peptide
2	Z	34	VAL	Peptide

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	2622	0	2495	133	0
1	B	2655	0	2522	127	0
2	C	534	0	557	33	0
2	Z	538	0	561	22	0
All	All	6349	0	6135	289	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 23.

All (289) 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:B:1077:GLN:HB3	1:B:1083:LEU:HA	1.53	0.91
1:A:1077:GLN:HB3	1:A:1083:LEU:HA	1.54	0.90
2:C:27:ILE:HA	2:C:31:ASP:HB2	1.61	0.81
1:B:112:PHE:O	1:B:119:CYS:N	2.14	0.81
1:B:75:LEU:HA	1:B:81:THR:HA	1.61	0.81
2:Z:27:ILE:HA	2:Z:31:ASP:HB2	1.61	0.80
1:A:112:PHE:O	1:A:119:CYS:N	2.16	0.77
1:B:150:LEU:HD22	1:B:1086:LEU:HD21	1.69	0.75
1:A:150:LEU:HD22	1:A:1086:LEU:HD21	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:ASN:HA	1:B:1037:PHE:HB3	1.69	0.74
1:A:185:GLN:NE2	1:A:189:ASN:OD1	2.23	0.71
1:A:1125:GLU:O	1:A:1129:PHE:N	2.20	0.70
1:B:185:GLN:NE2	1:B:189:ASN:OD1	2.25	0.70
1:A:1034:ASN:HA	1:A:1037:PHE:HB3	1.72	0.70
1:B:1062:THR:O	1:B:1070:SER:OG	2.10	0.69
1:A:1032:ARG:CZ	1:A:1032:ARG:HA	2.22	0.69
1:A:1062:THR:O	1:A:1070:SER:OG	2.10	0.69
1:B:1032:ARG:HA	1:B:1032:ARG:CZ	2.22	0.68
1:B:158:ARG:HD2	1:B:1070:SER:O	1.94	0.68
1:A:1165:MET:SD	1:A:1170:VAL:N	2.66	0.68
1:B:1125:GLU:O	1:B:1129:PHE:N	2.20	0.66
2:C:33:PRO:O	2:C:34:VAL:HG12	1.95	0.66
1:A:158:ARG:HD2	1:A:1070:SER:O	1.95	0.66
2:Z:33:PRO:O	2:Z:34:VAL:HG12	1.96	0.65
1:B:1103:PHE:CZ	1:B:1134:TYR:HB3	2.30	0.65
1:B:1115:VAL:HG12	1:B:1145:ILE:HB	1.79	0.65
1:A:1115:VAL:HG12	1:A:1145:ILE:HB	1.79	0.64
1:A:170:TYR:HB2	2:C:53:LEU:HD11	1.79	0.64
2:C:18:LEU:HD13	2:Z:59:TYR:HB3	1.78	0.63
1:B:1011:LEU:HD21	2:Z:71:SER:HA	1.80	0.63
1:B:3:LEU:HG	1:B:91:LEU:HD13	1.81	0.63
1:A:1103:PHE:CZ	1:A:1134:TYR:HB3	2.33	0.63
1:B:145:LYS:HA	1:B:148:GLU:HB2	1.82	0.62
1:A:140:ILE:HA	1:A:1115:VAL:HG23	1.82	0.62
1:B:8:VAL:HA	1:B:87:ASP:OD1	2.01	0.61
1:A:9:ILE:HD13	1:A:17:ARG:HG2	1.82	0.61
1:A:145:LYS:HA	1:A:148:GLU:HB2	1.83	0.61
1:A:8:VAL:HA	1:A:87:ASP:OD1	2.01	0.60
1:A:3:LEU:HG	1:A:91:LEU:HD13	1.82	0.60
1:B:9:ILE:HD13	1:B:17:ARG:HG2	1.83	0.60
1:A:173:ARG:NH1	2:C:58:GLU:OE1	2.34	0.60
1:B:140:ILE:HA	1:B:1115:VAL:HG23	1.83	0.60
1:A:1032:ARG:HH21	2:C:49:ARG:NH2	1.99	0.59
2:C:59:TYR:CE1	2:Z:51:LEU:HD21	2.36	0.59
1:A:45:ARG:HH21	1:A:140:ILE:HG22	1.67	0.59
1:A:7:ASP:HB2	1:A:88:ASP:HB2	1.83	0.59
1:B:74:ARG:NH2	1:B:76:ASN:H	2.01	0.59
1:B:121:LEU:HA	1:B:124:ILE:HG13	1.85	0.59
1:B:45:ARG:HH21	1:B:140:ILE:HG22	1.67	0.59
1:B:198:LEU:HD11	1:B:1000:ARG:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD11	1:A:1000:ARG:HD2	1.85	0.58
1:B:7:ASP:HB2	1:B:88:ASP:HB2	1.84	0.58
1:A:121:LEU:HA	1:A:124:ILE:HG13	1.86	0.58
1:B:1112:PRO:HA	1:B:1142:THR:HB	1.85	0.58
1:B:184:THR:HG22	2:Z:68:SER:HB2	1.86	0.57
1:B:172:THR:HB	1:B:173:ARG:HD2	1.86	0.57
1:A:172:THR:HB	1:A:173:ARG:HD2	1.85	0.57
1:A:1112:PRO:HA	1:A:1142:THR:HB	1.85	0.57
1:A:170:TYR:HB2	2:C:53:LEU:CD1	2.35	0.57
1:B:40:ILE:HD11	1:B:1163:VAL:HG21	1.88	0.56
1:B:1018:LEU:HD12	2:Z:67:LEU:HD12	1.87	0.56
1:B:85:ASP:O	1:B:103:ARG:HA	2.05	0.56
1:B:1017:THR:O	1:B:1020:GLN:HB3	2.05	0.56
1:A:40:ILE:HD11	1:A:1163:VAL:HG21	1.88	0.56
1:B:1093:GLU:O	1:B:1097:THR:HG23	2.06	0.55
1:B:112:PHE:O	1:B:118:PRO:HA	2.07	0.55
1:A:85:ASP:O	1:A:103:ARG:HA	2.07	0.55
1:A:3:LEU:HD11	1:A:89:HIS:NE2	2.22	0.55
1:A:89:HIS:N	1:A:100:VAL:O	2.39	0.55
1:B:3:LEU:HD11	1:B:89:HIS:NE2	2.22	0.54
1:A:1032:ARG:HE	2:C:49:ARG:CZ	2.20	0.54
1:A:142:SER:O	1:A:146:VAL:HG23	2.07	0.54
1:A:23:VAL:O	1:A:1143:GLN:NE2	2.40	0.54
1:A:1093:GLU:O	1:A:1097:THR:HG23	2.06	0.54
1:B:1133:GLN:O	1:B:1137:LYS:HG2	2.08	0.54
1:B:138:PHE:HB3	1:B:1113:PHE:HD2	1.71	0.54
1:A:138:PHE:HB3	1:A:1113:PHE:HD2	1.72	0.54
1:A:1133:GLN:O	1:A:1137:LYS:HG2	2.08	0.54
1:B:1153:THR:O	1:B:1157:ALA:N	2.41	0.53
1:A:1138:TYR:HA	1:A:1141:ASP:OD2	2.08	0.53
1:B:1107:LYS:HD3	1:B:1138:TYR:OH	2.08	0.53
1:B:23:VAL:O	1:B:1143:GLN:NE2	2.41	0.53
1:A:50:GLU:OE2	1:B:120:ARG:NH1	2.42	0.53
2:C:73:MET:SD	2:Z:29:ILE:HG23	2.48	0.53
1:A:1017:THR:O	1:A:1020:GLN:HB3	2.08	0.53
1:A:1153:THR:O	1:A:1157:ALA:N	2.42	0.53
1:B:142:SER:O	1:B:146:VAL:HG23	2.08	0.53
1:A:1040:ILE:HD11	1:A:1108:VAL:HG21	1.91	0.53
1:B:1138:TYR:HA	1:B:1141:ASP:OD2	2.08	0.53
1:B:1158:ASP:OD2	1:B:1159:VAL:HG23	2.08	0.53
1:B:1040:ILE:HD11	1:B:1108:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:VAL:HG13	2:C:36:LYS:N	2.24	0.52
1:A:1030:THR:HG22	1:A:1067:LEU:HD22	1.91	0.52
1:A:45:ARG:HD3	1:A:52:SER:HA	1.91	0.52
1:A:112:PHE:O	1:A:118:PRO:HA	2.09	0.52
1:B:45:ARG:HD3	1:B:52:SER:HA	1.92	0.52
1:A:187:ASN:ND2	2:C:71:SER:OG	2.27	0.52
1:A:184:THR:HG21	2:C:67:LEU:HB3	1.91	0.51
1:B:1034:ASN:HA	1:B:1037:PHE:CB	2.39	0.51
1:A:27:THR:OG1	1:A:1145:ILE:HD13	2.11	0.51
1:B:27:THR:OG1	1:B:1145:ILE:HD13	2.11	0.51
1:A:1000:ARG:O	1:A:1004:LEU:N	2.37	0.51
1:A:1059:LEU:HD23	1:A:1074:ILE:HG12	1.92	0.51
1:A:1053:GLY:N	1:A:1054:GLY:HA2	2.25	0.51
1:B:1059:LEU:HD23	1:B:1074:ILE:HG12	1.92	0.51
1:A:167:VAL:HG21	1:A:1029:MET:O	2.12	0.50
1:A:44:ILE:HG13	1:A:89:HIS:HE1	1.76	0.50
1:A:1158:ASP:OD2	1:A:1159:VAL:HG23	2.12	0.50
1:B:89:HIS:N	1:B:100:VAL:O	2.41	0.50
1:B:44:ILE:HG13	1:B:89:HIS:HE1	1.76	0.50
1:A:180:LYS:NZ	2:C:65:THR:OG1	2.44	0.50
1:B:81:THR:O	1:B:82:LEU:HD23	2.10	0.50
2:C:19:LEU:HD21	2:Z:59:TYR:CE2	2.46	0.50
1:B:1030:THR:HG22	1:B:1067:LEU:HD22	1.93	0.50
2:Z:34:VAL:HG13	2:Z:36:LYS:N	2.26	0.50
1:B:1086:LEU:HA	1:B:1089:LEU:HD12	1.93	0.50
1:B:1053:GLY:N	1:B:1054:GLY:HA2	2.27	0.49
1:B:143:GLN:NE2	1:B:1118:GLU:O	2.45	0.49
1:A:1135:LEU:HA	1:A:1138:TYR:HB2	1.94	0.49
1:A:1107:LYS:HD3	1:A:1138:TYR:OH	2.12	0.49
1:B:157:ARG:HB3	1:B:1072:VAL:HG13	1.95	0.49
1:A:1086:LEU:HA	1:A:1089:LEU:HD12	1.94	0.49
1:A:1031:LYS:HG2	2:C:49:ARG:HH22	1.78	0.49
1:A:1048:PHE:CD2	1:A:1057:ALA:HB2	2.48	0.48
1:A:1130:ARG:HA	1:A:1133:GLN:HB2	1.94	0.48
1:A:143:GLN:NE2	1:A:1118:GLU:O	2.45	0.48
2:C:29:ILE:HG23	2:Z:73:MET:SD	2.53	0.48
1:A:6:LEU:HB2	1:A:22:PHE:HE2	1.79	0.48
1:A:1043:HIS:HB3	1:A:1104:SER:HB2	1.95	0.48
1:A:107:SER:OG	1:A:108:GLY:HA2	2.13	0.48
1:A:1:MET:HB3	1:A:2:PHE:H	1.59	0.48
1:A:112:PHE:HB2	1:A:119:CYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1106:LEU:HD23	1:B:1138:TYR:HE2	1.78	0.48
1:B:188:LEU:HD13	1:B:1012:THR:HG23	1.96	0.48
1:A:6:LEU:HD22	1:A:44:ILE:HD11	1.96	0.47
1:B:1043:HIS:HB3	1:B:1104:SER:HB2	1.95	0.47
1:A:1034:ASN:HA	1:A:1037:PHE:CB	2.40	0.47
1:B:20:VAL:HG13	1:B:1161:TYR:CE2	2.49	0.47
1:B:1021:VAL:O	1:B:1025:MET:HG3	2.14	0.47
1:B:1130:ARG:HA	1:B:1133:GLN:HB2	1.95	0.47
1:A:157:ARG:HB3	1:A:1072:VAL:HG13	1.95	0.47
1:B:1135:LEU:HA	1:B:1138:TYR:HB2	1.95	0.47
1:B:3:LEU:HD11	1:B:89:HIS:CE1	2.49	0.47
1:A:1056:ARG:H	1:A:1077:GLN:HG3	1.80	0.47
1:B:6:LEU:HB2	1:B:22:PHE:HE2	1.78	0.47
2:C:11:PHE:O	2:C:17:LEU:HD11	2.14	0.47
2:Z:11:PHE:O	2:Z:17:LEU:HD11	2.15	0.47
1:A:87:ASP:O	1:A:101:THR:HA	2.15	0.47
1:A:1086:LEU:HD12	1:A:1089:LEU:HD12	1.97	0.47
1:A:6:LEU:HB2	1:A:22:PHE:CE2	2.50	0.47
1:B:1048:PHE:CD2	1:B:1057:ALA:HB2	2.49	0.47
1:B:1043:HIS:CB	1:B:1104:SER:HB2	2.45	0.47
1:B:112:PHE:HB2	1:B:119:CYS:O	2.14	0.47
1:B:75:LEU:HB3	1:B:81:THR:HB	1.97	0.47
1:A:1056:ARG:HD3	1:A:1077:GLN:NE2	2.30	0.47
1:A:20:VAL:HG13	1:A:1161:TYR:CE2	2.50	0.47
1:B:6:LEU:HB2	1:B:22:PHE:CE2	2.50	0.47
1:B:45:ARG:HE	1:B:140:ILE:HG21	1.80	0.47
1:A:3:LEU:HD11	1:A:89:HIS:CE1	2.49	0.46
2:C:19:LEU:HD21	2:Z:59:TYR:CD2	2.50	0.46
1:A:1136:LYS:HD2	1:A:1136:LYS:HA	1.76	0.46
1:B:1039:GLN:HE21	2:Z:42:LEU:HD13	1.80	0.46
1:A:1118:GLU:CD	1:A:1148:THR:HA	2.36	0.46
1:A:44:ILE:HD12	1:A:44:ILE:H	1.80	0.46
1:B:167:VAL:HG21	1:B:1029:MET:O	2.15	0.46
1:B:6:LEU:HD22	1:B:44:ILE:HD11	1.96	0.46
1:A:1043:HIS:CB	1:A:1104:SER:HB2	2.46	0.46
1:B:107:SER:OG	1:B:108:GLY:HA2	2.16	0.46
1:A:1033:PHE:CD2	1:A:1067:LEU:HD21	2.51	0.46
1:A:1106:LEU:HD23	1:A:1138:TYR:HE2	1.80	0.46
1:A:173:ARG:HB2	2:C:57:SER:HB2	1.97	0.46
1:B:3:LEU:N	1:B:1143:GLN:OE1	2.48	0.46
1:A:1003:PHE:HA	1:A:1006:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:PHE:HA	1:B:1006:GLU:HB3	1.97	0.46
1:A:3:LEU:N	1:A:1143:GLN:OE1	2.49	0.46
1:A:1056:ARG:HD3	1:A:1077:GLN:HE21	1.81	0.46
1:A:45:ARG:HE	1:A:140:ILE:HG21	1.81	0.45
1:B:1032:ARG:NH2	1:B:1035:ASP:OD2	2.48	0.45
1:B:44:ILE:HD12	1:B:44:ILE:H	1.81	0.45
1:A:1021:VAL:O	1:A:1025:MET:HG3	2.16	0.45
2:Z:14:PRO:O	2:Z:18:LEU:HG	2.16	0.45
1:A:180:LYS:HA	1:A:183:GLU:HG3	1.98	0.45
1:A:138:PHE:HB3	1:A:1113:PHE:CD2	2.51	0.45
1:A:43:ALA:O	1:A:47:VAL:HG23	2.17	0.45
1:B:138:PHE:HB3	1:B:1113:PHE:CD2	2.51	0.45
1:B:173:ARG:HD2	1:B:173:ARG:N	2.32	0.45
1:A:1039:GLN:NE2	2:C:42:LEU:HD13	2.32	0.45
1:B:1011:LEU:HD12	1:B:1011:LEU:HA	1.73	0.45
1:B:1056:ARG:HD3	1:B:1077:GLN:NE2	2.31	0.45
1:B:1118:GLU:CD	1:B:1148:THR:HA	2.37	0.45
1:A:188:LEU:HD13	1:A:1012:THR:HG23	1.98	0.45
1:B:87:ASP:O	1:B:101:THR:HA	2.16	0.45
1:B:1086:LEU:HD12	1:B:1089:LEU:HD12	1.98	0.45
1:B:1131:PHE:CZ	1:B:1135:LEU:HD11	2.52	0.45
1:B:16:GLU:O	1:B:18:ILE:HD12	2.17	0.45
1:A:178:GLU:O	1:A:182:PHE:HD1	2.00	0.45
1:B:41:THR:HG23	1:B:1147:ILE:HD13	1.99	0.45
2:C:70:LYS:HD2	2:C:73:MET:HE2	1.99	0.45
1:B:71:SER:N	1:B:75:LEU:HD11	2.32	0.45
1:A:1116:LEU:HD13	1:A:1146:VAL:HB	2.00	0.44
1:A:41:THR:HG23	1:A:1147:ILE:HD13	1.99	0.44
1:B:178:GLU:O	1:B:182:PHE:HD1	2.00	0.44
1:B:1033:PHE:CD2	1:B:1067:LEU:HD21	2.52	0.44
1:B:44:ILE:CG1	1:B:89:HIS:HE1	2.30	0.44
1:A:1131:PHE:CZ	1:A:1135:LEU:HD11	2.52	0.44
2:Z:66:LEU:HA	2:Z:69:ILE:HD12	1.99	0.44
1:B:145:LYS:O	1:B:148:GLU:HB2	2.18	0.44
1:B:1056:ARG:HB2	1:B:1077:GLN:HE21	1.83	0.44
1:B:20:VAL:HA	1:B:1161:TYR:HE2	1.83	0.44
1:A:1039:GLN:HE21	2:C:42:LEU:HD13	1.83	0.43
1:A:173:ARG:N	1:A:173:ARG:HD2	2.32	0.43
1:B:1056:ARG:H	1:B:1077:GLN:HG3	1.83	0.43
1:B:1136:LYS:O	1:B:1139:SER:OG	2.36	0.43
1:A:84:LEU:HA	1:A:104:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ARG:HA	1:B:107:SER:C	2.38	0.43
2:C:14:PRO:O	2:C:18:LEU:HG	2.18	0.43
2:Z:45:VAL:O	2:Z:49:ARG:HB2	2.17	0.43
1:A:44:ILE:CG1	1:A:89:HIS:HE1	2.31	0.43
1:B:1056:ARG:HD3	1:B:1077:GLN:HE21	1.83	0.43
1:B:112:PHE:CZ	1:B:121:LEU:HD21	2.54	0.43
1:B:155:GLU:O	1:B:158:ARG:HG2	2.19	0.43
2:C:19:LEU:HA	2:C:19:LEU:HD23	1.63	0.43
1:B:1136:LYS:HD2	1:B:1136:LYS:HA	1.75	0.43
1:A:3:LEU:HA	1:A:91:LEU:HA	2.01	0.43
1:B:1:MET:HB3	1:B:2:PHE:H	1.60	0.43
1:B:31:GLY:HA2	1:B:32:PRO:HD3	1.78	0.43
1:B:74:ARG:HE	1:B:74:ARG:HB3	1.17	0.43
1:A:81:THR:O	1:A:82:LEU:HD23	2.18	0.43
1:B:89:HIS:O	1:B:99:SER:HA	2.19	0.43
1:A:1011:LEU:HD12	1:A:1011:LEU:HA	1.74	0.43
1:A:106:ARG:HA	1:A:107:SER:C	2.39	0.43
2:C:34:VAL:HG13	2:C:35:ALA:N	2.34	0.43
1:A:1032:ARG:NH2	1:A:1035:ASP:OD2	2.51	0.43
1:A:145:LYS:O	1:A:148:GLU:HB2	2.19	0.43
2:Z:51:LEU:O	2:Z:54:ASP:N	2.52	0.43
1:B:1113:PHE:HD1	1:B:1113:PHE:HA	1.71	0.42
1:B:1115:VAL:HA	1:B:1145:ILE:O	2.19	0.42
2:C:18:LEU:HD22	2:Z:60:LEU:HA	2.01	0.42
1:A:1019:PHE:O	1:A:1023:GLU:HG3	2.19	0.42
1:B:1097:THR:O	1:B:1100:ALA:HB3	2.19	0.42
1:A:20:VAL:HA	1:A:1161:TYR:HE2	1.84	0.42
1:A:16:GLU:O	1:A:18:ILE:HD12	2.19	0.42
1:A:180:LYS:HD2	2:C:65:THR:HA	2.01	0.42
1:B:1152:GLY:O	1:B:1156:GLU:HB2	2.20	0.42
1:B:1116:LEU:HD13	1:B:1146:VAL:HB	2.02	0.42
1:A:31:GLY:HA2	1:A:32:PRO:HD3	1.79	0.42
1:B:105:TYR:C	1:B:108:GLY:HA3	2.40	0.42
1:A:99:SER:HB2	1:A:115:ASN:HA	2.02	0.42
1:B:20:VAL:HG13	1:B:1161:TYR:CD2	2.55	0.42
1:B:3:LEU:HA	1:B:91:LEU:HA	2.02	0.42
2:Z:34:VAL:HG13	2:Z:35:ALA:N	2.35	0.42
1:B:1060:ARG:HB3	1:B:1060:ARG:CZ	2.50	0.41
1:B:43:ALA:O	1:B:47:VAL:HG23	2.19	0.41
2:C:21:LEU:O	2:C:24:ARG:N	2.53	0.41
1:A:1032:ARG:HE	2:C:49:ARG:NH1	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:ARG:HB3	1:A:1060:ARG:CZ	2.50	0.41
1:A:1056:ARG:HB2	1:A:1077:GLN:HE21	1.85	0.41
1:A:188:LEU:HD21	1:A:1011:LEU:HD23	2.02	0.41
1:B:1060:ARG:HB3	1:B:1060:ARG:NH1	2.35	0.41
1:A:1113:PHE:HD1	1:A:1113:PHE:HA	1.70	0.41
1:A:89:HIS:O	1:A:99:SER:HA	2.21	0.41
2:C:66:LEU:HA	2:C:69:ILE:HD12	2.02	0.41
2:C:73:MET:HB2	2:C:73:MET:HE2	1.77	0.41
1:A:113:LEU:HB3	1:A:116:ASN:HA	2.02	0.41
1:A:112:PHE:CZ	1:A:121:LEU:HD21	2.55	0.41
2:C:18:LEU:O	2:C:22:ILE:HG13	2.20	0.41
2:Z:18:LEU:O	2:Z:22:ILE:HG13	2.21	0.41
1:B:180:LYS:HA	1:B:183:GLU:HG3	2.02	0.41
1:A:1152:GLY:O	1:A:1156:GLU:HB2	2.20	0.41
1:A:20:VAL:HG13	1:A:1161:TYR:CD2	2.56	0.41
1:A:8:VAL:O	1:A:17:ARG:HA	2.20	0.41
1:B:1125:GLU:HB3	1:B:1126:ALA:H	1.75	0.41
1:B:113:LEU:HB3	1:B:116:ASN:HA	2.03	0.41
1:A:1060:ARG:HB3	1:A:1060:ARG:NH1	2.36	0.41
1:A:1115:VAL:HA	1:A:1145:ILE:O	2.20	0.41
1:A:5:ARG:HB3	1:A:90:PHE:CB	2.51	0.41
1:B:169:LYS:HB2	1:B:169:LYS:HE3	1.95	0.41
1:B:5:ARG:HB3	1:B:90:PHE:CB	2.51	0.40
1:B:149:ILE:HG23	1:B:150:LEU:H	1.86	0.40
1:A:1055:GLY:HA3	1:A:1077:GLN:O	2.20	0.40
1:A:1077:GLN:HA	1:A:1078:PRO:HD2	1.96	0.40
1:B:113:LEU:HG	1:B:118:PRO:HA	2.02	0.40
2:Z:19:LEU:HA	2:Z:19:LEU:HD23	1.71	0.40
1:A:1032:ARG:HA	1:A:1032:ARG:NH1	2.37	0.40
1:A:1125:GLU:O	1:A:1128:VAL:N	2.55	0.40
1:A:1117:ASP:HA	1:A:1147:ILE:HG12	2.04	0.40
1:B:1000:ARG:O	1:B:1004:LEU:N	2.37	0.40
1:B:1018:LEU:HD23	1:B:1018:LEU:HA	2.00	0.40
1:B:1061:LEU:HD12	1:B:1061:LEU:HA	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	331/426 (78%)	302 (91%)	26 (8%)	3 (1%)	17	49
1	B	337/426 (79%)	305 (90%)	27 (8%)	5 (2%)	10	36
2	C	65/94 (69%)	58 (89%)	6 (9%)	1 (2%)	10	36
2	Z	65/94 (69%)	57 (88%)	7 (11%)	1 (2%)	10	36
All	All	798/1040 (77%)	722 (90%)	66 (8%)	10 (1%)	12	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	34	VAL
2	Z	34	VAL
1	A	125	ILE
1	A	1174	ILE
1	B	125	ILE
1	B	1174	ILE
1	A	1088	LEU
1	B	1088	LEU
1	B	74	ARG
1	B	149	ILE

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	268/373 (72%)	215 (80%)	53 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	269/373 (72%)	216 (80%)	53 (20%)	1 4
2	C	59/89 (66%)	48 (81%)	11 (19%)	1 5
2	Z	60/89 (67%)	49 (82%)	11 (18%)	1 5
All	All	656/924 (71%)	528 (80%)	128 (20%)	1 4

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LEU
1	A	9	ILE
1	A	27	THR
1	A	81	THR
1	A	83	THR
1	A	89	HIS
1	A	105	TYR
1	A	127	LEU
1	A	139	SER
1	A	160	ILE
1	A	167	VAL
1	A	172	THR
1	A	174	LYS
1	A	184	THR
1	A	190	ARG
1	A	191	VAL
1	A	196	HIS
1	A	198	LEU
1	A	997	VAL
1	A	1003	PHE
1	A	1004	LEU
1	A	1006	GLU
1	A	1012	THR
1	A	1013	GLU
1	A	1029	MET
1	A	1042	SER
1	A	1046	GLN
1	A	1059	LEU
1	A	1060	ARG
1	A	1062	THR
1	A	1063	ASP
1	A	1065	ASN

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Mol	Chain	Res	Type
1	A	1069	HIS
1	A	1072	VAL
1	A	1073	GLU
1	A	1088	LEU
1	A	1090	SER
1	A	1105	ILE
1	A	1111	VAL
1	A	1113	PHE
1	A	1120	GLU
1	A	1124	ASP
1	A	1125	GLU
1	A	1133	GLN
1	A	1134	TYR
1	A	1141	ASP
1	A	1146	VAL
1	A	1149	HIS
1	A	1150	ARG
1	A	1153	THR
1	A	1164	THR
1	A	1165	MET
1	B	1	MET
1	B	3	LEU
1	B	9	ILE
1	B	27	THR
1	B	74	ARG
1	B	75	LEU
1	B	81	THR
1	B	83	THR
1	B	89	HIS
1	B	105	TYR
1	B	127	LEU
1	B	139	SER
1	B	160	ILE
1	B	167	VAL
1	B	172	THR
1	B	174	LYS
1	B	184	THR
1	B	190	ARG
1	B	191	VAL
1	B	198	LEU
1	B	997	VAL
1	B	1003	PHE

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Mol	Chain	Res	Type
1	B	1004	LEU
1	B	1006	GLU
1	B	1012	THR
1	B	1013	GLU
1	B	1029	MET
1	B	1042	SER
1	B	1046	GLN
1	B	1059	LEU
1	B	1060	ARG
1	B	1062	THR
1	B	1063	ASP
1	B	1065	ASN
1	B	1069	HIS
1	B	1072	VAL
1	B	1073	GLU
1	B	1088	LEU
1	B	1090	SER
1	B	1105	ILE
1	B	1111	VAL
1	B	1113	PHE
1	B	1120	GLU
1	B	1124	ASP
1	B	1125	GLU
1	B	1133	GLN
1	B	1134	TYR
1	B	1141	ASP
1	B	1146	VAL
1	B	1149	HIS
1	B	1150	ARG
1	B	1153	THR
1	B	1164	THR
2	C	25	LEU
2	C	28	ASP
2	C	33	PRO
2	C	38	THR
2	C	40	GLN
2	C	47	THR
2	C	49	ARG
2	C	50	VAL
2	C	53	LEU
2	C	62	MET
2	C	67	LEU

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Mol	Chain	Res	Type
2	Z	25	LEU
2	Z	28	ASP
2	Z	33	PRO
2	Z	38	THR
2	Z	40	GLN
2	Z	47	THR
2	Z	49	ARG
2	Z	50	VAL
2	Z	53	LEU
2	Z	62	MET
2	Z	67	LEU

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	89	HIS
1	A	143	GLN
1	A	1077	GLN
1	B	89	HIS
1	B	143	GLN
1	B	1039	GLN
1	B	1077	GLN
2	Z	46	HIS

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 (i)

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	345/426 (80%)	0.26	16 (4%) 32 32	89, 126, 143, 160	0
1	B	351/426 (82%)	0.08	7 (1%) 65 64	64, 112, 138, 165	0
2	C	67/94 (71%)	-0.08	1 (1%) 73 72	73, 94, 108, 143	0
2	Z	67/94 (71%)	0.02	0 100 100	61, 95, 132, 148	0
All	All	830/1040 (79%)	0.13	24 (2%) 51 50	61, 115, 142, 165	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	LYS	3.9
1	A	97	GLU	3.6
1	A	1160	LEU	3.5
1	A	149	ILE	3.5
2	C	10	THR	3.5
1	A	150	LEU	3.2
1	A	118	PRO	3.0
1	A	1116	LEU	2.7
1	A	1074	ILE	2.5
1	B	1001	TYR	2.5
1	B	122	LYS	2.5
1	A	123	ASP	2.4
1	A	1108	VAL	2.4
1	B	110	SER	2.3
1	B	138	PHE	2.3
1	A	188	LEU	2.2
1	A	1119	VAL	2.2
1	A	141	ILE	2.2
1	A	28	ALA	2.1
1	B	149	ILE	2.1
1	A	126	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	123	ASP	2.1
1	A	110	SER	2.1
1	B	141	ILE	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 carbohydrates 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.