Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 04:04 AM EDT

PDB ID	:	4DNQ
Title	:	Crystal Structure of DAD2 S96A mutant
Authors	:	Hamiaux, C.
Deposited on	:	2012-02-08
Resolution	:	2.80 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 (1)) were used in the production of this report:

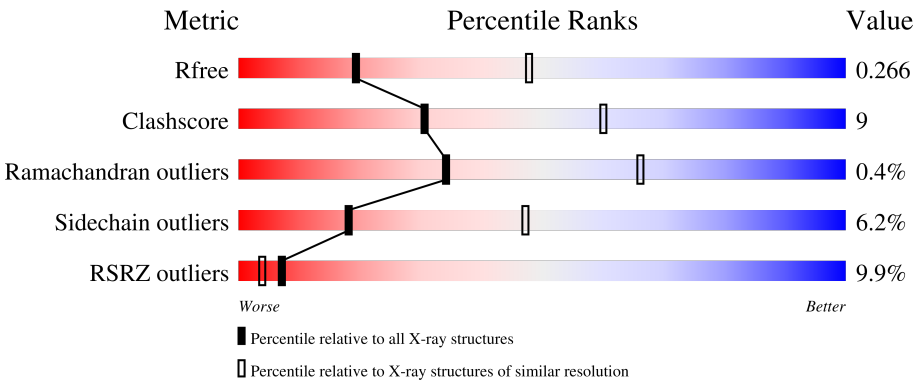
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	269	4% 78% 17% • •
1	B	269	4% 78% 17% • •
1	C	269	6% 78% 19% • •
1	D	269	5% 79% 18% • •
1	E	269	9% 80% 16% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	269	5% 81% 14%
1	G	269	7% 80% 16%
1	H	269	9% 78% 18%
1	I	269	9% 79% 17%
1	J	269	13% 80% 16%
1	K	269	14% 79% 16%
1	L	269	30% 78% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25042 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 DAD2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	2054	1320	359	367	8	0	0	0
1	B	262	2054	1320	359	367	8	0	0	0
1	C	263	2063	1325	361	369	8	0	0	0
1	D	263	2063	1325	361	369	8	0	0	0
1	E	262	2054	1320	359	367	8	0	0	0
1	F	263	2063	1325	361	369	8	0	0	0
1	G	263	2063	1325	361	369	8	0	0	0
1	H	262	2054	1320	359	367	8	0	0	0
1	I	264	2067	1327	362	370	8	0	0	0
1	J	263	2063	1325	361	369	8	0	0	0
1	K	262	2054	1320	359	367	8	0	0	0
1	L	264	2067	1327	362	370	8	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	33	33	33	0	0
2	B	27	27	27	0	0

Continued on next page...

Continued from previous page...

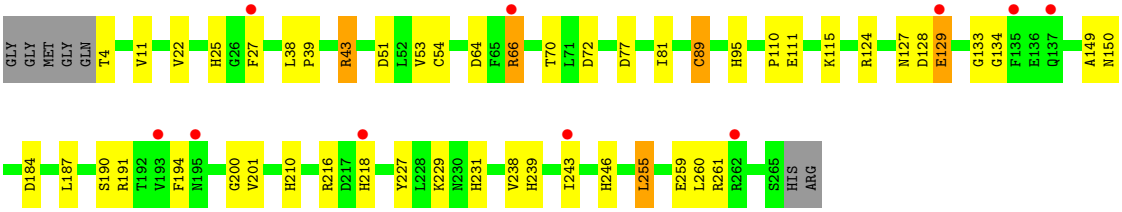
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	C	35	35	35	0	0
			Total	O		
2	D	32	32	32	0	0
			Total	O		
2	E	27	27	27	0	0
			Total	O		
2	F	27	27	27	0	0
			Total	O		
2	G	31	31	31	0	0
			Total	O		
2	H	24	24	24	0	0
			Total	O		
2	I	21	21	21	0	0
			Total	O		
2	J	12	12	12	0	0
			Total	O		
2	K	22	22	22	0	0
			Total	O		
2	L	32	32	32	0	0

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.

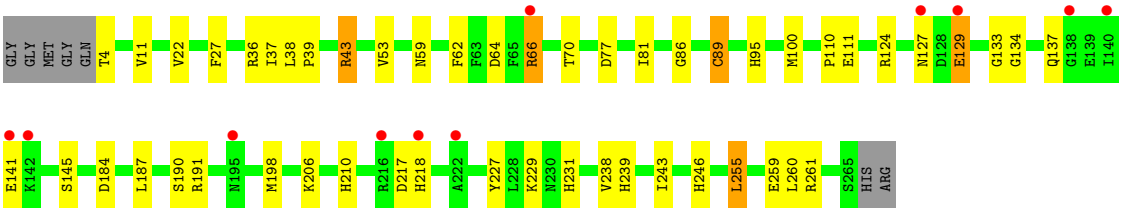
- Molecule 1: DAD2

Chain A:



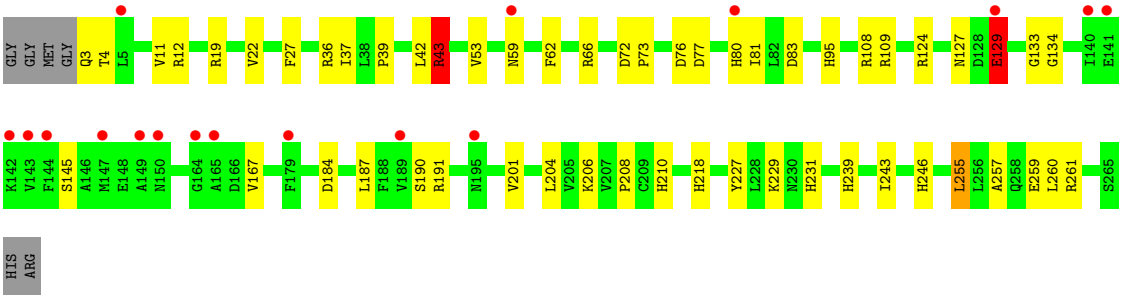
- Molecule 1: DAD2

Chain B:



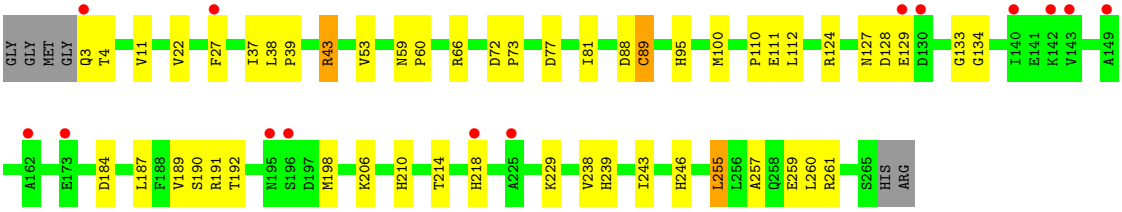
- Molecule 1: DAD2

Chain C:



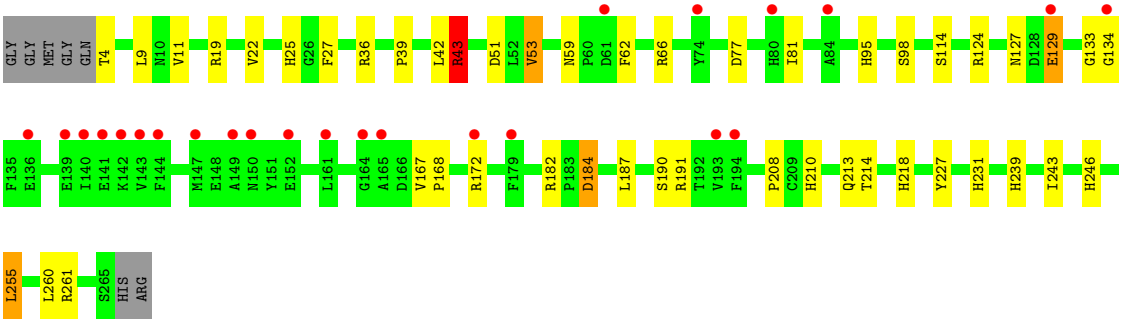
- Molecule 1: DAD2

Chain D:



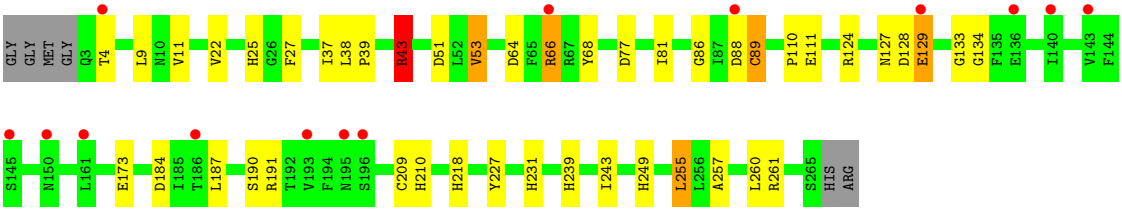
- Molecule 1: DAD2

Chain E:



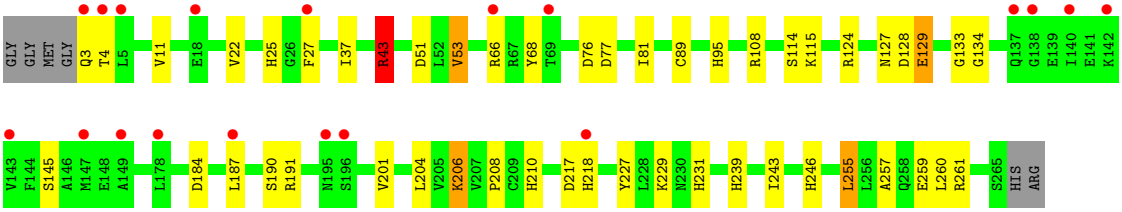
- Molecule 1: DAD2

Chain F:



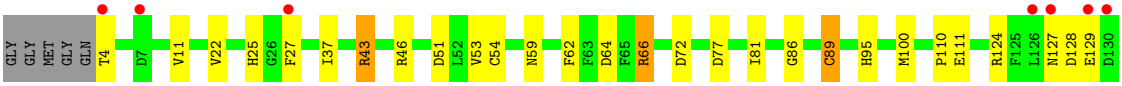
- Molecule 1: DAD2

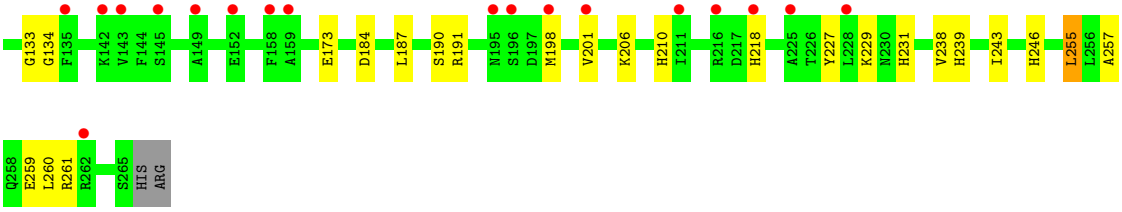
Chain G:



- Molecule 1: DAD2

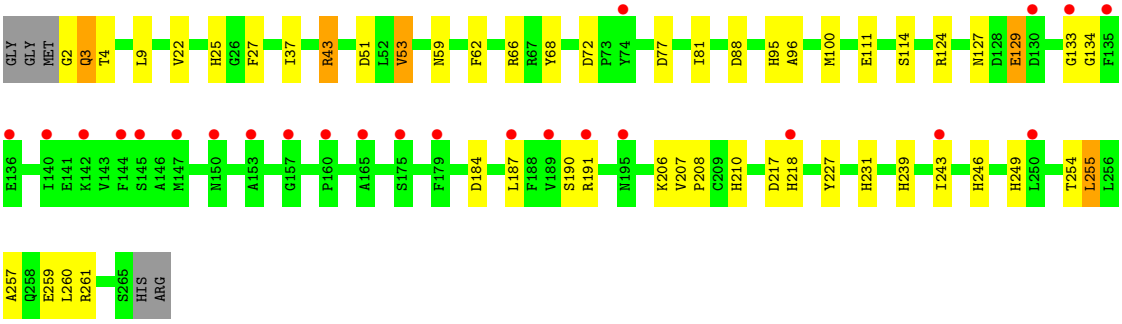
Chain H:





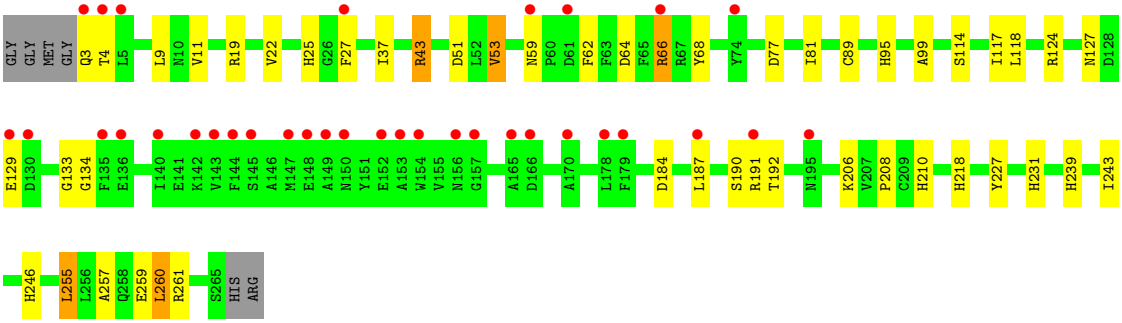
• Molecule 1: DAD2

Chain I:



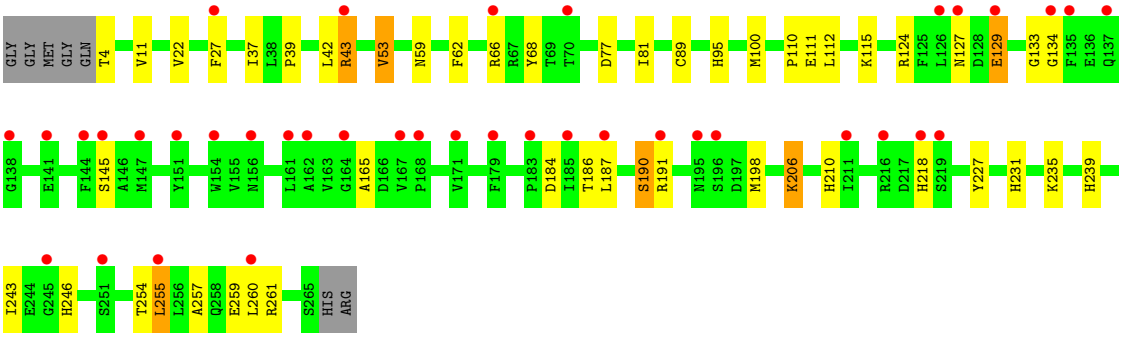
• Molecule 1: DAD2

Chain J:



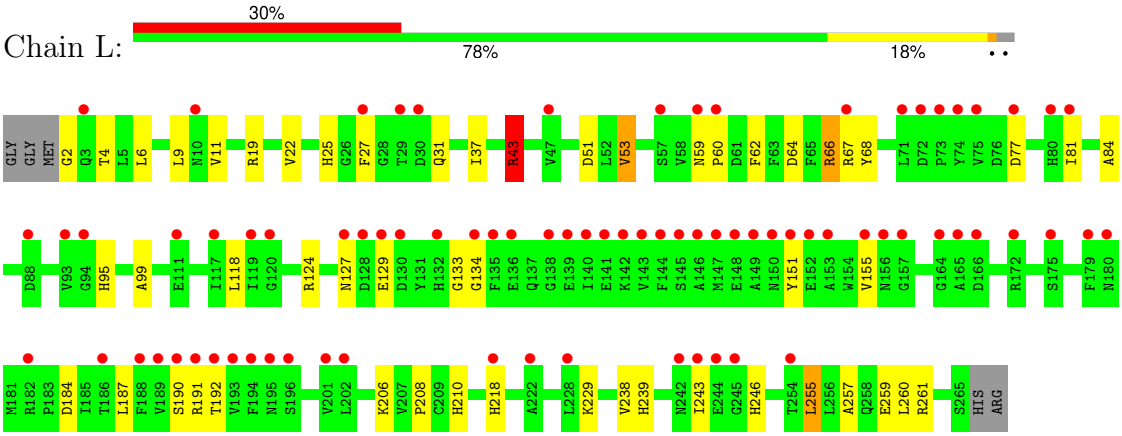
• Molecule 1: DAD2

Chain K:



• Molecule 1: DAD2

Chain L:


30%
78%
18%
GLY GLY MET G2 Q3 T4 L5 L6 L9 N10 V11 R19 V22 H25 G26 F27 G28 T29 D30 Q31 I37 R43 V47 D51 L52 V53 S57 V58 N59 P60 D61 F62 F63 D64 F65 R66 R67 Y68 L71 D72 P73 Y74 V75 D76 D77 H80 I81 A84
D88 V93 G94 H95 A99 E111 I117 L118 I119 G120 R124 N127 D128 E129 D130 Y131 H132 G133 G134 F135 E136 Q137 G138 E139 I140 E141 K142 V143 F144 S145 A146 M147 E148 A149 N150 Y151 E152 A153 W154 V155 N156 G157 G164 A165 D166 R172 S175 F179 N180
M181 R182 P183 D184 I185 T186 L187 F188 V189 S190 R191 T192 V193 F194 N195 S196 V201 L202 K206 V207 P208 C209 H210 H218 A222 L228 K229 V238 H239 N242 I243 E244 G245 H246 T254 L255 L256 A257 Q258 E259 L260 R261 S265 HIS ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	176.66Å 176.66Å 107.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.36 – 2.80 62.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.36-2.80) 100.0 (62.36-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.272 0.240 , 0.266	Depositor DCC
R_{free} test set	4632 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.046 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	25042	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3633e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.82	2/2105 (0.1%)	0.77	1/2865 (0.0%)
1	B	0.69	0/2105	0.75	1/2865 (0.0%)
1	C	0.70	0/2114	0.75	2/2877 (0.1%)
1	D	0.75	1/2114 (0.0%)	0.77	1/2877 (0.0%)
1	E	0.74	0/2105	0.71	1/2865 (0.0%)
1	F	0.76	2/2114 (0.1%)	0.75	2/2877 (0.1%)
1	G	0.72	1/2114 (0.0%)	0.74	1/2877 (0.0%)
1	H	0.75	2/2105 (0.1%)	0.75	1/2865 (0.0%)
1	I	0.70	0/2118	0.73	0/2882
1	J	0.64	0/2114	0.70	1/2877 (0.0%)
1	K	0.70	1/2105 (0.0%)	0.74	2/2865 (0.1%)
1	L	0.68	0/2118	0.70	1/2882 (0.0%)
All	All	0.72	9/25331 (0.0%)	0.74	14/34474 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	89	CYS	CB-SG	-12.59	1.60	1.82
1	A	89	CYS	CB-SG	-11.16	1.63	1.82
1	A	54	CYS	CB-SG	-7.76	1.69	1.82
1	G	89	CYS	CB-SG	-6.99	1.70	1.82
1	H	89	CYS	CB-SG	-6.10	1.71	1.82
1	D	89	CYS	CB-SG	-5.92	1.72	1.81
1	H	54	CYS	CB-SG	-5.81	1.72	1.81
1	F	209	CYS	CB-SG	-5.57	1.72	1.81
1	F	173	GLU	CD-OE2	5.01	1.31	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	89	CYS	CA-CB-SG	12.01	135.62	114.00
1	B	89	CYS	CA-CB-SG	10.46	132.83	114.00
1	D	89	CYS	CA-CB-SG	8.35	129.03	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	89	CYS	CB-CA-C	-8.08	94.23	110.40
1	H	89	CYS	CA-CB-SG	7.47	127.45	114.00
1	C	109	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	G	43	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	43	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	F	89	CYS	CA-CB-SG	5.87	124.56	114.00
1	A	89	CYS	CA-CB-SG	5.75	124.36	114.00
1	E	43	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	J	89	CYS	CA-CB-SG	5.41	123.74	114.00
1	L	43	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	F	43	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	2054	0	2034	44	0
1	B	2054	0	2034	43	0
1	C	2063	0	2042	61	0
1	D	2063	0	2042	35	0
1	E	2054	0	2034	54	0
1	F	2063	0	2042	40	0
1	G	2063	0	2042	43	0
1	H	2054	0	2034	44	0
1	I	2067	0	2045	36	1
1	J	2063	0	2042	36	0
1	K	2054	0	2034	44	0
1	L	2067	0	2045	49	0
2	A	33	0	0	3	0
2	B	27	0	0	2	0
2	C	35	0	0	1	0
2	D	32	0	0	2	0
2	E	27	0	0	5	0
2	F	27	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	31	0	0	0	0
2	H	24	0	0	4	0
2	I	21	0	0	3	0
2	J	12	0	0	1	0
2	K	22	0	0	2	0
2	L	32	0	0	4	0
All	All	25042	0	24470	451	1

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 9.

All (451) 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:F:88:ASP:OD2	1:L:19:ARG:HD3	1.42	1.16
1:C:36:ARG:HD3	1:G:108:ARG:HD2	1.34	1.09
1:E:36:ARG:HG3	2:E:306:HOH:O	1.50	1.09
1:A:70:THR:HG21	1:K:254:THR:HG21	1.10	1.05
1:F:88:ASP:OD2	1:L:19:ARG:CD	2.06	1.03
1:A:70:THR:CG2	1:K:254:THR:HG21	1.94	0.98
1:I:210:HIS:HD2	1:I:239:HIS:HE1	1.11	0.98
1:J:210:HIS:HD2	1:J:239:HIS:HE1	1.12	0.97
1:A:70:THR:HG21	1:K:254:THR:CG2	1.95	0.96
1:C:210:HIS:HD2	1:C:239:HIS:HE1	1.12	0.96
1:L:210:HIS:HD2	1:L:239:HIS:HE1	1.14	0.95
1:E:210:HIS:HD2	1:E:239:HIS:HE1	1.15	0.94
1:L:127:ASN:HD22	1:L:133:GLY:H	1.17	0.93
1:H:210:HIS:HD2	1:H:239:HIS:HE1	1.13	0.92
1:G:210:HIS:HD2	1:G:239:HIS:HE1	1.14	0.92
1:D:210:HIS:HD2	1:D:239:HIS:HE1	1.19	0.90
1:A:111:GLU:HB2	1:I:114:SER:O	1.71	0.90
1:K:210:HIS:HD2	1:K:239:HIS:HE1	1.18	0.90
1:D:127:ASN:HD22	1:D:133:GLY:H	1.19	0.89
1:A:210:HIS:HD2	1:A:239:HIS:HE1	1.20	0.88
1:B:111:GLU:HB3	1:J:208:PRO:HG2	1.52	0.87
1:C:36:ARG:CD	1:G:108:ARG:HD2	2.04	0.87
1:H:127:ASN:HD22	1:H:133:GLY:H	1.20	0.87
1:F:210:HIS:HD2	1:F:239:HIS:HE1	1.17	0.86
1:G:114:SER:O	1:K:111:GLU:HB2	1.74	0.86
1:A:127:ASN:HD22	1:A:133:GLY:H	1.19	0.85
1:C:12:ARG:NH1	2:C:311:HOH:O	2.08	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ASN:HD22	1:E:133:GLY:H	1.24	0.84
1:J:127:ASN:HD22	1:J:133:GLY:H	1.26	0.84
1:B:210:HIS:HD2	1:B:239:HIS:HE1	1.20	0.83
1:G:127:ASN:HD22	1:G:133:GLY:H	1.24	0.83
1:C:108:ARG:HD2	1:E:36:ARG:HD3	1.61	0.82
1:I:127:ASN:HD22	1:I:133:GLY:H	1.23	0.81
1:F:88:ASP:HB3	1:L:19:ARG:NH1	1.96	0.81
1:C:127:ASN:HD22	1:C:133:GLY:H	1.28	0.81
1:B:127:ASN:HD22	1:B:133:GLY:H	1.26	0.80
1:A:201:VAL:HG12	1:K:39:PRO:HB3	1.62	0.80
1:I:43:ARG:HG2	1:I:43:ARG:HH11	1.47	0.80
1:L:127:ASN:ND2	1:L:133:GLY:H	1.81	0.79
1:F:127:ASN:HD22	1:F:133:GLY:H	1.27	0.78
1:H:43:ARG:HH11	1:H:43:ARG:CG	1.97	0.78
1:K:43:ARG:CG	1:K:43:ARG:HH11	1.97	0.77
1:H:127:ASN:ND2	1:H:133:GLY:H	1.81	0.77
1:K:127:ASN:HD22	1:K:133:GLY:H	1.32	0.77
1:D:127:ASN:ND2	1:D:133:GLY:H	1.82	0.77
1:L:210:HIS:CD2	1:L:239:HIS:HE1	2.03	0.77
1:E:210:HIS:CD2	1:E:239:HIS:HE1	2.03	0.77
1:A:43:ARG:CG	1:A:43:ARG:HH11	1.98	0.77
1:C:42:LEU:HD11	1:G:204:LEU:HD21	1.67	0.76
1:D:43:ARG:CG	1:D:43:ARG:HH11	1.98	0.76
1:B:95:HIS:CD2	2:B:322:HOH:O	2.38	0.76
1:C:108:ARG:HD2	1:E:36:ARG:CD	2.14	0.76
1:C:108:ARG:HD2	1:E:36:ARG:NE	2.01	0.76
1:H:210:HIS:CD2	1:H:239:HIS:HE1	2.00	0.76
1:B:43:ARG:HH11	1:B:43:ARG:CG	1.98	0.75
1:B:111:GLU:HB2	1:J:114:SER:O	1.87	0.75
1:I:127:ASN:ND2	1:I:133:GLY:H	1.85	0.75
1:L:127:ASN:HD21	1:L:134:GLY:H	1.34	0.75
1:J:43:ARG:HH11	1:J:43:ARG:CG	2.00	0.75
1:F:43:ARG:CG	1:F:43:ARG:HH11	2.00	0.75
1:G:127:ASN:HD21	1:G:134:GLY:H	1.33	0.74
1:J:210:HIS:CD2	1:J:239:HIS:HE1	2.01	0.74
1:C:127:ASN:HD21	1:C:134:GLY:H	1.36	0.74
1:F:127:ASN:HD21	1:F:134:GLY:H	1.35	0.74
1:E:127:ASN:HD21	1:E:134:GLY:H	1.36	0.74
1:G:210:HIS:CD2	1:G:239:HIS:HE1	2.02	0.74
1:H:127:ASN:HD21	1:H:134:GLY:H	1.33	0.74
1:A:127:ASN:ND2	1:A:133:GLY:H	1.85	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:ASN:HD21	1:J:134:GLY:H	1.36	0.74
1:I:210:HIS:CD2	1:I:239:HIS:HE1	2.01	0.73
1:I:127:ASN:HD21	1:I:134:GLY:H	1.33	0.73
1:C:204:LEU:HD12	1:E:39:PRO:HG3	1.69	0.73
1:B:43:ARG:HH11	1:B:43:ARG:HG2	1.53	0.73
1:C:210:HIS:HD2	1:C:239:HIS:CE1	2.03	0.73
1:L:43:ARG:HG2	1:L:43:ARG:HH11	1.53	0.72
1:H:43:ARG:HH11	1:H:43:ARG:HG2	1.55	0.72
1:C:36:ARG:CZ	1:G:108:ARG:NH1	2.52	0.72
1:C:210:HIS:CD2	1:C:239:HIS:HE1	2.02	0.72
1:I:43:ARG:HH11	1:I:43:ARG:CG	2.02	0.72
1:L:43:ARG:HH11	1:L:43:ARG:CG	2.01	0.72
1:F:210:HIS:CD2	1:F:239:HIS:HE1	2.04	0.71
1:E:210:HIS:HD2	1:E:239:HIS:CE1	2.05	0.71
1:D:127:ASN:HD21	1:D:134:GLY:H	1.36	0.71
1:A:127:ASN:HD21	1:A:134:GLY:H	1.36	0.71
1:D:210:HIS:HD2	1:D:239:HIS:CE1	2.08	0.71
1:A:43:ARG:HH11	1:A:43:ARG:HG2	1.55	0.70
1:C:43:ARG:HH11	1:C:43:ARG:CG	2.04	0.70
1:K:127:ASN:HD21	1:K:134:GLY:H	1.39	0.70
1:B:77:ASP:O	1:B:81:ILE:HG12	1.91	0.70
1:C:36:ARG:HD3	1:G:108:ARG:CD	2.18	0.70
1:C:39:PRO:HG3	1:G:204:LEU:HD12	1.73	0.70
1:G:43:ARG:HH11	1:G:43:ARG:CG	2.05	0.70
1:E:43:ARG:HH11	1:E:43:ARG:CG	2.05	0.69
1:E:127:ASN:ND2	1:E:133:GLY:H	1.90	0.69
1:I:210:HIS:HD2	1:I:239:HIS:CE1	2.01	0.69
1:F:77:ASP:O	1:F:81:ILE:HG12	1.93	0.69
1:G:208:PRO:HG2	1:K:111:GLU:HB3	1.74	0.69
1:J:127:ASN:ND2	1:J:133:GLY:H	1.90	0.69
1:A:149:ALA:HA	1:B:191:ARG:NH2	2.08	0.68
1:F:43:ARG:HH11	1:F:43:ARG:HG2	1.57	0.68
1:G:77:ASP:O	1:G:81:ILE:HG12	1.93	0.68
1:G:127:ASN:ND2	1:G:133:GLY:H	1.91	0.68
1:L:77:ASP:O	1:L:81:ILE:HG12	1.94	0.68
1:A:216:ARG:NH2	2:A:312:HOH:O	2.21	0.68
1:H:77:ASP:O	1:H:81:ILE:HG12	1.94	0.67
1:C:43:ARG:HH11	1:C:43:ARG:HG2	1.59	0.67
1:C:127:ASN:ND2	1:C:133:GLY:H	1.92	0.67
1:D:43:ARG:HH11	1:D:43:ARG:HG2	1.59	0.67
1:L:31:GLN:HA	2:L:324:HOH:O	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASN:ND2	1:B:133:GLY:H	1.93	0.67
1:K:210:HIS:CD2	1:K:239:HIS:HE1	2.07	0.67
1:H:95:HIS:CD2	2:H:302:HOH:O	2.49	0.66
1:B:127:ASN:HD21	1:B:134:GLY:H	1.41	0.66
1:A:111:GLU:HB3	1:I:208:PRO:HG2	1.78	0.66
1:E:43:ARG:HH11	1:E:43:ARG:HG2	1.58	0.66
1:C:77:ASP:O	1:C:81:ILE:HG12	1.96	0.66
1:F:127:ASN:ND2	1:F:133:GLY:H	1.92	0.66
1:B:210:HIS:CD2	1:B:239:HIS:HE1	2.10	0.66
1:D:95:HIS:CD2	2:D:315:HOH:O	2.49	0.65
1:J:43:ARG:HH11	1:J:43:ARG:HG2	1.60	0.65
1:F:86:GLY:O	1:L:19:ARG:NH2	2.30	0.64
1:A:210:HIS:CD2	1:A:239:HIS:HE1	2.08	0.64
1:C:39:PRO:HG3	1:G:204:LEU:CD1	2.28	0.64
1:A:194:PHE:HE2	2:A:332:HOH:O	1.80	0.63
1:H:210:HIS:HD2	1:H:239:HIS:CE1	2.06	0.63
1:K:43:ARG:HH11	1:K:43:ARG:HG2	1.64	0.63
1:D:210:HIS:CD2	1:D:239:HIS:HE1	2.10	0.63
1:A:111:GLU:CB	1:I:114:SER:O	2.47	0.62
1:H:95:HIS:HD2	2:H:302:HOH:O	1.84	0.61
1:D:261:ARG:HG2	1:D:261:ARG:HH11	1.66	0.61
1:E:36:ARG:HB2	2:E:306:HOH:O	2.00	0.61
1:B:95:HIS:HD2	2:B:322:HOH:O	1.80	0.61
1:C:108:ARG:NH1	1:E:36:ARG:NH2	2.49	0.61
1:K:77:ASP:O	1:K:81:ILE:HG12	2.00	0.61
1:E:187:LEU:HD11	1:E:191:ARG:NH1	2.15	0.61
1:G:210:HIS:HD2	1:G:239:HIS:CE1	2.06	0.60
1:J:210:HIS:HD2	1:J:239:HIS:CE1	2.04	0.60
1:B:210:HIS:HD2	1:B:239:HIS:CE1	2.12	0.60
1:G:43:ARG:HH11	1:G:43:ARG:HG2	1.65	0.60
1:C:108:ARG:NH1	1:E:36:ARG:CZ	2.65	0.60
1:G:208:PRO:HG3	1:K:110:PRO:HG2	1.82	0.60
1:F:187:LEU:HD11	1:F:191:ARG:NH1	2.17	0.60
1:F:210:HIS:HD2	1:F:239:HIS:CE1	2.09	0.60
1:B:100:MET:SD	1:B:198:MET:HE2	2.42	0.59
1:F:37:ILE:HD12	1:F:257:ALA:HB2	1.83	0.59
1:K:127:ASN:ND2	1:K:133:GLY:H	1.99	0.59
1:L:210:HIS:HD2	1:L:239:HIS:CE1	2.06	0.59
1:E:36:ARG:CB	2:E:306:HOH:O	2.49	0.59
1:I:261:ARG:HG2	1:I:261:ARG:HH11	1.68	0.59
1:C:201:VAL:HG12	1:E:39:PRO:CB	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:GLU:HB3	1:L:208:PRO:HG2	1.86	0.58
1:E:114:SER:O	1:H:111:GLU:HB2	2.04	0.58
1:G:187:LEU:HD11	1:G:191:ARG:NH1	2.18	0.58
1:C:12:ARG:NH1	1:K:235:LYS:HG3	2.18	0.58
1:B:36:ARG:HH12	1:H:72:ASP:CG	2.07	0.58
1:G:37:ILE:HD12	1:G:257:ALA:HB2	1.86	0.58
1:J:77:ASP:O	1:J:81:ILE:HG12	2.03	0.58
1:E:77:ASP:O	1:E:81:ILE:HG12	2.04	0.57
1:I:2:GLY:O	1:I:3:GLN:HB2	2.03	0.57
1:I:100:MET:HG2	2:I:302:HOH:O	2.04	0.57
1:D:77:ASP:O	1:D:81:ILE:HG12	2.05	0.57
1:C:204:LEU:CD1	1:E:39:PRO:HG3	2.34	0.56
1:K:261:ARG:HG2	1:K:261:ARG:HH11	1.71	0.56
1:D:37:ILE:HD12	1:D:257:ALA:HB2	1.88	0.56
1:D:187:LEU:HD11	1:D:191:ARG:NH1	2.21	0.56
1:J:187:LEU:HD11	1:J:191:ARG:NH1	2.20	0.56
1:B:187:LEU:HD11	1:B:191:ARG:NH1	2.21	0.56
1:C:19:ARG:HG2	1:D:88:ASP:OD2	2.06	0.56
1:L:187:LEU:HD11	1:L:191:ARG:NH1	2.20	0.56
1:B:39:PRO:HB3	1:H:201:VAL:HG12	1.88	0.56
1:I:187:LEU:HD11	1:I:191:ARG:NH1	2.21	0.56
1:A:150:ASN:HB2	1:B:141:GLU:OE2	2.06	0.55
1:G:127:ASN:ND2	1:G:134:GLY:H	2.03	0.55
1:C:83:ASP:OD2	1:E:172:ARG:NE	2.39	0.55
1:C:129:GLU:OE2	1:C:129:GLU:HA	2.05	0.55
1:E:208:PRO:HG2	1:H:111:GLU:HB3	1.88	0.55
1:G:114:SER:O	1:K:111:GLU:CB	2.51	0.55
1:B:36:ARG:NH1	1:H:72:ASP:CG	2.60	0.55
1:C:187:LEU:HD11	1:C:191:ARG:NH1	2.21	0.55
1:I:77:ASP:O	1:I:81:ILE:HG12	2.06	0.55
1:A:77:ASP:O	1:A:81:ILE:HG12	2.06	0.54
1:L:2:GLY:N	1:L:84:ALA:CB	2.70	0.54
1:H:173:GLU:OE2	2:H:312:HOH:O	2.18	0.54
1:C:36:ARG:NH2	1:G:108:ARG:NH1	2.55	0.54
1:E:129:GLU:OE2	1:E:129:GLU:HA	2.08	0.54
1:I:129:GLU:HA	1:I:129:GLU:OE2	2.07	0.54
1:A:110:PRO:HG2	1:I:208:PRO:HG3	1.88	0.54
1:A:210:HIS:HD2	1:A:239:HIS:CE1	2.12	0.54
1:H:46:ARG:HD2	2:H:321:HOH:O	2.08	0.54
1:K:43:ARG:HH11	1:K:43:ARG:HG3	1.72	0.54
1:C:36:ARG:NE	1:G:108:ARG:HD2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:261:ARG:HH11	1:J:261:ARG:HG2	1.73	0.53
1:L:37:ILE:HD12	1:L:257:ALA:HB2	1.90	0.53
1:L:95:HIS:HE1	1:L:246:HIS:O	1.91	0.53
1:C:37:ILE:HD12	1:C:257:ALA:HB2	1.90	0.53
1:D:127:ASN:ND2	1:D:134:GLY:H	2.06	0.53
1:I:127:ASN:ND2	1:I:134:GLY:H	2.05	0.53
1:B:39:PRO:CB	1:H:201:VAL:HG12	2.38	0.53
1:C:108:ARG:CD	1:E:36:ARG:HD3	2.36	0.53
1:K:165:ALA:HB2	2:K:305:HOH:O	2.08	0.53
1:K:210:HIS:HD2	1:K:239:HIS:CE1	2.10	0.53
1:K:187:LEU:HD11	1:K:191:ARG:NH1	2.24	0.53
1:A:129:GLU:OE2	1:A:129:GLU:HA	2.08	0.53
1:H:261:ARG:HG2	1:H:261:ARG:HH11	1.73	0.53
1:L:60:PRO:HA	2:L:305:HOH:O	2.08	0.53
1:H:227:TYR:O	1:H:231:HIS:HD2	1.92	0.52
1:A:261:ARG:HG2	1:A:261:ARG:HH11	1.74	0.52
1:G:129:GLU:OE2	1:G:129:GLU:HA	2.10	0.52
1:F:88:ASP:OD2	1:L:19:ARG:CG	2.57	0.52
1:F:127:ASN:ND2	1:F:134:GLY:H	2.06	0.52
1:K:95:HIS:HE1	1:K:246:HIS:O	1.93	0.52
1:A:187:LEU:HD11	1:A:191:ARG:NH1	2.25	0.51
1:I:37:ILE:HD12	1:I:257:ALA:HB2	1.92	0.51
1:C:227:TYR:O	1:C:231:HIS:HD2	1.94	0.51
1:C:59:ASN:HB3	1:C:62:PHE:HD2	1.76	0.51
1:F:129:GLU:OE2	1:F:129:GLU:HA	2.11	0.51
1:L:127:ASN:ND2	1:L:134:GLY:H	2.06	0.51
1:L:239:HIS:HD2	1:L:259:GLU:OE1	1.93	0.51
1:F:128:ASP:HA	2:F:318:HOH:O	2.10	0.51
1:B:127:ASN:ND2	1:B:134:GLY:H	2.09	0.51
1:B:261:ARG:HG2	1:B:261:ARG:HH11	1.75	0.51
1:E:208:PRO:HG3	1:H:110:PRO:HG2	1.93	0.50
1:J:9:LEU:HD21	1:J:53:VAL:HG13	1.93	0.50
1:A:243:ILE:HD11	1:A:255:LEU:HB3	1.93	0.50
1:K:129:GLU:OE2	1:K:129:GLU:HA	2.11	0.50
1:H:210:HIS:CD2	1:H:239:HIS:CE1	2.91	0.50
1:G:261:ARG:HG2	1:G:261:ARG:HH11	1.77	0.50
1:J:127:ASN:ND2	1:J:134:GLY:H	2.07	0.50
1:A:115:LYS:HZ3	1:A:210:HIS:HE1	1.60	0.50
1:D:243:ILE:HD11	1:D:255:LEU:HB3	1.93	0.50
1:J:59:ASN:HB3	1:J:62:PHE:HD2	1.77	0.50
1:L:192:THR:HA	2:L:323:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ASN:ND2	1:D:133:GLY:N	2.56	0.50
1:H:100:MET:SD	1:H:198:MET:HE2	2.52	0.50
1:L:2:GLY:O	1:L:6:LEU:HG	2.12	0.50
1:H:243:ILE:HD11	1:H:255:LEU:HB3	1.92	0.50
1:I:95:HIS:HE1	1:I:246:HIS:O	1.95	0.50
1:K:165:ALA:CB	2:K:305:HOH:O	2.60	0.50
1:G:11:VAL:CG2	1:G:81:ILE:HD12	2.42	0.49
1:B:129:GLU:HA	1:B:129:GLU:OE2	2.12	0.49
1:E:59:ASN:HB3	1:E:62:PHE:HD2	1.77	0.49
1:H:127:ASN:ND2	1:H:134:GLY:H	2.04	0.49
1:J:37:ILE:HD12	1:J:257:ALA:HB2	1.93	0.49
1:B:36:ARG:HH12	1:H:72:ASP:HB3	1.77	0.49
1:B:243:ILE:HD11	1:B:255:LEU:HB3	1.94	0.49
1:L:261:ARG:HH11	1:L:261:ARG:HG2	1.75	0.49
1:I:243:ILE:HD11	1:I:255:LEU:HB3	1.94	0.49
1:B:86:GLY:HA2	1:J:19:ARG:NH2	2.27	0.49
1:C:201:VAL:HG12	1:E:39:PRO:HB3	1.93	0.49
1:H:37:ILE:HD12	1:H:257:ALA:HB2	1.94	0.49
1:E:261:ARG:HH11	1:E:261:ARG:HG2	1.78	0.48
1:C:76:ASP:OD2	1:E:167:VAL:HG13	2.12	0.48
1:E:95:HIS:HE1	1:E:246:HIS:O	1.95	0.48
1:A:111:GLU:HA	2:I:305:HOH:O	2.14	0.48
1:F:88:ASP:OD2	1:L:19:ARG:NE	2.46	0.48
1:H:95:HIS:HE1	1:H:246:HIS:O	1.96	0.48
1:I:239:HIS:HD2	1:I:259:GLU:OE1	1.96	0.48
1:F:53:VAL:HG21	1:F:68:TYR:CZ	2.49	0.48
1:G:227:TYR:O	1:G:231:HIS:HD2	1.96	0.48
1:J:129:GLU:OE2	1:J:129:GLU:HA	2.13	0.48
1:B:36:ARG:HH12	1:H:72:ASP:CB	2.27	0.48
1:C:108:ARG:CZ	1:E:36:ARG:NH2	2.76	0.48
1:E:43:ARG:CG	1:E:43:ARG:NH1	2.73	0.48
1:H:206:LYS:HA	1:H:206:LYS:HD3	1.64	0.48
1:D:95:HIS:HE1	1:D:246:HIS:O	1.96	0.48
1:E:127:ASN:ND2	1:E:134:GLY:H	2.07	0.48
1:L:67:ARG:NH2	2:L:307:HOH:O	2.47	0.48
1:A:127:ASN:ND2	1:A:133:GLY:N	2.58	0.47
1:C:167:VAL:HG13	1:G:76:ASP:OD2	2.13	0.47
1:E:36:ARG:CG	2:E:306:HOH:O	2.26	0.47
1:D:100:MET:SD	1:D:198:MET:HE2	2.53	0.47
1:D:129:GLU:HA	1:D:129:GLU:OE2	2.13	0.47
1:L:2:GLY:N	1:L:84:ALA:HB2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:OD2	1:K:254:THR:OG1	2.32	0.47
1:C:80:HIS:ND1	1:E:168:PRO:HB2	2.29	0.47
1:F:25:HIS:NE2	1:F:51:ASP:HA	2.28	0.47
1:I:25:HIS:NE2	1:I:51:ASP:HA	2.30	0.47
1:C:12:ARG:HH11	1:K:235:LYS:HG3	1.79	0.47
1:A:127:ASN:ND2	1:A:134:GLY:H	2.09	0.47
1:B:206:LYS:HA	1:B:206:LYS:HD3	1.62	0.47
1:J:11:VAL:CG2	1:J:81:ILE:HD12	2.45	0.47
1:K:127:ASN:ND2	1:K:134:GLY:H	2.09	0.47
1:B:110:PRO:HG2	1:J:208:PRO:HG3	1.97	0.47
1:C:11:VAL:CG2	1:C:81:ILE:HD12	2.45	0.47
1:C:243:ILE:HD11	1:C:255:LEU:HB3	1.97	0.47
1:G:53:VAL:HG21	1:G:68:TYR:CE1	2.50	0.47
1:K:11:VAL:CG2	1:K:81:ILE:HD12	2.45	0.47
1:C:201:VAL:HA	1:E:39:PRO:HB3	1.96	0.47
1:I:43:ARG:HG2	1:I:43:ARG:NH1	2.23	0.46
1:J:206:LYS:HD3	1:J:206:LYS:HA	1.65	0.46
1:D:11:VAL:CG2	1:D:81:ILE:HD12	2.44	0.46
1:L:11:VAL:CG2	1:L:81:ILE:HD12	2.45	0.46
1:H:127:ASN:ND2	1:H:133:GLY:N	2.59	0.46
1:K:243:ILE:HD11	1:K:255:LEU:HB3	1.98	0.46
1:E:25:HIS:NE2	1:E:51:ASP:HA	2.30	0.46
1:H:59:ASN:HB3	1:H:62:PHE:HD2	1.79	0.46
1:G:95:HIS:HE1	1:G:246:HIS:O	1.98	0.46
1:G:243:ILE:HD11	1:G:255:LEU:HB3	1.97	0.46
1:J:239:HIS:HD2	1:J:259:GLU:OE1	1.98	0.46
1:K:206:LYS:HA	1:K:206:LYS:HD3	1.62	0.46
1:F:9:LEU:HD21	1:F:53:VAL:HG13	1.98	0.46
1:H:187:LEU:HD11	1:H:191:ARG:NH1	2.30	0.46
1:D:95:HIS:HD2	2:D:315:HOH:O	1.90	0.46
1:H:129:GLU:OE2	1:H:129:GLU:HA	2.16	0.46
1:I:59:ASN:HB3	1:I:62:PHE:HD2	1.79	0.46
1:J:192:THR:HA	2:J:301:HOH:O	2.15	0.46
1:L:127:ASN:ND2	1:L:133:GLY:N	2.57	0.46
1:B:43:ARG:HG2	1:B:43:ARG:NH1	2.27	0.46
1:B:59:ASN:HB3	1:B:62:PHE:HD2	1.79	0.45
1:B:64:ASP:OD1	1:B:66:ARG:HG3	2.16	0.45
1:I:210:HIS:CD2	1:I:239:HIS:CE1	2.89	0.45
1:H:11:VAL:CG2	1:H:81:ILE:HD12	2.46	0.45
1:C:95:HIS:HE1	1:C:246:HIS:O	1.99	0.45
1:L:59:ASN:HB3	1:L:62:PHE:HD2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:HIS:HD2	1:D:259:GLU:OE1	1.99	0.45
1:G:25:HIS:NE2	1:G:51:ASP:HA	2.32	0.45
1:C:229:LYS:HE3	1:C:229:LYS:HB3	1.87	0.45
1:F:88:ASP:OD2	1:L:19:ARG:NH1	2.50	0.45
1:H:229:LYS:HG3	1:H:238:VAL:HG23	1.98	0.45
1:J:210:HIS:CD2	1:J:239:HIS:CE1	2.91	0.45
1:B:239:HIS:HD2	1:B:259:GLU:OE1	2.00	0.45
1:C:204:LEU:HD21	1:E:42:LEU:HD11	1.99	0.44
1:A:95:HIS:HE1	1:A:246:HIS:O	2.00	0.44
1:F:53:VAL:HG21	1:F:68:TYR:CE1	2.52	0.44
1:I:43:ARG:CG	1:I:43:ARG:NH1	2.71	0.44
1:L:129:GLU:OE2	1:L:129:GLU:HA	2.16	0.44
1:E:227:TYR:O	1:E:231:HIS:HD2	2.00	0.44
1:C:208:PRO:HG3	1:D:110:PRO:HG2	1.98	0.44
1:L:43:ARG:HG2	1:L:43:ARG:NH1	2.28	0.44
1:I:96:ALA:HB1	2:I:321:HOH:O	2.17	0.44
1:J:243:ILE:HD11	1:J:255:LEU:HB3	1.99	0.44
1:K:59:ASN:HB3	1:K:62:PHE:HD2	1.83	0.44
1:A:229:LYS:HG3	1:A:238:VAL:HG23	1.99	0.44
1:B:37:ILE:HD13	1:B:37:ILE:HA	1.77	0.44
1:C:19:ARG:CG	1:D:88:ASP:OD2	2.65	0.44
1:I:217:ASP:C	1:I:217:ASP:OD1	2.56	0.44
1:C:108:ARG:CD	1:E:36:ARG:NE	2.78	0.44
1:C:261:ARG:HG2	1:C:261:ARG:HH11	1.83	0.44
1:F:64:ASP:OD1	1:F:66:ARG:HG3	2.18	0.44
1:K:43:ARG:CG	1:K:43:ARG:NH1	2.67	0.44
1:B:11:VAL:CG2	1:B:81:ILE:HD12	2.48	0.44
1:J:25:HIS:NE2	1:J:51:ASP:HA	2.33	0.44
1:C:210:HIS:CD2	1:C:239:HIS:CE1	2.92	0.44
1:D:187:LEU:HD11	1:D:191:ARG:HH11	1.82	0.44
1:G:210:HIS:CD2	1:G:239:HIS:CE1	2.92	0.43
1:G:217:ASP:C	1:G:217:ASP:OD1	2.56	0.43
1:D:206:LYS:HA	1:D:206:LYS:HD3	1.61	0.43
1:E:127:ASN:ND2	1:E:133:GLY:N	2.63	0.43
1:E:182:ARG:NH1	1:E:184:ASP:OD2	2.48	0.43
1:I:53:VAL:HG21	1:I:68:TYR:CZ	2.52	0.43
1:K:227:TYR:O	1:K:231:HIS:HD2	2.00	0.43
1:A:150:ASN:ND2	1:B:137:GLN:OE1	2.51	0.43
1:C:108:ARG:HD2	1:E:36:ARG:CZ	2.47	0.43
1:F:11:VAL:CG2	1:F:81:ILE:HD12	2.48	0.43
1:K:210:HIS:CD2	1:K:239:HIS:CE1	2.96	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:GLN:NE2	2:E:318:HOH:O	2.51	0.43
1:L:2:GLY:N	1:L:84:ALA:HB1	2.33	0.43
1:A:25:HIS:NE2	1:A:51:ASP:HA	2.34	0.43
1:G:206:LYS:HA	1:G:206:LYS:HD3	1.65	0.43
1:J:99:ALA:HB1	1:J:118:LEU:HD22	2.00	0.43
1:K:37:ILE:HD12	1:K:257:ALA:HB2	1.99	0.43
1:A:11:VAL:CG2	1:A:81:ILE:HD12	2.48	0.43
1:C:208:PRO:HG2	1:D:111:GLU:HB3	1.99	0.43
1:D:189:VAL:O	1:D:192:THR:HB	2.19	0.43
1:E:9:LEU:HD21	1:E:53:VAL:HG13	2.01	0.43
1:E:187:LEU:HD11	1:E:191:ARG:HH11	1.82	0.43
1:L:9:LEU:HD21	1:L:53:VAL:HG13	2.01	0.43
1:E:43:ARG:HG2	1:E:43:ARG:NH1	2.30	0.43
1:F:43:ARG:HG2	1:F:43:ARG:NH1	2.31	0.43
2:A:333:HOH:O	1:I:111:GLU:HB3	2.18	0.43
1:D:59:ASN:HA	1:D:60:PRO:HD3	1.91	0.43
1:L:151:TYR:O	1:L:155:VAL:HG23	2.19	0.43
1:F:37:ILE:HD13	1:F:37:ILE:HA	1.75	0.43
1:F:127:ASN:ND2	1:F:133:GLY:N	2.65	0.43
1:F:128:ASP:O	1:F:129:GLU:C	2.58	0.43
1:F:261:ARG:HG2	1:F:261:ARG:HH11	1.83	0.43
1:A:200:GLY:O	1:K:42:LEU:HD12	2.19	0.42
1:G:239:HIS:HD2	1:G:259:GLU:OE1	2.02	0.42
1:J:37:ILE:HD13	1:J:37:ILE:HA	1.83	0.42
1:A:38:LEU:N	1:A:39:PRO:CD	2.83	0.42
1:J:95:HIS:HE1	1:J:246:HIS:O	2.01	0.42
1:F:243:ILE:HD11	1:F:255:LEU:HB3	2.00	0.42
1:D:38:LEU:HB3	1:D:39:PRO:HD3	2.01	0.42
1:L:206:LYS:HA	1:L:206:LYS:HD3	1.65	0.42
1:F:110:PRO:HG2	1:L:208:PRO:HG3	2.02	0.42
1:I:206:LYS:HA	1:I:206:LYS:HD3	1.57	0.42
1:L:229:LYS:HG3	1:L:238:VAL:HG23	2.01	0.42
1:A:227:TYR:O	1:A:231:HIS:HD2	2.03	0.42
1:L:210:HIS:CD2	1:L:239:HIS:CE1	2.93	0.42
1:C:127:ASN:ND2	1:C:134:GLY:H	2.11	0.42
1:G:115:LYS:HZ3	1:G:210:HIS:HE1	1.68	0.42
1:A:64:ASP:OD1	1:A:66:ARG:HG3	2.20	0.42
1:C:239:HIS:HD2	1:C:259:GLU:OE1	2.03	0.42
1:D:214:THR:HB	1:D:243:ILE:O	2.20	0.42
1:F:210:HIS:CD2	1:F:239:HIS:CE1	2.96	0.42
1:L:25:HIS:NE2	1:L:51:ASP:HA	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:243:ILE:HD11	1:L:255:LEU:HB3	2.01	0.42
1:H:25:HIS:NE2	1:H:51:ASP:HA	2.35	0.41
1:H:43:ARG:HG2	1:H:43:ARG:NH1	2.30	0.41
1:K:53:VAL:HG21	1:K:68:TYR:CE1	2.55	0.41
1:B:229:LYS:HG3	1:B:238:VAL:HG23	2.01	0.41
1:D:72:ASP:HB2	1:D:73:PRO:CD	2.51	0.41
1:E:19:ARG:HH21	1:H:86:GLY:HA2	1.84	0.41
1:J:227:TYR:O	1:J:231:HIS:HD2	2.02	0.41
1:K:100:MET:SD	1:K:198:MET:HE2	2.60	0.41
1:L:64:ASP:OD1	1:L:66:ARG:HG3	2.20	0.41
1:B:39:PRO:CG	1:H:201:VAL:HG12	2.51	0.41
1:B:95:HIS:HE1	1:B:246:HIS:O	2.02	0.41
1:F:88:ASP:OD2	1:L:19:ARG:CZ	2.68	0.41
1:D:229:LYS:HG3	1:D:238:VAL:HG23	2.02	0.41
1:E:214:THR:HB	1:E:243:ILE:O	2.20	0.41
1:F:227:TYR:O	1:F:231:HIS:HD2	2.03	0.41
1:J:53:VAL:HG21	1:J:68:TYR:CZ	2.55	0.41
1:G:127:ASN:ND2	1:G:133:GLY:N	2.64	0.41
1:H:64:ASP:OD1	1:H:66:ARG:HG3	2.20	0.41
1:J:43:ARG:HH11	1:J:43:ARG:HG3	1.81	0.41
1:K:112:LEU:HD12	1:K:112:LEU:HA	1.92	0.41
1:K:53:VAL:HG21	1:K:68:TYR:CZ	2.56	0.41
1:K:115:LYS:HZ3	1:K:210:HIS:HE1	1.68	0.41
1:A:115:LYS:NZ	1:A:210:HIS:CE1	2.89	0.41
1:A:239:HIS:HD2	1:A:259:GLU:OE1	2.03	0.41
1:E:243:ILE:HD11	1:E:255:LEU:HB3	2.02	0.41
1:J:117:ILE:HD13	1:J:260:LEU:HD12	2.01	0.41
1:K:239:HIS:HD2	1:K:259:GLU:OE1	2.03	0.41
1:A:115:LYS:NZ	1:A:210:HIS:HE1	2.17	0.41
1:A:128:ASP:O	1:A:129:GLU:C	2.60	0.41
1:C:43:ARG:CG	1:C:43:ARG:NH1	2.73	0.41
1:F:86:GLY:C	1:L:19:ARG:NH2	2.73	0.41
1:G:53:VAL:HG21	1:G:68:TYR:CZ	2.55	0.41
1:G:128:ASP:O	1:G:129:GLU:C	2.58	0.41
1:C:206:LYS:HA	1:C:206:LYS:HD3	1.61	0.41
1:D:128:ASP:O	1:D:129:GLU:C	2.58	0.41
1:H:128:ASP:O	1:H:129:GLU:C	2.59	0.41
1:J:127:ASN:ND2	1:J:133:GLY:N	2.64	0.41
1:K:186:THR:O	1:K:190:SER:HB2	2.20	0.41
1:C:72:ASP:HB2	1:C:73:PRO:HD3	2.03	0.41
1:F:38:LEU:HB3	1:F:39:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:239:HIS:HD2	1:H:259:GLU:OE1	2.04	0.41
1:I:187:LEU:HD11	1:I:191:ARG:HH11	1.83	0.41
1:B:217:ASP:C	1:B:217:ASP:OD1	2.59	0.40
1:L:53:VAL:HG21	1:L:68:TYR:CE1	2.56	0.40
1:B:38:LEU:HB3	1:B:39:PRO:HD3	2.03	0.40
1:I:9:LEU:HD21	1:I:53:VAL:HG13	2.02	0.40
1:J:64:ASP:OD1	1:J:66:ARG:HG3	2.20	0.40
1:A:43:ARG:HH11	1:A:43:ARG:HG3	1.83	0.40
1:B:227:TYR:O	1:B:231:HIS:HD2	2.05	0.40
1:C:80:HIS:ND1	1:E:168:PRO:CB	2.84	0.40
1:E:11:VAL:CG2	1:E:81:ILE:HD12	2.52	0.40
1:G:37:ILE:HD13	1:G:37:ILE:HA	1.85	0.40
1:I:227:TYR:O	1:I:231:HIS:HD2	2.04	0.40
1:L:99:ALA:HB1	1:L:118:LEU:HD22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:ASP:OD2	1:I:254:THR:OG1[2_545]	1.83	0.37

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	260/269 (97%)	251 (96%)	8 (3%)	1 (0%)	34	66
1	B	260/269 (97%)	247 (95%)	12 (5%)	1 (0%)	34	66
1	C	261/269 (97%)	252 (97%)	7 (3%)	2 (1%)	19	49
1	D	261/269 (97%)	250 (96%)	10 (4%)	1 (0%)	34	66
1	E	260/269 (97%)	249 (96%)	10 (4%)	1 (0%)	34	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	261/269 (97%)	251 (96%)	9 (3%)	1 (0%)	34	66
1	G	261/269 (97%)	251 (96%)	9 (3%)	1 (0%)	34	66
1	H	260/269 (97%)	252 (97%)	7 (3%)	1 (0%)	34	66
1	I	262/269 (97%)	252 (96%)	8 (3%)	2 (1%)	19	49
1	J	261/269 (97%)	253 (97%)	7 (3%)	1 (0%)	34	66
1	K	260/269 (97%)	250 (96%)	9 (4%)	1 (0%)	34	66
1	L	262/269 (97%)	250 (95%)	11 (4%)	1 (0%)	34	66
All	All	3129/3228 (97%)	3008 (96%)	107 (3%)	14 (0%)	34	66

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	3	GLN
1	I	184	ASP
1	A	184	ASP
1	B	184	ASP
1	C	184	ASP
1	D	184	ASP
1	E	184	ASP
1	F	184	ASP
1	G	184	ASP
1	J	184	ASP
1	L	184	ASP
1	H	184	ASP
1	K	184	ASP
1	C	129	GLU

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	219/223 (98%)	206 (94%)	13 (6%)	19	49
1	B	219/223 (98%)	204 (93%)	15 (7%)	16	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	220/223 (99%)	206 (94%)	14 (6%)	17	45
1	D	220/223 (99%)	206 (94%)	14 (6%)	17	45
1	E	219/223 (98%)	206 (94%)	13 (6%)	19	49
1	F	220/223 (99%)	206 (94%)	14 (6%)	17	45
1	G	220/223 (99%)	203 (92%)	17 (8%)	13	35
1	H	219/223 (98%)	207 (94%)	12 (6%)	21	52
1	I	220/223 (99%)	205 (93%)	15 (7%)	16	42
1	J	220/223 (99%)	208 (94%)	12 (6%)	21	52
1	K	219/223 (98%)	205 (94%)	14 (6%)	17	45
1	L	220/223 (99%)	209 (95%)	11 (5%)	24	56
All	All	2635/2676 (98%)	2471 (94%)	164 (6%)	18	47

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	22	VAL
1	A	27	PHE
1	A	43	ARG
1	A	53	VAL
1	A	66	ARG
1	A	89	CYS
1	A	124	ARG
1	A	129	GLU
1	A	190	SER
1	A	218	HIS
1	A	255	LEU
1	A	260	LEU
1	B	4	THR
1	B	22	VAL
1	B	27	PHE
1	B	43	ARG
1	B	53	VAL
1	B	66	ARG
1	B	70	THR
1	B	89	CYS
1	B	124	ARG
1	B	129	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	145	SER
1	B	190	SER
1	B	218	HIS
1	B	255	LEU
1	B	260	LEU
1	C	3	GLN
1	C	4	THR
1	C	22	VAL
1	C	27	PHE
1	C	43	ARG
1	C	53	VAL
1	C	66	ARG
1	C	124	ARG
1	C	129	GLU
1	C	145	SER
1	C	190	SER
1	C	218	HIS
1	C	255	LEU
1	C	260	LEU
1	D	3	GLN
1	D	4	THR
1	D	22	VAL
1	D	27	PHE
1	D	43	ARG
1	D	53	VAL
1	D	66	ARG
1	D	89	CYS
1	D	112	LEU
1	D	124	ARG
1	D	190	SER
1	D	218	HIS
1	D	255	LEU
1	D	260	LEU
1	E	4	THR
1	E	22	VAL
1	E	27	PHE
1	E	43	ARG
1	E	53	VAL
1	E	66	ARG
1	E	98	SER
1	E	124	ARG
1	E	129	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	190	SER
1	E	218	HIS
1	E	255	LEU
1	E	260	LEU
1	F	4	THR
1	F	22	VAL
1	F	27	PHE
1	F	43	ARG
1	F	53	VAL
1	F	66	ARG
1	F	89	CYS
1	F	124	ARG
1	F	129	GLU
1	F	190	SER
1	F	218	HIS
1	F	249	HIS
1	F	255	LEU
1	F	260	LEU
1	G	3	GLN
1	G	4	THR
1	G	22	VAL
1	G	27	PHE
1	G	43	ARG
1	G	53	VAL
1	G	66	ARG
1	G	124	ARG
1	G	129	GLU
1	G	145	SER
1	G	190	SER
1	G	201	VAL
1	G	206	LYS
1	G	218	HIS
1	G	229	LYS
1	G	255	LEU
1	G	260	LEU
1	H	4	THR
1	H	22	VAL
1	H	27	PHE
1	H	43	ARG
1	H	53	VAL
1	H	66	ARG
1	H	89	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	124	ARG
1	H	190	SER
1	H	218	HIS
1	H	255	LEU
1	H	260	LEU
1	I	4	THR
1	I	22	VAL
1	I	27	PHE
1	I	43	ARG
1	I	53	VAL
1	I	66	ARG
1	I	88	ASP
1	I	124	ARG
1	I	129	GLU
1	I	190	SER
1	I	207	VAL
1	I	218	HIS
1	I	249	HIS
1	I	255	LEU
1	I	260	LEU
1	J	3	GLN
1	J	4	THR
1	J	22	VAL
1	J	27	PHE
1	J	43	ARG
1	J	53	VAL
1	J	66	ARG
1	J	124	ARG
1	J	190	SER
1	J	218	HIS
1	J	255	LEU
1	J	260	LEU
1	K	4	THR
1	K	22	VAL
1	K	27	PHE
1	K	43	ARG
1	K	53	VAL
1	K	66	ARG
1	K	124	ARG
1	K	129	GLU
1	K	145	SER
1	K	190	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	206	LYS
1	K	218	HIS
1	K	255	LEU
1	K	260	LEU
1	L	4	THR
1	L	22	VAL
1	L	27	PHE
1	L	43	ARG
1	L	53	VAL
1	L	66	ARG
1	L	124	ARG
1	L	190	SER
1	L	218	HIS
1	L	255	LEU
1	L	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	80	HIS
1	A	95	HIS
1	A	127	ASN
1	A	180	ASN
1	A	210	HIS
1	A	213	GLN
1	A	231	HIS
1	A	236	ASN
1	A	239	HIS
1	B	10	ASN
1	B	95	HIS
1	B	127	ASN
1	B	210	HIS
1	B	213	GLN
1	B	231	HIS
1	B	236	ASN
1	B	239	HIS
1	C	95	HIS
1	C	127	ASN
1	C	210	HIS
1	C	213	GLN
1	C	231	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	239	HIS
1	D	31	GLN
1	D	95	HIS
1	D	127	ASN
1	D	210	HIS
1	D	213	GLN
1	D	231	HIS
1	D	236	ASN
1	D	239	HIS
1	E	95	HIS
1	E	127	ASN
1	E	210	HIS
1	E	213	GLN
1	E	231	HIS
1	E	239	HIS
1	F	10	ASN
1	F	31	GLN
1	F	95	HIS
1	F	127	ASN
1	F	210	HIS
1	F	213	GLN
1	F	231	HIS
1	F	236	ASN
1	F	239	HIS
1	G	31	GLN
1	G	95	HIS
1	G	127	ASN
1	G	210	HIS
1	G	213	GLN
1	G	231	HIS
1	G	236	ASN
1	G	239	HIS
1	H	95	HIS
1	H	127	ASN
1	H	210	HIS
1	H	213	GLN
1	H	231	HIS
1	H	236	ASN
1	H	239	HIS
1	I	95	HIS
1	I	127	ASN
1	I	210	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	213	GLN
1	I	231	HIS
1	I	236	ASN
1	I	239	HIS
1	J	95	HIS
1	J	127	ASN
1	J	210	HIS
1	J	213	GLN
1	J	231	HIS
1	J	236	ASN
1	J	239	HIS
1	K	10	ASN
1	K	95	HIS
1	K	127	ASN
1	K	210	HIS
1	K	213	GLN
1	K	231	HIS
1	K	239	HIS
1	L	95	HIS
1	L	127	ASN
1	L	210	HIS
1	L	213	GLN
1	L	231	HIS
1	L	236	ASN
1	L	239	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 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	262/269 (97%)	0.04	10 (3%)	40	30	21, 38, 63, 76	0
1	B	262/269 (97%)	0.19	11 (4%)	36	26	29, 47, 72, 89	0
1	C	263/269 (97%)	0.24	17 (6%)	18	11	24, 45, 75, 93	0
1	D	263/269 (97%)	0.19	14 (5%)	26	17	25, 43, 70, 85	0
1	E	262/269 (97%)	0.38	24 (9%)	9	5	27, 47, 80, 105	0
1	F	263/269 (97%)	0.32	14 (5%)	26	17	29, 43, 68, 80	0
1	G	263/269 (97%)	0.32	19 (7%)	15	8	27, 45, 69, 87	0
1	H	262/269 (97%)	0.43	25 (9%)	8	4	27, 46, 72, 97	0
1	I	264/269 (98%)	0.42	24 (9%)	9	5	26, 53, 119, 145	0
1	J	263/269 (97%)	0.62	34 (12%)	3	2	32, 60, 132, 168	0
1	K	262/269 (97%)	0.74	39 (14%)	2	1	35, 59, 102, 124	0
1	L	264/269 (98%)	1.40	80 (30%)	0	0	42, 58, 86, 100	0
All	All	3153/3228 (97%)	0.44	311 (9%)	7	4	21, 49, 90, 168	0

All (311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	138	GLY	11.5
1	J	147	MET	9.0
1	L	189	VAL	7.7
1	L	80	HIS	7.7
1	J	179	PHE	7.3
1	L	195	ASN	6.7
1	L	164	GLY	6.2
1	K	218	HIS	6.0
1	G	149	ALA	5.6
1	L	140	ILE	5.5
1	J	144	PHE	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	196	SER	5.2
1	L	146	ALA	5.1
1	L	193	VAL	5.1
1	I	179	PHE	5.1
1	L	74	TYR	4.9
1	H	195	ASN	4.9
1	L	152	GLU	4.9
1	F	143	VAL	4.9
1	K	137	GLN	4.9
1	L	71	LEU	4.9
1	L	75	VAL	4.8
1	K	168	PRO	4.8
1	L	244	GLU	4.7
1	H	159	ALA	4.6
1	E	143	VAL	4.5
1	F	195	ASN	4.5
1	J	149	ALA	4.4
1	I	195	ASN	4.4
1	K	161	LEU	4.4
1	L	179	PHE	4.4
1	L	180	ASN	4.4
1	K	135	PHE	4.3
1	H	129	GLU	4.3
1	H	143	VAL	4.3
1	L	194	PHE	4.2
1	K	162	ALA	4.1
1	L	182	ARG	4.1
1	L	134	GLY	4.1
1	I	147	MET	4.0
1	K	195	ASN	4.0
1	D	196	SER	3.9
1	I	145	SER	3.9
1	L	155	VAL	3.9
1	E	165	ALA	3.9
1	E	144	PHE	3.9
1	I	191	ARG	3.9
1	H	225	ALA	3.9
1	K	251	SER	3.9
1	D	143	VAL	3.8
1	L	202	LEU	3.8
1	B	129	GLU	3.8
1	H	152	GLU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	192	THR	3.8
1	K	187	LEU	3.8
1	L	191	ARG	3.8
1	H	218	HIS	3.8
1	L	149	ALA	3.8
1	A	129	GLU	3.8
1	L	3	GLN	3.7
1	E	149	ALA	3.7
1	L	120	GLY	3.7
1	B	195	ASN	3.7
1	J	66	ARG	3.7
1	L	150	ASN	3.7
1	J	157	GLY	3.6
1	F	140	ILE	3.6
1	L	129	GLU	3.6
1	F	136	GLU	3.6
1	H	262	ARG	3.5
1	A	66	ARG	3.5
1	L	29	THR	3.5
1	H	211	ILE	3.5
1	C	195	ASN	3.5
1	D	195	ASN	3.5
1	K	127	ASN	3.5
1	E	179	PHE	3.4
1	G	143	VAL	3.4
1	K	126	LEU	3.4
1	D	149	ALA	3.4
1	L	151	TYR	3.3
1	K	171	VAL	3.3
1	B	141	GLU	3.3
1	E	139	GLU	3.3
1	J	135	PHE	3.3
1	J	143	VAL	3.3
1	K	145	SER	3.3
1	F	150	ASN	3.3
1	K	156	ASN	3.3
1	E	140	ILE	3.3
1	L	148	GLU	3.2
1	J	74	TYR	3.2
1	L	145	SER	3.2
1	L	243	ILE	3.2
1	C	165	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	153	ALA	3.2
1	G	3	GLN	3.2
1	C	5	LEU	3.2
1	L	186	THR	3.2
1	L	153	ALA	3.2
1	F	193	VAL	3.2
1	J	5	LEU	3.2
1	H	135	PHE	3.1
1	J	191	ARG	3.1
1	I	165	ALA	3.1
1	L	201	VAL	3.1
1	L	138	GLY	3.1
1	K	129	GLU	3.1
1	L	222	ALA	3.1
1	H	126	LEU	3.1
1	K	141	GLU	3.1
1	L	141	GLU	3.1
1	D	130	ASP	3.1
1	E	142	LYS	3.1
1	L	130	ASP	3.1
1	K	219	SER	3.0
1	J	154	TRP	3.0
1	K	66	ARG	3.0
1	K	154	TRP	3.0
1	C	141	GLU	3.0
1	E	80	HIS	3.0
1	G	137	GLN	3.0
1	J	140	ILE	3.0
1	C	144	PHE	3.0
1	E	164	GLY	3.0
1	K	151	TYR	3.0
1	F	196	SER	3.0
1	K	43	ARG	3.0
1	C	129	GLU	3.0
1	L	27	PHE	3.0
1	F	145	SER	3.0
1	D	3	GLN	3.0
1	I	218	HIS	3.0
1	L	60	PRO	2.9
1	D	129	GLU	2.9
1	E	194	PHE	2.9
1	L	144	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	195	ASN	2.9
1	E	147	MET	2.9
1	J	153	ALA	2.9
1	E	172	ARG	2.9
1	G	66	ARG	2.9
1	J	187	LEU	2.9
1	L	218	HIS	2.9
1	H	216	ARG	2.9
1	B	218	HIS	2.9
1	L	94	GLY	2.9
1	B	222	ALA	2.9
1	G	178	LEU	2.9
1	L	59	ASN	2.8
1	L	135	PHE	2.8
1	K	196	SER	2.8
1	I	157	GLY	2.8
1	L	30	ASP	2.8
1	E	193	VAL	2.8
1	H	142	LYS	2.8
1	F	4	THR	2.8
1	E	136	GLU	2.8
1	B	127	ASN	2.8
1	L	196	SER	2.8
1	J	129	GLU	2.8
1	J	150	ASN	2.8
1	C	164	GLY	2.7
1	K	191	ARG	2.7
1	L	136	GLU	2.7
1	L	93	VAL	2.7
1	H	27	PHE	2.7
1	E	74	TYR	2.7
1	K	211	ILE	2.7
1	J	61	ASP	2.7
1	J	136	GLU	2.7
1	H	198	MET	2.7
1	L	132	HIS	2.7
1	I	140	ILE	2.7
1	H	228	LEU	2.7
1	K	27	PHE	2.7
1	E	61	ASP	2.7
1	J	130	ASP	2.7
1	I	135	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	140	ILE	2.6
1	C	150	ASN	2.6
1	I	142	LYS	2.6
1	L	190	SER	2.6
1	C	59	ASN	2.6
1	J	170	ALA	2.6
1	J	152	GLU	2.6
1	I	130	ASP	2.6
1	G	195	ASN	2.6
1	C	179	PHE	2.6
1	L	119	ILE	2.6
1	K	255	LEU	2.6
1	K	164	GLY	2.6
1	J	165	ALA	2.6
1	F	186	THR	2.6
1	G	142	LYS	2.6
1	K	134	GLY	2.6
1	L	10	ASN	2.6
1	L	72	ASP	2.6
1	L	242	ASN	2.6
1	K	260	LEU	2.5
1	E	150	ASN	2.5
1	F	66	ARG	2.5
1	L	228	LEU	2.5
1	C	147	MET	2.5
1	H	201	VAL	2.5
1	L	128	ASP	2.5
1	D	225	ALA	2.5
1	F	161	LEU	2.5
1	A	27	PHE	2.5
1	J	148	GLU	2.5
1	J	59	ASN	2.5
1	G	27	PHE	2.5
1	L	77	ASP	2.5
1	L	147	MET	2.5
1	E	129	GLU	2.5
1	K	179	PHE	2.5
1	J	178	LEU	2.5
1	A	193	VAL	2.4
1	D	27	PHE	2.4
1	L	143	VAL	2.4
1	G	187	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	156	ASN	2.4
1	L	157	GLY	2.4
1	I	74	TYR	2.4
1	J	145	SER	2.4
1	K	245	GLY	2.4
1	L	166	ASP	2.4
1	C	149	ALA	2.4
1	K	70	THR	2.4
1	L	175	SER	2.4
1	L	117	ILE	2.4
1	D	140	ILE	2.4
1	J	4	THR	2.4
1	G	4	THR	2.4
1	H	145	SER	2.4
1	B	66	ARG	2.4
1	I	144	PHE	2.4
1	L	254	THR	2.4
1	D	173	GLU	2.3
1	G	18	GLU	2.3
1	E	152	GLU	2.3
1	L	188	PHE	2.3
1	A	262	ARG	2.3
1	I	189	VAL	2.3
1	L	47	VAL	2.3
1	L	57	SER	2.3
1	B	140	ILE	2.3
1	E	134	GLY	2.3
1	G	140	ILE	2.3
1	F	129	GLU	2.3
1	A	243	ILE	2.2
1	H	158	PHE	2.2
1	L	139	GLU	2.2
1	G	218	HIS	2.2
1	J	142	LYS	2.2
1	I	136	GLU	2.2
1	H	127	ASN	2.2
1	I	160	PRO	2.2
1	G	138	GLY	2.2
1	C	80	HIS	2.2
1	D	218	HIS	2.2
1	L	142	LYS	2.2
1	J	166	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	88	ASP	2.2
1	I	175	SER	2.2
1	F	88	ASP	2.2
1	L	73	PRO	2.2
1	B	138	GLY	2.2
1	A	195	ASN	2.2
1	E	161	LEU	2.1
1	H	7	ASP	2.1
1	C	142	LYS	2.1
1	C	143	VAL	2.1
1	I	133	GLY	2.1
1	I	150	ASN	2.1
1	K	185	ILE	2.1
1	L	111	GLU	2.1
1	L	156	ASN	2.1
1	A	135	PHE	2.1
1	B	216	ARG	2.1
1	A	218	HIS	2.1
1	B	142	LYS	2.1
1	K	216	ARG	2.1
1	L	172	ARG	2.1
1	L	81	ILE	2.1
1	I	187	LEU	2.1
1	L	245	GLY	2.1
1	L	67	ARG	2.1
1	H	130	ASP	2.1
1	J	3	GLN	2.1
1	D	162	ALA	2.1
1	I	243	ILE	2.1
1	C	189	VAL	2.1
1	G	5	LEU	2.1
1	K	144	PHE	2.1
1	H	4	THR	2.1
1	H	149	ALA	2.1
1	D	142	LYS	2.1
1	J	27	PHE	2.1
1	G	196	SER	2.0
1	E	84	ALA	2.0
1	E	141	GLU	2.0
1	K	167	VAL	2.0
1	L	165	ALA	2.0
1	K	147	MET	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	137	GLN	2.0
1	I	250	LEU	2.0
1	L	127	ASN	2.0
1	G	69	THR	2.0
1	G	147	MET	2.0
1	K	183	PRO	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.