Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 06:32 PM JST

PDB ID	:	6M09
Title	:	The ligand-free structure of the chloroplast protein At3g03890
Authors	:	Wang, J.; Liu, L.
Deposited on	:	2020-02-20
Resolution	:	2.10 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

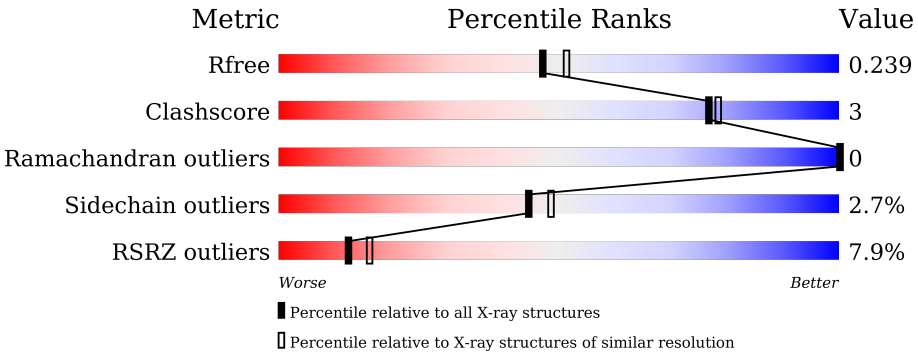
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	292	6% 79% • • 16%
1	B	292	8% 78% 7% • 14%
1	C	292	7% 77% 6% • 16%
1	D	292	7% 80% 6% 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8084 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 AT3G03890 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	4	0
			1856	1172	317	356	11			
1	B	252	Total	C	N	O	S	0	4	0
			1901	1205	327	358	11			
1	C	246	Total	C	N	O	S	0	5	0
			1859	1174	317	357	11			
1	D	253	Total	C	N	O	S	0	3	0
			1900	1201	327	361	11			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP Q8LDU1
A	31	GLY	-	expression tag	UNP Q8LDU1
A	32	SER	-	expression tag	UNP Q8LDU1
A	33	SER	-	expression tag	UNP Q8LDU1
A	34	HIS	-	expression tag	UNP Q8LDU1
A	35	HIS	-	expression tag	UNP Q8LDU1
A	36	HIS	-	expression tag	UNP Q8LDU1
A	37	HIS	-	expression tag	UNP Q8LDU1
A	38	HIS	-	expression tag	UNP Q8LDU1
A	39	HIS	-	expression tag	UNP Q8LDU1
A	40	SER	-	expression tag	UNP Q8LDU1
A	41	SER	-	expression tag	UNP Q8LDU1
A	42	GLY	-	expression tag	UNP Q8LDU1
A	43	LEU	-	expression tag	UNP Q8LDU1
A	44	VAL	-	expression tag	UNP Q8LDU1
A	45	PRO	-	expression tag	UNP Q8LDU1
A	46	ARG	-	expression tag	UNP Q8LDU1
A	47	GLY	-	expression tag	UNP Q8LDU1
A	48	SER	-	expression tag	UNP Q8LDU1
A	49	HIS	-	expression tag	UNP Q8LDU1
A	50	MET	-	expression tag	UNP Q8LDU1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ALA	-	expression tag	UNP Q8LDU1
A	52	SER	-	expression tag	UNP Q8LDU1
A	53	MET	-	expression tag	UNP Q8LDU1
A	54	THR	-	expression tag	UNP Q8LDU1
A	55	GLY	-	expression tag	UNP Q8LDU1
A	56	GLY	-	expression tag	UNP Q8LDU1
A	57	GLN	-	expression tag	UNP Q8LDU1
A	58	GLN	-	expression tag	UNP Q8LDU1
A	59	MET	-	expression tag	UNP Q8LDU1
A	60	GLY	-	expression tag	UNP Q8LDU1
A	61	ARG	-	expression tag	UNP Q8LDU1
A	62	GLY	-	expression tag	UNP Q8LDU1
B	30	MET	-	expression tag	UNP Q8LDU1
B	31	GLY	-	expression tag	UNP Q8LDU1
B	32	SER	-	expression tag	UNP Q8LDU1
B	33	SER	-	expression tag	UNP Q8LDU1
B	34	HIS	-	expression tag	UNP Q8LDU1
B	35	HIS	-	expression tag	UNP Q8LDU1
B	36	HIS	-	expression tag	UNP Q8LDU1
B	37	HIS	-	expression tag	UNP Q8LDU1
B	38	HIS	-	expression tag	UNP Q8LDU1
B	39	HIS	-	expression tag	UNP Q8LDU1
B	40	SER	-	expression tag	UNP Q8LDU1
B	41	SER	-	expression tag	UNP Q8LDU1
B	42	GLY	-	expression tag	UNP Q8LDU1
B	43	LEU	-	expression tag	UNP Q8LDU1
B	44	VAL	-	expression tag	UNP Q8LDU1
B	45	PRO	-	expression tag	UNP Q8LDU1
B	46	ARG	-	expression tag	UNP Q8LDU1
B	47	GLY	-	expression tag	UNP Q8LDU1
B	48	SER	-	expression tag	UNP Q8LDU1
B	49	HIS	-	expression tag	UNP Q8LDU1
B	50	MET	-	expression tag	UNP Q8LDU1
B	51	ALA	-	expression tag	UNP Q8LDU1
B	52	SER	-	expression tag	UNP Q8LDU1
B	53	MET	-	expression tag	UNP Q8LDU1
B	54	THR	-	expression tag	UNP Q8LDU1
B	55	GLY	-	expression tag	UNP Q8LDU1
B	56	GLY	-	expression tag	UNP Q8LDU1
B	57	GLN	-	expression tag	UNP Q8LDU1
B	58	GLN	-	expression tag	UNP Q8LDU1
B	59	MET	-	expression tag	UNP Q8LDU1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	60	GLY	-	expression tag	UNP Q8LDU1
B	61	ARG	-	expression tag	UNP Q8LDU1
B	62	GLY	-	expression tag	UNP Q8LDU1
C	30	MET	-	expression tag	UNP Q8LDU1
C	31	GLY	-	expression tag	UNP Q8LDU1
C	32	SER	-	expression tag	UNP Q8LDU1
C	33	SER	-	expression tag	UNP Q8LDU1
C	34	HIS	-	expression tag	UNP Q8LDU1
C	35	HIS	-	expression tag	UNP Q8LDU1
C	36	HIS	-	expression tag	UNP Q8LDU1
C	37	HIS	-	expression tag	UNP Q8LDU1
C	38	HIS	-	expression tag	UNP Q8LDU1
C	39	HIS	-	expression tag	UNP Q8LDU1
C	40	SER	-	expression tag	UNP Q8LDU1
C	41	SER	-	expression tag	UNP Q8LDU1
C	42	GLY	-	expression tag	UNP Q8LDU1
C	43	LEU	-	expression tag	UNP Q8LDU1
C	44	VAL	-	expression tag	UNP Q8LDU1
C	45	PRO	-	expression tag	UNP Q8LDU1
C	46	ARG	-	expression tag	UNP Q8LDU1
C	47	GLY	-	expression tag	UNP Q8LDU1
C	48	SER	-	expression tag	UNP Q8LDU1
C	49	HIS	-	expression tag	UNP Q8LDU1
C	50	MET	-	expression tag	UNP Q8LDU1
C	51	ALA	-	expression tag	UNP Q8LDU1
C	52	SER	-	expression tag	UNP Q8LDU1
C	53	MET	-	expression tag	UNP Q8LDU1
C	54	THR	-	expression tag	UNP Q8LDU1
C	55	GLY	-	expression tag	UNP Q8LDU1
C	56	GLY	-	expression tag	UNP Q8LDU1
C	57	GLN	-	expression tag	UNP Q8LDU1
C	58	GLN	-	expression tag	UNP Q8LDU1
C	59	MET	-	expression tag	UNP Q8LDU1
C	60	GLY	-	expression tag	UNP Q8LDU1
C	61	ARG	-	expression tag	UNP Q8LDU1
C	62	GLY	-	expression tag	UNP Q8LDU1
D	30	MET	-	expression tag	UNP Q8LDU1
D	31	GLY	-	expression tag	UNP Q8LDU1
D	32	SER	-	expression tag	UNP Q8LDU1
D	33	SER	-	expression tag	UNP Q8LDU1
D	34	HIS	-	expression tag	UNP Q8LDU1
D	35	HIS	-	expression tag	UNP Q8LDU1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	36	HIS	-	expression tag	UNP Q8LDU1
D	37	HIS	-	expression tag	UNP Q8LDU1
D	38	HIS	-	expression tag	UNP Q8LDU1
D	39	HIS	-	expression tag	UNP Q8LDU1
D	40	SER	-	expression tag	UNP Q8LDU1
D	41	SER	-	expression tag	UNP Q8LDU1
D	42	GLY	-	expression tag	UNP Q8LDU1
D	43	LEU	-	expression tag	UNP Q8LDU1
D	44	VAL	-	expression tag	UNP Q8LDU1
D	45	PRO	-	expression tag	UNP Q8LDU1
D	46	ARG	-	expression tag	UNP Q8LDU1
D	47	GLY	-	expression tag	UNP Q8LDU1
D	48	SER	-	expression tag	UNP Q8LDU1
D	49	HIS	-	expression tag	UNP Q8LDU1
D	50	MET	-	expression tag	UNP Q8LDU1
D	51	ALA	-	expression tag	UNP Q8LDU1
D	52	SER	-	expression tag	UNP Q8LDU1
D	53	MET	-	expression tag	UNP Q8LDU1
D	54	THR	-	expression tag	UNP Q8LDU1
D	55	GLY	-	expression tag	UNP Q8LDU1
D	56	GLY	-	expression tag	UNP Q8LDU1
D	57	GLN	-	expression tag	UNP Q8LDU1
D	58	GLN	-	expression tag	UNP Q8LDU1
D	59	MET	-	expression tag	UNP Q8LDU1
D	60	GLY	-	expression tag	UNP Q8LDU1
D	61	ARG	-	expression tag	UNP Q8LDU1
D	62	GLY	-	expression tag	UNP Q8LDU1

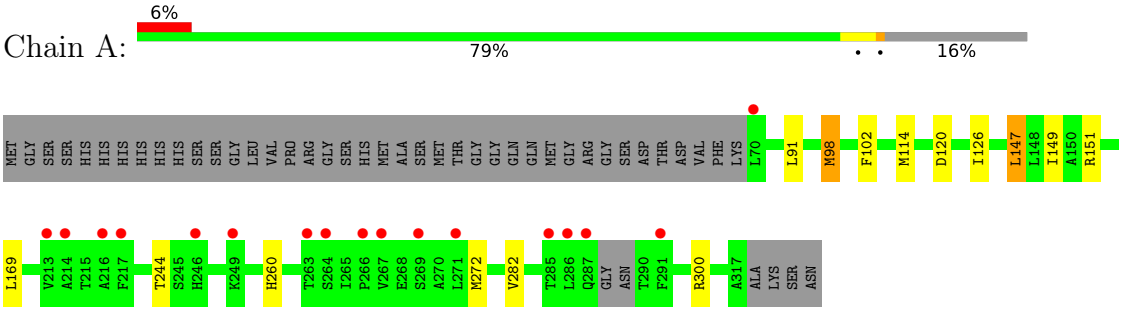
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	151	Total 151	O 151	0	0
2	B	128	Total 128	O 128	0	0
2	C	131	Total 131	O 131	0	0
2	D	158	Total 158	O 158	0	0

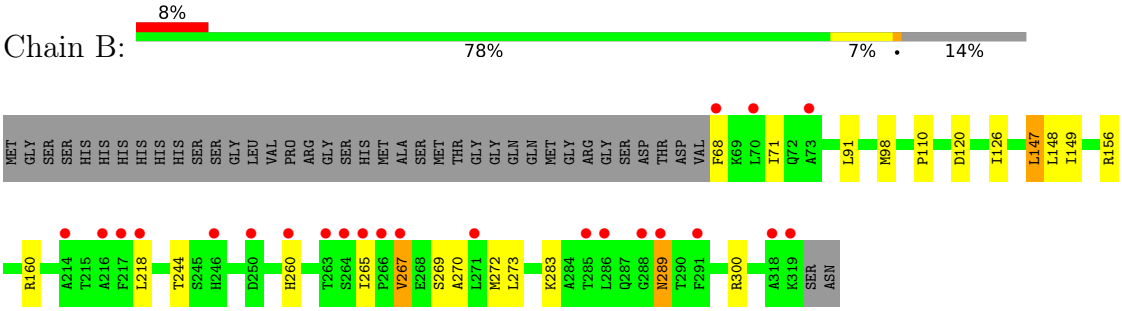
3 Residue-property plots (i)

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.

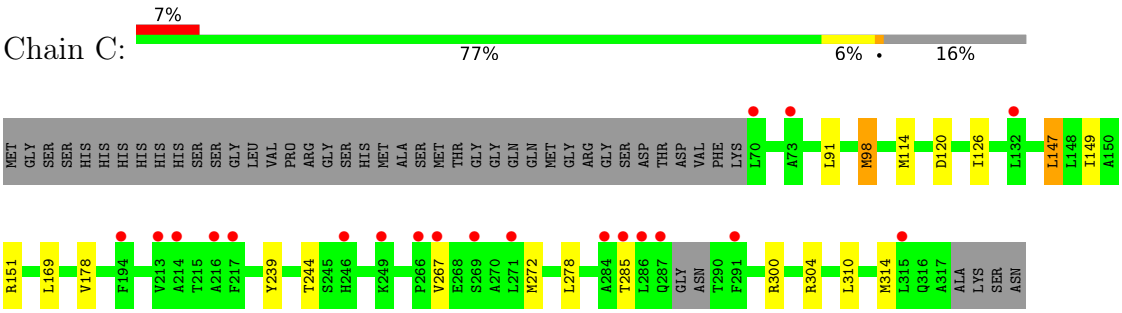
• Molecule 1: AT3G03890 protein



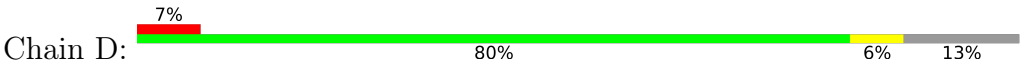
• Molecule 1: AT3G03890 protein

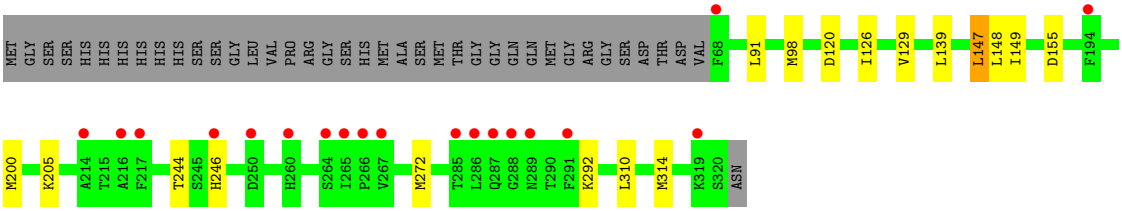


• Molecule 1: AT3G03890 protein



• Molecule 1: AT3G03890 protein




MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER ASP THR ASP VAL F68 L91 M98 D120 I126 V129 L139 L147 L148 I149 D155 F194
M200 K205 A214 T215 A216 F217 T244 S245 H246 D250 H260 S264 I265 P266 V267 M272 T285 L286 Q287 G288 N289 T290 F291 K292 L310 M314 K319 S320 ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.93Å 79.96Å 80.15Å 99.63° 109.80° 104.48°	Depositor
Resolution (Å)	37.76 – 2.10 41.46 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.0 (37.76-2.10) 87.0 (41.46-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.10Å)	Xtriage
Refinement program	PHENIX v1.12	Depositor
R, R_{free}	0.200 , 0.239 0.200 , 0.239	Depositor DCC
R_{free} test set	3358 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8084	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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	0.28	0/1904	0.48	0/2586
1	B	0.27	0/1947	0.47	0/2643
1	C	0.27	0/1910	0.47	0/2594
1	D	0.27	0/1945	0.49	0/2640
All	All	0.27	0/7706	0.48	0/10463

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

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	1856	0	1782	10	0
1	B	1901	0	1856	15	0
1	C	1859	0	1787	11	0
1	D	1900	0	1857	13	0
2	A	151	0	0	2	0
2	B	128	0	0	4	0
2	C	131	0	0	1	0
2	D	158	0	0	2	0
All	All	8084	0	7282	44	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 3.

All (44) 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:147:LEU:HD13	1:A:149:ILE:HD11	1.61	0.83
1:D:147:LEU:HD13	1:D:149[A]:ILE:HD11	1.61	0.82
1:C:98[A]:MET:HB3	1:D:98[A]:MET:HE2	1.79	0.65
1:A:151:ARG:NH2	2:A:404:HOH:O	2.29	0.63
1:C:151:ARG:NH1	2:C:403:HOH:O	2.32	0.62
1:B:147:LEU:HD13	1:B:149[A]:ILE:HD11	1.80	0.62
1:D:246:HIS:NE2	2:D:405:HOH:O	2.31	0.61
1:C:98[B]:MET:HE2	1:D:98[B]:MET:HB3	1.84	0.59
1:D:129:VAL:HG21	1:D:200:MET:HE2	1.84	0.58
1:D:205:LYS:NZ	2:D:409:HOH:O	2.36	0.58
1:B:265:ILE:HG22	1:B:267:VAL:HG12	1.86	0.58
1:A:98[A]:MET:HB3	1:B:98[A]:MET:HE2	1.87	0.56
1:B:68:PHE:N	2:B:405:HOH:O	2.38	0.56
1:C:120:ASP:HB3	1:C:126:ILE:HD11	1.87	0.55
1:A:98[A]:MET:HG3	1:A:114:MET:SD	2.48	0.53
1:B:273:LEU:HD21	1:B:283:LYS:HE3	1.91	0.53
1:B:289:ASN:N	1:B:289:ASN:OD1	2.43	0.51
1:C:98[A]:MET:HG3	1:C:114:MET:SD	2.50	0.51
1:B:300:ARG:NE	2:B:409:HOH:O	2.44	0.50
1:B:120:ASP:HB3	1:B:126:ILE:HD11	1.94	0.50
1:D:120:ASP:HB3	1:D:126:ILE:HD11	1.93	0.50
1:C:244:THR:HG22	1:C:272:MET:HG2	1.95	0.49
1:A:120:ASP:HB3	1:A:126:ILE:HD11	1.95	0.48
1:B:156:ARG:NH2	2:B:410:HOH:O	2.47	0.48
1:C:239:TYR:CD1	1:C:304:ARG:HD3	2.49	0.47
1:B:244:THR:HG22	1:B:272:MET:HB3	1.95	0.47
1:B:160:ARG:NH2	2:B:411:HOH:O	2.47	0.47
1:A:102:PHE:HE2	1:B:110:PRO:HD3	1.80	0.47
1:C:147:LEU:HD13	1:C:149:ILE:HD11	1.96	0.46
1:D:244:THR:HG22	1:D:272:MET:HB3	1.97	0.45
1:B:98[B]:MET:HG3	1:B:148:LEU:HD23	1.98	0.45
1:C:126:ILE:HG21	1:C:178:VAL:HG13	1.99	0.45
1:A:98[B]:MET:HE2	1:B:98[B]:MET:HB3	1.99	0.44
1:C:278:LEU:HD21	1:C:300:ARG:NH1	2.32	0.44
1:D:310:LEU:O	1:D:314:MET:HG3	2.18	0.44
1:B:267:VAL:HG21	1:B:270:ALA:HB2	1.99	0.43
1:D:129:VAL:HG21	1:D:200:MET:CE	2.47	0.43
1:D:139:LEU:HD13	1:D:200:MET:HE3	2.01	0.43
1:C:310:LEU:O	1:C:314:MET:HG3	2.18	0.43
1:A:300:ARG:NH1	2:A:407:HOH:O	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:THR:HG22	1:A:272:MET:HG2	2.02	0.42
1:A:272:MET:HA	1:A:282:VAL:HG12	2.01	0.42
1:D:148:LEU:O	1:D:149[B]:ILE:HD13	2.20	0.41
1:D:155:ASP:OD2	1:D:292:LYS:NZ	2.49	0.41

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	246/292 (84%)	244 (99%)	2 (1%)	0	100	100
1	B	254/292 (87%)	251 (99%)	3 (1%)	0	100	100
1	C	247/292 (85%)	244 (99%)	3 (1%)	0	100	100
1	D	254/292 (87%)	251 (99%)	3 (1%)	0	100	100
All	All	1001/1168 (86%)	990 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	193/244 (79%)	187 (97%)	6 (3%)	40	43
1	B	197/244 (81%)	189 (96%)	8 (4%)	30	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	194/244 (80%)	187 (96%)	7 (4%)	35 36
1	D	198/244 (81%)	196 (99%)	2 (1%)	76 82
All	All	782/976 (80%)	759 (97%)	23 (3%)	44 46

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	98[A]	MET
1	A	98[B]	MET
1	A	147	LEU
1	A	169	LEU
1	A	260	HIS
1	B	71	ILE
1	B	91	LEU
1	B	147	LEU
1	B	218	LEU
1	B	260	HIS
1	B	267	VAL
1	B	269	SER
1	B	289	ASN
1	C	91	LEU
1	C	98[A]	MET
1	C	98[B]	MET
1	C	147	LEU
1	C	169	LEU
1	C	267	VAL
1	C	285	THR
1	D	91	LEU
1	D	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	261	ASN

5.3.3 RNA

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

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	246/292 (84%)	0.16	17 (6%)	16	21	11, 29, 66, 73	2 (0%)
1	B	252/292 (86%)	0.26	23 (9%)	9	12	13, 31, 65, 76	2 (0%)
1	C	246/292 (84%)	0.29	20 (8%)	12	15	14, 32, 65, 76	3 (1%)
1	D	253/292 (86%)	0.22	19 (7%)	14	18	12, 29, 64, 80	5 (1%)
All	All	997/1168 (85%)	0.23	79 (7%)	12	16	11, 30, 65, 80	12 (1%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	214	ALA	9.2
1	B	216	ALA	5.4
1	C	217	PHE	5.3
1	C	266	PRO	5.0
1	B	214	ALA	4.9
1	C	216	ALA	4.8
1	D	286	LEU	4.3
1	C	285	THR	4.1
1	B	319	LYS	4.1
1	C	73	ALA	4.1
1	D	287	GLN	4.1
1	A	214	ALA	4.1
1	B	291	PHE	4.0
1	B	267	VAL	4.0
1	B	70	LEU	3.9
1	B	266	PRO	3.9
1	A	216	ALA	3.9
1	C	267	VAL	3.8
1	D	267	VAL	3.8
1	D	216	ALA	3.8
1	B	288	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	286	LEU	3.5
1	D	217	PHE	3.5
1	C	291	PHE	3.4
1	D	214	ALA	3.4
1	C	70	LEU	3.4
1	A	213	VAL	3.3
1	A	286	LEU	3.3
1	B	218	LEU	3.3
1	A	271	LEU	3.2
1	A	217	PHE	3.2
1	D	68	PHE	3.1
1	D	265	ILE	3.1
1	D	266	PRO	3.1
1	B	289	ASN	3.0
1	B	217	PHE	2.9
1	C	249	LYS	2.9
1	A	266	PRO	2.9
1	D	246	HIS	2.9
1	C	284	ALA	2.9
1	C	271	LEU	2.9
1	B	264	SER	2.8
1	D	291	PHE	2.8
1	A	285	THR	2.8
1	A	267	VAL	2.8
1	D	264	SER	2.8
1	B	265	ILE	2.7
1	B	68	PHE	2.7
1	B	286	LEU	2.7
1	D	289	ASN	2.7
1	A	246	HIS	2.7
1	C	287	GLN	2.6
1	C	246	HIS	2.6
1	D	260	HIS	2.6
1	D	250	ASP	2.5
1	A	287	GLN	2.4
1	D	288	GLY	2.4
1	B	285	THR	2.4
1	B	271	LEU	2.4
1	C	269	SER	2.3
1	C	194	PHE	2.3
1	D	319	LYS	2.3
1	A	291	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	213	VAL	2.3
1	B	263	THR	2.3
1	A	269	SER	2.3
1	D	285	THR	2.2
1	A	264	SER	2.2
1	A	249	LYS	2.2
1	D	194	PHE	2.1
1	B	73	ALA	2.1
1	A	263	THR	2.1
1	A	70	LEU	2.1
1	B	318	ALA	2.1
1	B	260	HIS	2.1
1	C	315	LEU	2.1
1	B	250	ASP	2.1
1	B	246	HIS	2.0
1	C	132	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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.