



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:05 pm BST

PDB ID : 4FD3
Title : Crystal structure of apo-formed ymtOAR1
Authors : Zhang, Y.; Gao, Y.; Ning, F.; Niu, L.; Teng, M.
Deposited on : 2012-05-26
Resolution : 2.60 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

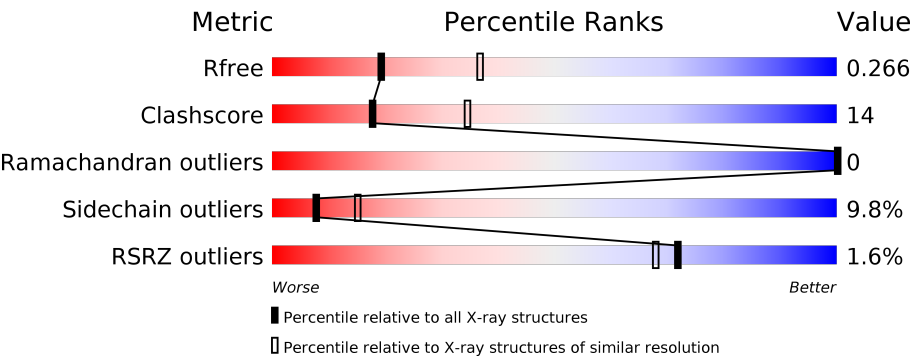
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. 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	286	<div><div>%</div><div><div></div><div>65%</div><div>21%</div><div>•</div><div>11%</div></div></div>
1	B	286	<div><div></div><div>65%</div><div>20%</div><div>•</div><div>12%</div></div>
1	C	286	<div><div></div><div>65%</div><div>20%</div><div>•</div><div>13%</div></div>
1	D	286	<div><div>3%</div><div></div><div>67%</div><div>22%</div><div>5%</div><div>6%</div></div>
1	E	286	<div><div>2%</div><div></div><div>62%</div><div>23%</div><div>•</div><div>13%</div></div>
1	F	286	<div><div>2%</div><div></div><div>66%</div><div>17%</div><div>•</div><div>14%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11328 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 3-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1865	1189	320	342	14			
1	B	253	Total	C	N	O	S	0	0	0
			1903	1212	323	353	15			
1	C	250	Total	C	N	O	S	0	0	0
			1878	1198	319	346	15			
1	D	268	Total	C	N	O	S	0	0	0
			1961	1248	338	360	15			
1	E	250	Total	C	N	O	S	0	0	0
			1837	1174	311	337	15			
1	F	246	Total	C	N	O	S	0	0	0
			1820	1161	312	333	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	LEU	-	EXPRESSION TAG	UNP P35731
A	280	GLU	-	EXPRESSION TAG	UNP P35731
A	281	HIS	-	EXPRESSION TAG	UNP P35731
A	282	HIS	-	EXPRESSION TAG	UNP P35731
A	283	HIS	-	EXPRESSION TAG	UNP P35731
A	284	HIS	-	EXPRESSION TAG	UNP P35731
A	285	HIS	-	EXPRESSION TAG	UNP P35731
A	286	HIS	-	EXPRESSION TAG	UNP P35731
B	279	LEU	-	EXPRESSION TAG	UNP P35731
B	280	GLU	-	EXPRESSION TAG	UNP P35731
B	281	HIS	-	EXPRESSION TAG	UNP P35731
B	282	HIS	-	EXPRESSION TAG	UNP P35731
B	283	HIS	-	EXPRESSION TAG	UNP P35731
B	284	HIS	-	EXPRESSION TAG	UNP P35731
B	285	HIS	-	EXPRESSION TAG	UNP P35731
B	286	HIS	-	EXPRESSION TAG	UNP P35731
C	279	LEU	-	EXPRESSION TAG	UNP P35731

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Chain	Residue	Modelled	Actual	Comment	Reference
C	280	GLU	-	EXPRESSION TAG	UNP P35731
C	281	HIS	-	EXPRESSION TAG	UNP P35731
C	282	HIS	-	EXPRESSION TAG	UNP P35731
C	283	HIS	-	EXPRESSION TAG	UNP P35731
C	284	HIS	-	EXPRESSION TAG	UNP P35731
C	285	HIS	-	EXPRESSION TAG	UNP P35731
C	286	HIS	-	EXPRESSION TAG	UNP P35731
D	279	LEU	-	EXPRESSION TAG	UNP P35731
D	280	GLU	-	EXPRESSION TAG	UNP P35731
D	281	HIS	-	EXPRESSION TAG	UNP P35731
D	282	HIS	-	EXPRESSION TAG	UNP P35731
D	283	HIS	-	EXPRESSION TAG	UNP P35731
D	284	HIS	-	EXPRESSION TAG	UNP P35731
D	285	HIS	-	EXPRESSION TAG	UNP P35731
D	286	HIS	-	EXPRESSION TAG	UNP P35731
E	279	LEU	-	EXPRESSION TAG	UNP P35731
E	280	GLU	-	EXPRESSION TAG	UNP P35731
E	281	HIS	-	EXPRESSION TAG	UNP P35731
E	282	HIS	-	EXPRESSION TAG	UNP P35731
E	283	HIS	-	EXPRESSION TAG	UNP P35731
E	284	HIS	-	EXPRESSION TAG	UNP P35731
E	285	HIS	-	EXPRESSION TAG	UNP P35731
E	286	HIS	-	EXPRESSION TAG	UNP P35731
F	279	LEU	-	EXPRESSION TAG	UNP P35731
F	280	GLU	-	EXPRESSION TAG	UNP P35731
F	281	HIS	-	EXPRESSION TAG	UNP P35731
F	282	HIS	-	EXPRESSION TAG	UNP P35731
F	283	HIS	-	EXPRESSION TAG	UNP P35731
F	284	HIS	-	EXPRESSION TAG	UNP P35731
F	285	HIS	-	EXPRESSION TAG	UNP P35731
F	286	HIS	-	EXPRESSION TAG	UNP P35731

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	15	Total O 15 15	0	0
2	C	16	Total O 16 16	0	0
2	D	9	Total O 9 9	0	0

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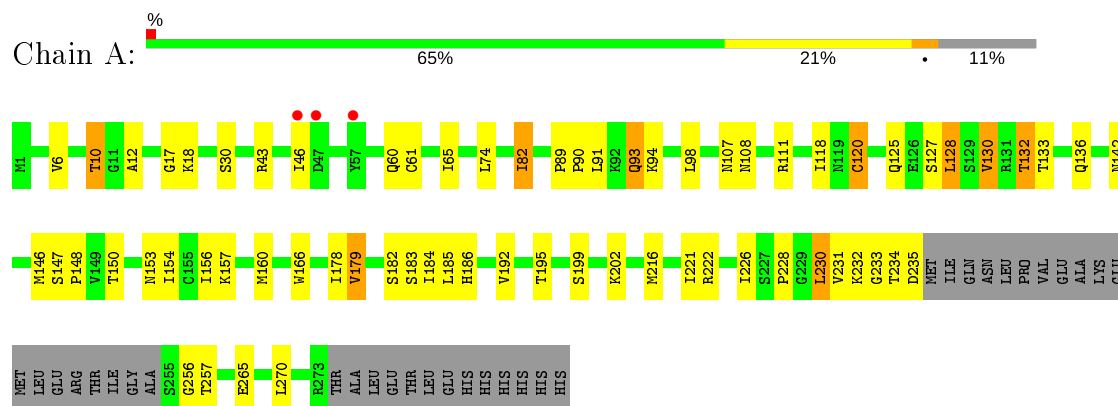
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	9	Total	O	0	0
			9	9		
2	F	9	Total	O	0	0
			9	9		

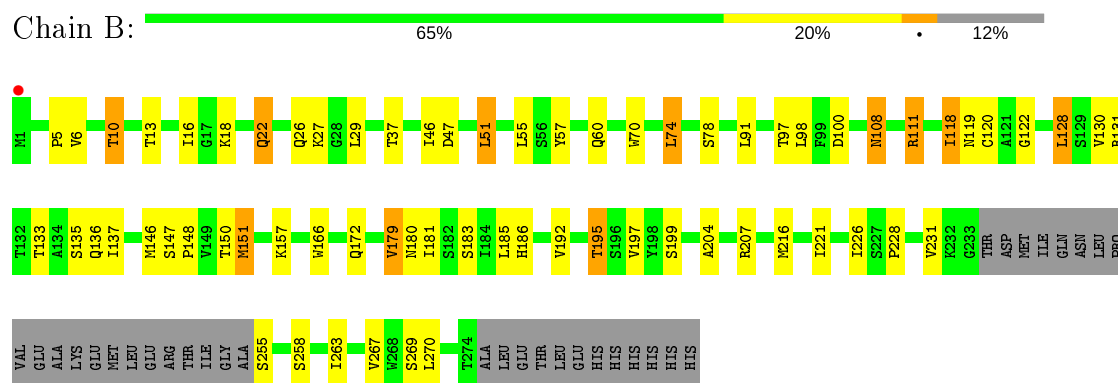
3 Residue-property plots

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.

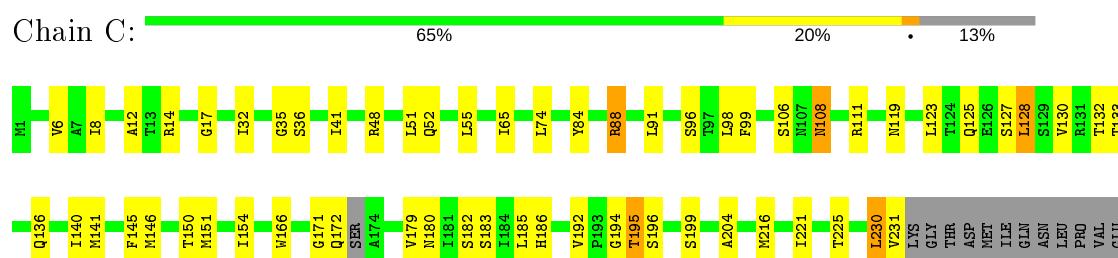
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



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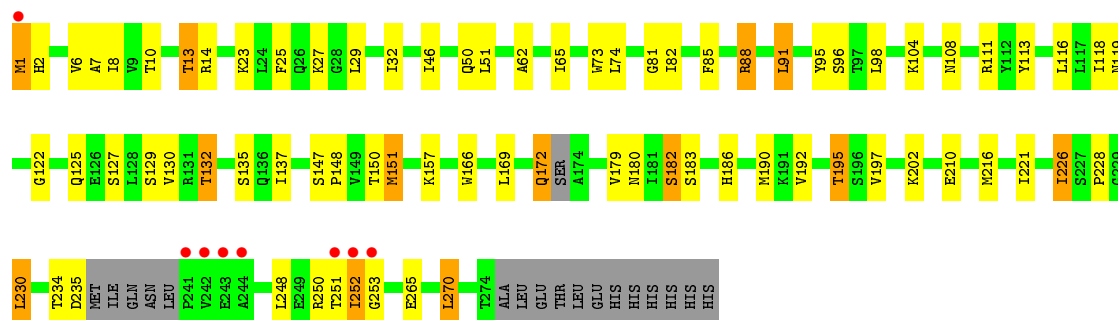


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

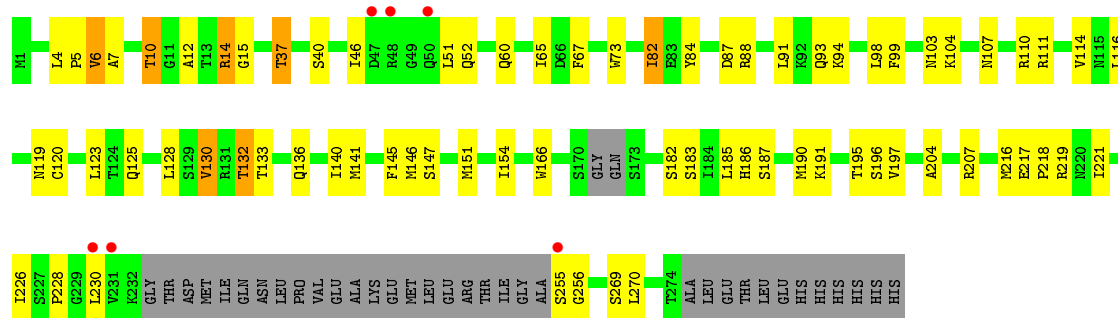




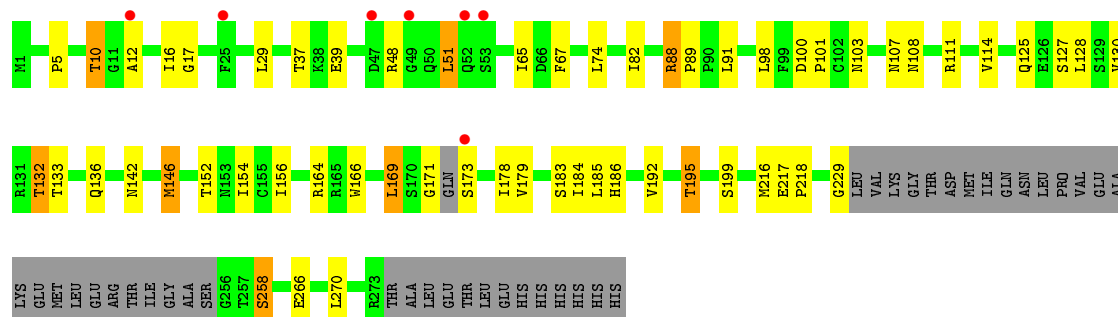
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.83Å 170.83Å 316.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 2.60 41.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.20-2.60) 98.4 (41.08-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.73 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.229 , 0.274 0.225 , 0.266	Depositor DCC
R_{free} test set	3577 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11328	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.62	2/1905 (0.1%)	0.64	0/2598
1	B	0.67	0/1944	0.67	1/2644 (0.0%)
1	C	0.62	0/1918	0.69	0/2609
1	D	0.57	0/2002	0.64	0/2727
1	E	0.61	0/1876	0.73	1/2559 (0.0%)
1	F	0.57	0/1859	0.61	0/2532
All	All	0.61	2/11504 (0.0%)	0.66	2/15669 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	GLU	CD-OE2	7.67	1.34	1.25
1	A	120	CYS	CB-SG	-5.02	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	14	ARG	N-CA-C	5.96	127.10	111.00
1	B	122	GLY	N-CA-C	5.38	126.56	113.10

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	1865	0	1778	61	0
1	B	1903	0	1847	47	0
1	C	1878	0	1815	46	0
1	D	1961	0	1859	63	0
1	E	1837	0	1751	47	0
1	F	1820	0	1744	48	0
2	A	6	0	0	0	0
2	B	15	0	0	0	0
2	C	16	0	0	0	0
2	D	9	0	0	0	0
2	E	9	0	0	2	0
2	F	9	0	0	0	0
All	All	11328	0	10794	300	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 14.

All (300) 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:230:LEU:H	1:A:230:LEU:CD1	1.56	1.18
1:C:171:GLY:HA3	1:C:172:GLN:CB	1.71	1.18
1:D:1:MET:H2	1:D:2:HIS:HA	1.07	1.09
1:A:230:LEU:HD12	1:A:230:LEU:N	1.52	1.08
1:D:1:MET:N	1:D:2:HIS:HA	1.58	1.08
1:D:88:ARG:HG2	1:D:88:ARG:HH11	0.95	1.06
1:A:231:VAL:HG23	1:A:233:GLY:H	1.16	1.05
1:D:1:MET:N	1:D:2:HIS:CA	2.22	1.03
1:D:1:MET:HG2	1:D:1:MET:O	1.61	0.99
1:D:88:ARG:HG2	1:D:88:ARG:NH1	1.73	0.98
1:D:1:MET:H3	1:D:2:HIS:C	1.66	0.96
1:E:185:LEU:HD23	1:E:195:THR:HG21	1.45	0.96
1:A:230:LEU:HD12	1:A:230:LEU:H	0.79	0.95
1:F:12:ALA:CB	1:F:17:GLY:HA3	1.97	0.94
1:E:12:ALA:HB2	1:E:120:CYS:SG	2.08	0.93
1:F:133:THR:H	1:F:136:GLN:HE21	1.17	0.92
1:D:230:LEU:HD12	1:D:230:LEU:N	1.82	0.92
1:C:171:GLY:CA	1:C:172:GLN:CB	2.48	0.91
1:B:10:THR:HG21	1:B:119:ASN:OD1	1.70	0.91
1:D:192:VAL:O	1:D:195:THR:HB	1.69	0.90
1:D:230:LEU:H	1:D:230:LEU:HD12	1.36	0.90
1:D:1:MET:H3	1:D:2:HIS:CA	1.85	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:ALA:HB1	1:F:17:GLY:HA3	1.57	0.86
1:F:74:LEU:HD21	1:F:154:ILE:HD11	1.57	0.86
1:A:231:VAL:HG23	1:A:233:GLY:N	1.91	0.84
1:C:230:LEU:O	1:C:231:VAL:HG23	1.79	0.82
1:A:133:THR:H	1:A:136:GLN:NE2	1.77	0.82
1:D:13:THR:CG2	1:D:14:ARG:HE	1.93	0.80
1:C:111:ARG:HD3	1:C:166:TRP:CZ2	2.17	0.80
1:A:118:ILE:HD13	1:A:179:VAL:HG13	1.63	0.80
1:A:185:LEU:HD23	1:A:195:THR:HG21	1.63	0.80
1:D:230:LEU:H	1:D:230:LEU:CD1	1.95	0.79
1:B:133:THR:H	1:B:136:GLN:NE2	1.80	0.79
1:D:23:LYS:HE3	1:D:265:GLU:OE2	1.82	0.79
1:C:133:THR:H	1:C:136:GLN:HE21	1.28	0.78
1:C:185:LEU:HD23	1:C:195:THR:HG21	1.63	0.78
1:D:98:LEU:HD13	1:D:151:MET:HE1	1.65	0.78
1:B:192:VAL:O	1:B:195:THR:HB	1.83	0.78
1:E:14:ARG:N	1:E:15:GLY:HA2	2.00	0.77
1:A:46:ILE:H	1:A:60:GLN:HE22	1.32	0.77
1:B:133:THR:H	1:B:136:GLN:HE21	1.32	0.77
1:F:266:GLU:O	1:F:270:LEU:HD12	1.84	0.76
1:A:111:ARG:HD3	1:A:166:TRP:CZ2	2.21	0.76
1:F:133:THR:H	1:F:136:GLN:NE2	1.83	0.75
1:E:46:ILE:H	1:E:60:GLN:HE22	1.35	0.74
1:D:65:ILE:HD11	1:D:73:TRP:CE3	2.24	0.73
1:C:133:THR:H	1:C:136:GLN:NE2	1.87	0.72
1:B:46:ILE:H	1:B:60:GLN:HE22	1.36	0.72
1:F:48:ARG:HA	1:F:51:LEU:HB2	1.71	0.71
1:C:127:SER:OG	1:C:132:THR:HG22	1.90	0.71
1:A:195:THR:O	1:A:195:THR:HG22	1.90	0.70
1:F:183:SER:O	1:F:186:HIS:HD2	1.75	0.69
1:E:104:LYS:HE3	2:E:305:HOH:O	1.90	0.69
1:E:195:THR:HG22	1:E:195:THR:O	1.92	0.69
1:F:127:SER:OG	1:F:132:THR:HG22	1.92	0.69
1:A:12:ALA:HB1	1:A:17:GLY:HA3	1.75	0.69
1:C:36:SER:HA	1:C:65:ILE:O	1.92	0.69
1:F:133:THR:N	1:F:136:GLN:HE21	1.90	0.68
1:F:192:VAL:O	1:F:195:THR:HB	1.93	0.68
1:E:111:ARG:HD3	1:E:166:TRP:CZ2	2.29	0.68
1:F:229:GLY:H	1:F:258:SER:HB2	1.59	0.68
1:A:107:ASN:OD1	1:A:107:ASN:C	2.33	0.67
1:B:10:THR:CG2	1:B:119:ASN:OD1	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:O	1:A:132:THR:HG23	1.95	0.66
1:D:234:THR:O	1:D:235:ASP:C	2.30	0.66
1:B:157:LYS:HD2	1:E:130:VAL:HG22	1.78	0.66
1:E:104:LYS:CE	2:E:305:HOH:O	2.42	0.65
1:E:216:MET:HE2	1:E:221:ILE:HG13	1.78	0.65
1:C:48:ARG:O	1:C:52:GLN:HG3	1.96	0.64
1:D:169:LEU:O	1:D:172:GLN:HB3	1.98	0.63
1:F:88:ARG:HB2	1:F:89:PRO:CD	2.28	0.63
1:B:151:MET:HA	1:B:151:MET:CE	2.28	0.63
1:B:111:ARG:HD3	1:B:166:TRP:CE2	2.34	0.63
1:C:183:SER:O	1:C:186:HIS:HD2	1.82	0.63
1:D:13:THR:HG22	1:D:14:ARG:HE	1.62	0.63
1:F:12:ALA:HB1	1:F:17:GLY:CA	2.28	0.63
1:D:88:ARG:CG	1:D:88:ARG:HH11	1.89	0.62
1:E:226:ILE:HG22	1:E:228:PRO:HD3	1.80	0.62
1:A:133:THR:H	1:A:136:GLN:HE21	1.43	0.62
1:A:12:ALA:CB	1:A:17:GLY:HA3	2.29	0.62
1:B:111:ARG:HD3	1:B:166:TRP:CZ2	2.34	0.62
1:A:18:LYS:HG3	1:A:43:ARG:O	1.99	0.62
1:C:128:LEU:O	1:C:132:THR:HG23	1.99	0.61
1:C:185:LEU:HD23	1:C:195:THR:CG2	2.30	0.61
1:F:65:ILE:HD11	1:F:98:LEU:HD21	1.83	0.61
1:A:231:VAL:C	1:A:233:GLY:H	2.05	0.60
1:C:108:ASN:H	1:C:108:ASN:HD22	1.48	0.60
1:D:111:ARG:HD3	1:D:166:TRP:CZ2	2.37	0.60
1:E:65:ILE:HD11	1:E:73:TRP:CE3	2.35	0.59
1:A:6:VAL:HG22	1:A:30:SER:HB2	1.85	0.59
1:D:1:MET:N	1:D:2:HIS:C	2.47	0.59
1:B:46:ILE:HD11	1:B:51:LEU:HD13	1.84	0.59
1:F:111:ARG:HD3	1:F:166:TRP:CZ2	2.38	0.59
1:A:231:VAL:C	1:A:233:GLY:N	2.51	0.59
1:E:107:ASN:OD1	1:E:107:ASN:C	2.41	0.59
1:C:8:ILE:HG12	1:C:32:ILE:HB	1.85	0.58
1:A:182:SER:OG	1:A:183:SER:N	2.36	0.58
1:B:26:GLN:HE21	1:B:27:LYS:NZ	2.01	0.58
1:F:74:LEU:CD2	1:F:154:ILE:HD11	2.31	0.58
1:D:250:ARG:O	1:D:252:ILE:N	2.37	0.58
1:A:127:SER:OG	1:A:132:THR:HG22	2.03	0.58
1:D:118:ILE:HG23	1:D:179:VAL:HG22	1.86	0.57
1:C:65:ILE:HD11	1:C:98:LEU:HD21	1.86	0.57
1:E:216:MET:CE	1:E:221:ILE:HG13	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:THR:HG23	1:F:67:PHE:HE2	1.69	0.57
1:C:230:LEU:O	1:C:231:VAL:CG2	2.52	0.56
1:B:157:LYS:CD	1:E:130:VAL:HG22	2.34	0.56
1:F:171:GLY:O	1:F:173:SER:N	2.38	0.56
1:C:125:GLN:HE21	1:C:132:THR:HG21	1.71	0.56
1:C:192:VAL:O	1:C:195:THR:HB	2.06	0.56
1:F:125:GLN:HE21	1:F:132:THR:HG21	1.71	0.56
1:D:252:ILE:HG23	1:D:253:GLY:N	2.21	0.56
1:D:216:MET:HE2	1:D:221:ILE:HB	1.88	0.55
1:F:185:LEU:HD23	1:F:195:THR:HG21	1.88	0.55
1:F:37:THR:HG22	1:F:39:GLU:H	1.72	0.55
1:A:118:ILE:CD1	1:A:179:VAL:HG13	2.36	0.55
1:B:5:PRO:HG2	1:B:29:LEU:HD22	1.89	0.55
1:E:107:ASN:OD1	1:E:110:ARG:N	2.40	0.55
1:F:133:THR:OG1	1:F:136:GLN:HG3	2.07	0.55
1:C:216:MET:CE	1:C:221:ILE:HD12	2.37	0.55
1:D:183:SER:O	1:D:186:HIS:HD2	1.89	0.54
1:B:204:ALA:HB2	1:E:204:ALA:HB2	1.89	0.54
1:A:157:LYS:HG2	1:C:91:LEU:HD13	1.88	0.54
1:C:195:THR:CG2	1:C:199:SER:OG	2.56	0.54
1:C:216:MET:HE2	1:C:221:ILE:HB	1.88	0.54
1:A:226:ILE:HG22	1:A:228:PRO:HD3	1.90	0.54
1:D:157:LYS:HG2	1:F:91:LEU:HD13	1.89	0.54
1:D:23:LYS:CE	1:D:265:GLU:OE2	2.56	0.54
1:B:183:SER:O	1:B:186:HIS:HD2	1.90	0.54
1:D:65:ILE:HD11	1:D:73:TRP:CD2	2.43	0.54
1:E:93:GLN:HG3	1:E:94:LYS:N	2.23	0.53
1:F:88:ARG:HB2	1:F:89:PRO:HD3	1.91	0.53
1:A:10:THR:O	1:A:120:CYS:HB2	2.09	0.53
1:A:128:LEU:O	1:A:132:THR:CG2	2.56	0.53
1:C:231:VAL:HA	1:C:258:SER:O	2.09	0.53
1:A:234:THR:CG2	1:A:235:ASP:N	2.70	0.53
1:A:93:GLN:HE21	1:A:94:LYS:N	2.06	0.53
1:B:195:THR:HG22	1:B:199:SER:HG	1.73	0.53
1:B:216:MET:CE	1:B:221:ILE:HD12	2.38	0.53
1:B:195:THR:HG22	1:B:199:SER:OG	2.07	0.53
1:F:103:ASN:HD22	1:F:111:ARG:NH2	2.07	0.53
1:D:195:THR:O	1:D:195:THR:CG2	2.57	0.53
1:A:234:THR:HG22	1:A:235:ASP:N	2.22	0.52
1:B:26:GLN:HE21	1:B:27:LYS:HZ3	1.57	0.52
1:E:103:ASN:OD1	1:E:111:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HD11	1:A:98:LEU:HD21	1.92	0.52
1:E:6:VAL:HG22	1:E:114:VAL:HG22	1.91	0.52
1:C:123:LEU:HD23	1:C:140:ILE:HA	1.92	0.51
1:E:46:ILE:HD11	1:E:51:LEU:HD13	1.91	0.51
1:D:127:SER:OG	1:D:132:THR:HG23	2.11	0.51
1:A:195:THR:HG22	1:A:199:SER:OG	2.10	0.51
1:C:35:GLY:HA3	1:C:41:ILE:HG23	1.93	0.51
1:F:111:ARG:HD3	1:F:166:TRP:CH2	2.46	0.51
1:B:130:VAL:HG12	1:B:131:ARG:HG3	1.92	0.51
1:A:153:ASN:OD1	1:D:129:SER:OG	2.29	0.50
1:C:99:PHE:CZ	1:C:154:ILE:HG22	2.46	0.50
1:D:190:MET:CE	1:D:248:LEU:CB	2.89	0.50
1:A:226:ILE:HD11	1:A:270:LEU:HD22	1.93	0.50
1:C:195:THR:CG2	1:C:195:THR:O	2.59	0.50
1:A:142:ASN:HA	1:A:146:MET:HB2	1.93	0.50
1:D:125:GLN:HE21	1:D:132:THR:HG21	1.77	0.50
1:F:195:THR:CG2	1:F:199:SER:OG	2.60	0.50
1:F:5:PRO:HG2	1:F:29:LEU:HD22	1.94	0.50
1:D:62:ALA:HB3	1:D:82:ILE:HG23	1.93	0.50
1:D:127:SER:OG	1:D:132:THR:CG2	2.60	0.49
1:E:125:GLN:HE21	1:E:132:THR:HG21	1.77	0.49
1:A:195:THR:CG2	1:A:195:THR:O	2.57	0.49
1:A:231:VAL:O	1:A:233:GLY:N	2.45	0.49
1:E:141:MET:HB3	1:E:146:MET:HE1	1.94	0.49
1:C:183:SER:O	1:C:186:HIS:CD2	2.65	0.49
1:E:93:GLN:NE2	1:E:104:LYS:HD3	2.27	0.49
1:F:142:ASN:HA	1:F:146:MET:HB2	1.93	0.49
1:F:12:ALA:HB2	1:F:17:GLY:HA3	1.87	0.49
1:A:130:VAL:CG2	1:D:157:LYS:HG3	2.43	0.49
1:A:82:ILE:HD11	1:A:90:PRO:CB	2.43	0.49
1:F:103:ASN:HD22	1:F:111:ARG:HH22	1.61	0.49
1:F:183:SER:O	1:F:186:HIS:CD2	2.62	0.49
1:F:125:GLN:NE2	1:F:132:THR:HG21	2.28	0.48
1:D:250:ARG:O	1:D:251:THR:C	2.51	0.48
1:E:182:SER:OG	1:E:183:SER:N	2.45	0.48
1:C:35:GLY:HA3	1:C:41:ILE:CG2	2.44	0.48
1:D:182:SER:HA	1:D:202:LYS:HD2	1.94	0.48
1:E:185:LEU:HD12	1:E:185:LEU:N	2.28	0.48
1:D:190:MET:HE1	1:D:248:LEU:CB	2.44	0.48
1:F:195:THR:HG22	1:F:199:SER:OG	2.13	0.48
1:B:195:THR:CG2	1:B:199:SER:OG	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:THR:O	1:F:195:THR:CG2	2.62	0.47
1:E:133:THR:OG1	1:E:136:GLN:HG3	2.14	0.47
1:F:100:ASP:N	1:F:101:PRO:CD	2.77	0.47
1:F:88:ARG:CB	1:F:89:PRO:CD	2.92	0.47
1:A:231:VAL:HG23	1:A:233:GLY:CA	2.44	0.47
1:B:207:ARG:NH2	1:E:190:MET:O	2.48	0.47
1:B:18:LYS:O	1:B:22:GLN:HB2	2.14	0.47
1:B:118:ILE:HD12	1:B:267:VAL:HG11	1.96	0.47
1:E:46:ILE:HG12	1:E:60:GLN:NE2	2.29	0.47
1:B:216:MET:HE3	1:B:221:ILE:HD12	1.96	0.47
1:C:141:MET:HB3	1:C:146:MET:CE	2.45	0.47
1:A:182:SER:O	1:A:228:PRO:HD2	2.15	0.47
1:F:166:TRP:HB2	1:F:169:LEU:HD22	1.96	0.47
1:E:133:THR:H	1:E:136:GLN:HE21	1.63	0.46
1:D:183:SER:O	1:D:186:HIS:CD2	2.69	0.46
1:D:62:ALA:HB3	1:D:82:ILE:CG2	2.45	0.46
1:C:141:MET:HB3	1:C:146:MET:HE2	1.98	0.46
1:A:160:MET:HG2	1:C:88:ARG:HH21	1.81	0.46
1:B:195:THR:CG2	1:B:199:SER:HG	2.28	0.46
1:A:118:ILE:HD13	1:A:179:VAL:CG1	2.39	0.46
1:E:99:PHE:CZ	1:E:154:ILE:HG22	2.51	0.46
1:B:185:LEU:HD23	1:B:195:THR:HG21	1.97	0.46
1:B:226:ILE:HG22	1:B:228:PRO:HD3	1.99	0.46
1:A:130:VAL:HG22	1:D:157:LYS:HG3	1.96	0.46
1:E:37:THR:HG23	1:E:40:SER:HB2	1.99	0.45
1:B:120:CYS:HA	1:B:181:ILE:HD12	1.98	0.45
1:D:182:SER:O	1:D:228:PRO:HD2	2.16	0.45
1:E:98:LEU:HD13	1:E:151:MET:HE1	1.99	0.45
1:A:230:LEU:HD13	1:A:256:GLY:O	2.17	0.45
1:D:137:ILE:HG12	1:D:197:VAL:HG21	1.99	0.45
1:D:166:TRP:HZ3	1:F:108:ASN:HD22	1.65	0.45
1:B:195:THR:O	1:B:195:THR:CG2	2.65	0.44
1:B:46:ILE:HG12	1:B:60:GLN:NE2	2.32	0.44
1:C:185:LEU:CD2	1:C:195:THR:HG21	2.40	0.44
1:E:98:LEU:HD13	1:E:151:MET:CE	2.46	0.44
1:E:217:GLU:N	1:E:218:PRO:HD2	2.33	0.44
1:D:166:TRP:O	1:D:169:LEU:HB2	2.18	0.44
1:F:152:THR:HG23	1:F:178:ILE:HG21	1.99	0.44
1:B:119:ASN:HB2	1:B:180:ASN:OD1	2.18	0.44
1:D:74:LEU:HD11	1:D:150:THR:HG21	2.00	0.44
1:B:108:ASN:HD22	1:B:108:ASN:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:PHE:CE2	1:C:154:ILE:HG22	2.53	0.44
1:C:230:LEU:O	1:C:231:VAL:CB	2.65	0.44
1:B:26:GLN:NE2	1:B:27:LYS:NZ	2.65	0.44
1:C:119:ASN:HB2	1:C:180:ASN:OD1	2.17	0.44
1:A:184:ILE:HG23	1:A:185:LEU:HD12	2.00	0.44
1:A:231:VAL:O	1:A:232:LYS:C	2.56	0.44
1:E:216:MET:HE1	1:E:219:ARG:HG3	1.99	0.44
1:A:183:SER:O	1:A:186:HIS:HD2	2.01	0.44
1:D:252:ILE:CG2	1:D:253:GLY:N	2.78	0.44
1:C:99:PHE:HE2	1:C:154:ILE:CG2	2.31	0.43
1:E:145:PHE:CE1	1:E:204:ALA:HB1	2.53	0.43
1:E:10:THR:HG21	1:E:119:ASN:OD1	2.18	0.43
1:A:147:SER:HB2	1:A:148:PRO:HD3	1.99	0.43
1:C:51:LEU:HD21	1:C:84:TYR:HB3	2.01	0.43
1:D:85:PHE:HE2	1:D:91:LEU:HB2	1.82	0.43
1:F:217:GLU:N	1:F:218:PRO:HD2	2.34	0.43
1:A:192:VAL:O	1:A:195:THR:HB	2.18	0.43
1:B:108:ASN:N	1:B:108:ASN:HD22	2.17	0.43
1:B:74:LEU:HD11	1:B:150:THR:HG21	2.00	0.43
1:A:46:ILE:N	1:A:60:GLN:HE22	2.10	0.43
1:C:195:THR:HG23	1:C:195:THR:O	2.18	0.43
1:F:127:SER:OG	1:F:132:THR:CG2	2.64	0.43
1:A:156:ILE:HG13	1:A:178:ILE:CD1	2.49	0.43
1:A:182:SER:HA	1:A:202:LYS:HD2	2.01	0.43
1:B:147:SER:HB2	1:B:148:PRO:HD3	2.01	0.43
1:C:125:GLN:HG2	1:C:194:GLY:O	2.19	0.43
1:D:147:SER:HB2	1:D:148:PRO:HD3	2.01	0.42
1:A:216:MET:CE	1:A:221:ILE:HB	2.50	0.42
1:B:118:ILE:HG23	1:B:179:VAL:HG22	2.01	0.42
1:D:8:ILE:HG12	1:D:32:ILE:HB	2.00	0.42
1:E:255:SER:OG	1:E:256:GLY:N	2.52	0.42
1:E:4:LEU:HA	1:E:5:PRO:HD3	1.92	0.42
1:B:137:ILE:HG12	1:B:197:VAL:HG21	2.02	0.42
1:D:166:TRP:CZ3	1:F:107:ASN:HB2	2.55	0.42
1:A:89:PRO:HA	1:A:90:PRO:HD3	1.88	0.42
1:F:156:ILE:HG23	1:F:216:MET:HE1	2.02	0.42
1:B:70:TRP:CZ3	1:B:146:MET:HG2	2.54	0.42
1:D:81:GLY:HA3	1:D:95:TYR:HE2	1.84	0.42
1:F:12:ALA:CB	1:F:17:GLY:CA	2.83	0.42
1:C:145:PHE:CE1	1:C:204:ALA:HB1	2.55	0.42
1:C:74:LEU:HD11	1:C:150:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LYS:NZ	1:D:27:LYS:HE3	2.33	0.42
1:E:82:ILE:HD11	1:E:84:TYR:CZ	2.54	0.42
1:B:57:TYR:C	1:B:57:TYR:CD2	2.94	0.42
1:D:226:ILE:HD11	1:D:270:LEU:HD22	2.02	0.42
1:B:128:LEU:HD23	1:B:131:ARG:NH1	2.35	0.41
1:D:119:ASN:HB2	1:D:180:ASN:OD1	2.20	0.41
1:E:67:PHE:CD1	1:E:147:SER:HB3	2.56	0.41
1:A:74:LEU:HD11	1:A:150:THR:HG21	2.03	0.41
1:B:97:THR:H	1:B:100:ASP:HB2	1.85	0.41
1:D:13:THR:HG21	1:D:122:GLY:O	2.20	0.41
1:E:125:GLN:NE2	1:E:132:THR:HG21	2.35	0.41
1:D:250:ARG:C	1:D:252:ILE:N	2.73	0.41
1:D:6:VAL:HG13	1:D:113:TYR:O	2.21	0.41
1:D:25:PHE:HB3	1:D:50:GLN:NE2	2.35	0.41
1:A:65:ILE:HD11	1:A:98:LEU:CD2	2.50	0.41
1:C:12:ALA:HB1	1:C:17:GLY:HA3	2.02	0.41
1:F:185:LEU:HD23	1:F:195:THR:CG2	2.51	0.41
1:B:16:ILE:HD11	1:B:231:VAL:HG21	2.02	0.41
1:E:7:ALA:HA	1:E:116:LEU:O	2.21	0.41
1:E:123:LEU:HD23	1:E:140:ILE:HA	2.03	0.41
1:E:186:HIS:CD2	1:E:187:SER:HB3	2.55	0.41
1:B:18:LYS:NZ	1:B:47:ASP:OD1	2.54	0.41
1:A:125:GLN:HE21	1:A:132:THR:HG21	1.86	0.41
1:A:230:LEU:N	1:A:230:LEU:CD1	2.30	0.40
1:D:7:ALA:HA	1:D:116:LEU:O	2.21	0.40
1:B:263:ILE:O	1:B:267:VAL:HG23	2.22	0.40
1:C:99:PHE:CE2	1:C:154:ILE:CG2	3.05	0.40
1:A:230:LEU:CD1	1:A:256:GLY:O	2.70	0.40
1:E:87:ASP:N	1:E:87:ASP:OD1	2.52	0.40
1:F:169:LEU:HA	1:F:169:LEU:HD12	1.67	0.40
1:A:93:GLN:HE21	1:A:94:LYS:H	1.68	0.40
1:C:230:LEU:C	1:C:231:VAL:HG23	2.41	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	250/286 (87%)	245 (98%)	5 (2%)	0	100	100
1	B	249/286 (87%)	242 (97%)	7 (3%)	0	100	100
1	C	244/286 (85%)	240 (98%)	4 (2%)	0	100	100
1	D	262/286 (92%)	253 (97%)	9 (3%)	0	100	100
1	E	244/286 (85%)	239 (98%)	5 (2%)	0	100	100
1	F	240/286 (84%)	230 (96%)	10 (4%)	0	100	100
All	All	1489/1716 (87%)	1449 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	187/250 (75%)	173 (92%)	14 (8%)	13	27
1	B	199/250 (80%)	175 (88%)	24 (12%)	5	9
1	C	194/250 (78%)	176 (91%)	18 (9%)	9	17
1	D	194/250 (78%)	171 (88%)	23 (12%)	5	9
1	E	185/250 (74%)	168 (91%)	17 (9%)	9	17
1	F	185/250 (74%)	169 (91%)	16 (9%)	10	20
All	All	1144/1500 (76%)	1032 (90%)	112 (10%)	8	15

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	61	CYS
1	A	82	ILE

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Mol	Chain	Res	Type
1	A	91	LEU
1	A	93	GLN
1	A	108	ASN
1	A	128	LEU
1	A	130	VAL
1	A	132	THR
1	A	154	ILE
1	A	179	VAL
1	A	222	ARG
1	A	230	LEU
1	A	257	THR
1	B	6	VAL
1	B	10	THR
1	B	13	THR
1	B	22	GLN
1	B	37	THR
1	B	51	LEU
1	B	55	LEU
1	B	74	LEU
1	B	78	SER
1	B	91	LEU
1	B	98	LEU
1	B	108	ASN
1	B	111	ARG
1	B	118	ILE
1	B	128	LEU
1	B	135	SER
1	B	151	MET
1	B	172	GLN
1	B	179	VAL
1	B	195	THR
1	B	255	SER
1	B	258	SER
1	B	269	SER
1	B	270	LEU
1	C	6	VAL
1	C	14	ARG
1	C	55	LEU
1	C	88	ARG
1	C	96	SER
1	C	106	SER
1	C	108	ASN

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Mol	Chain	Res	Type
1	C	128	LEU
1	C	130	VAL
1	C	151	MET
1	C	179	VAL
1	C	182	SER
1	C	195	THR
1	C	196	SER
1	C	225	THR
1	C	230	LEU
1	C	255	SER
1	C	270	LEU
1	D	1	MET
1	D	10	THR
1	D	13	THR
1	D	29	LEU
1	D	46	ILE
1	D	51	LEU
1	D	88	ARG
1	D	91	LEU
1	D	96	SER
1	D	104	LYS
1	D	108	ASN
1	D	130	VAL
1	D	132	THR
1	D	135	SER
1	D	151	MET
1	D	172	GLN
1	D	182	SER
1	D	195	THR
1	D	210	GLU
1	D	226	ILE
1	D	230	LEU
1	D	252	ILE
1	D	270	LEU
1	E	6	VAL
1	E	10	THR
1	E	37	THR
1	E	52	GLN
1	E	82	ILE
1	E	88	ARG
1	E	91	LEU
1	E	128	LEU

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Mol	Chain	Res	Type
1	E	130	VAL
1	E	132	THR
1	E	191	LYS
1	E	196	SER
1	E	197	VAL
1	E	207	ARG
1	E	230	LEU
1	E	269	SER
1	E	270	LEU
1	F	10	THR
1	F	16	ILE
1	F	51	LEU
1	F	82	ILE
1	F	88	ARG
1	F	114	VAL
1	F	128	LEU
1	F	130	VAL
1	F	132	THR
1	F	146	MET
1	F	164	ARG
1	F	169	LEU
1	F	179	VAL
1	F	184	ILE
1	F	195	THR
1	F	258	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	93	GLN
1	A	108	ASN
1	A	115	ASN
1	A	136	GLN
1	A	186	HIS
1	B	26	GLN
1	B	60	GLN
1	B	93	GLN
1	B	108	ASN
1	B	115	ASN
1	B	136	GLN
1	B	153	ASN

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Mol	Chain	Res	Type
1	B	186	HIS
1	C	108	ASN
1	C	136	GLN
1	C	153	ASN
1	C	186	HIS
1	D	2	HIS
1	D	153	ASN
1	D	186	HIS
1	E	60	GLN
1	E	115	ASN
1	E	136	GLN
1	F	103	ASN
1	F	115	ASN
1	F	136	GLN
1	F	153	ASN
1	F	186	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	254/286 (88%)	-0.18	3 (1%) 79 76	28, 45, 68, 83	0
1	B	253/286 (88%)	-0.35	1 (0%) 92 91	21, 39, 54, 63	0
1	C	250/286 (87%)	-0.42	0 100 100	20, 37, 54, 60	0
1	D	268/286 (93%)	-0.21	8 (2%) 50 43	20, 44, 66, 90	0
1	E	250/286 (87%)	-0.15	6 (2%) 59 53	23, 45, 66, 69	0
1	F	246/286 (86%)	-0.15	7 (2%) 53 46	32, 45, 71, 78	0
All	All	1521/1716 (88%)	-0.24	25 (1%) 72 68	20, 42, 64, 90	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	255	SER	4.0
1	D	242	VAL	3.5
1	E	230	LEU	3.5
1	D	241	PRO	3.5
1	F	53	SER	3.3
1	A	47	ASP	3.2
1	A	46	ILE	3.0
1	F	47	ASP	2.8
1	E	231	VAL	2.7
1	D	244	ALA	2.7
1	D	243	GLU	2.7
1	E	47	ASP	2.7
1	F	25	PHE	2.6
1	D	253	GLY	2.5
1	E	50	GLN	2.5
1	F	52	GLN	2.5
1	F	173	SER	2.5
1	F	49	GLY	2.4
1	D	1	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	12	ALA	2.2
1	A	57	TYR	2.2
1	D	251	THR	2.2
1	B	1	MET	2.1
1	E	48	ARG	2.1
1	D	252	ILE	2.1

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.