



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:10 pm BST

PDB ID : 1OQB
Title : The Crystal Structure of the one-iron form of the di-iron center in Stearoyl
Acyl Carrier Protein Desaturase from Ricinus Communis (Castor Bean).
Authors : Moche, M.; Shanklin, J.; Ghoshal, A.K.; Lindqvist, Y.
Deposited on : 2003-03-07
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 ⓘ 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

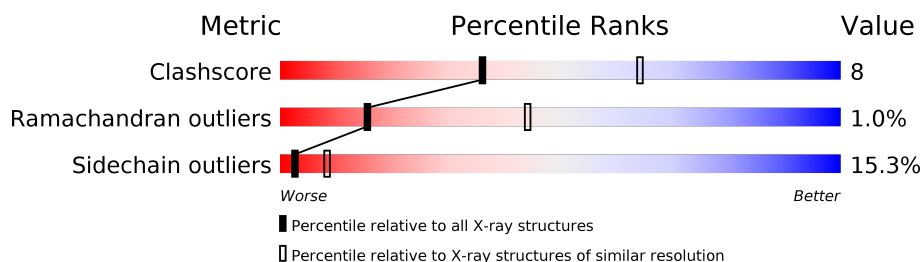
1 Overall quality at a glance

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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	363	66% 25% 5% 5%
1	B	363	65% 25% 5% 5%
1	C	363	66% 25% 5% 5%
1	D	363	67% 24% 5% 5%
1	E	363	67% 25% 5% 5%
1	F	363	68% 23% 5% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16847 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 Acyl-[acyl-carrier protein] desaturase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			
1	B	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			
1	C	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			
1	D	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			
1	E	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			
1	F	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

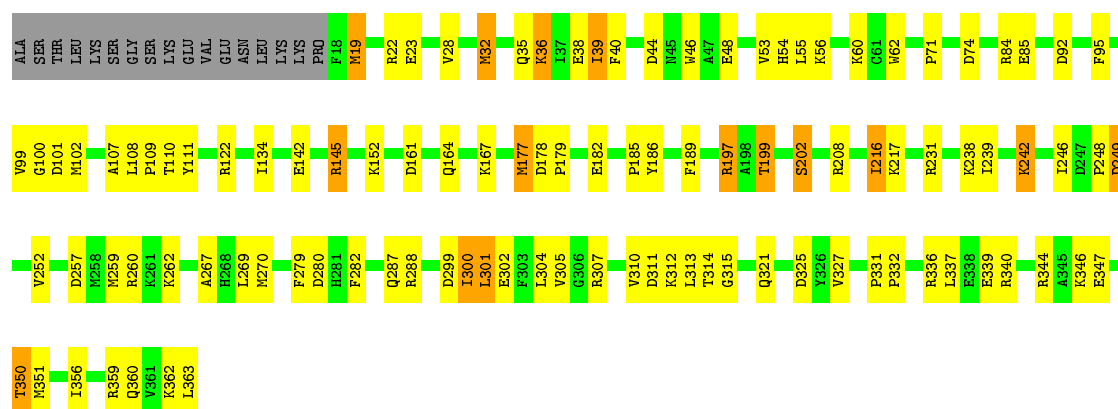
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	1	Total 1	O 1	0	0
3	C	1	Total 1	O 1	0	0
3	D	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0

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. 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. 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.

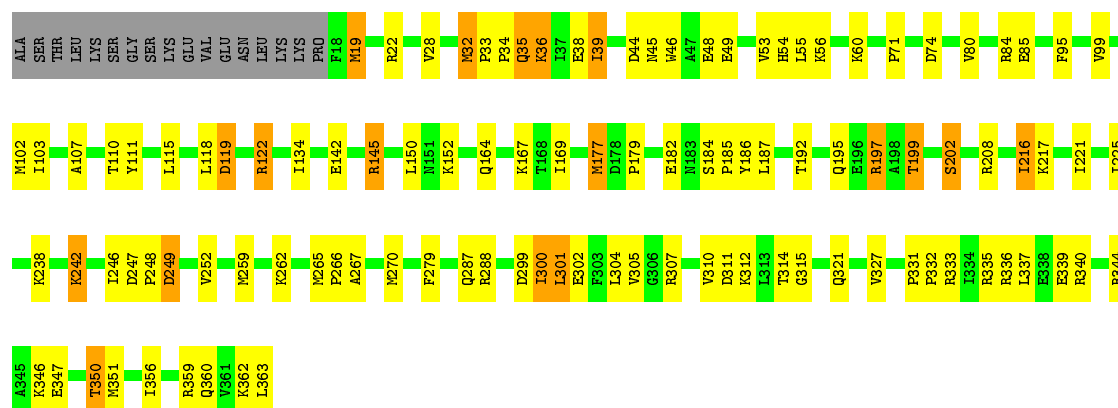
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain A: 



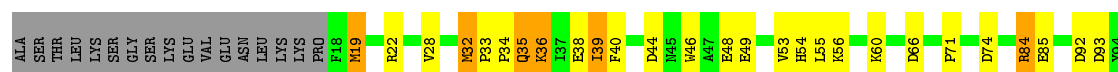
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

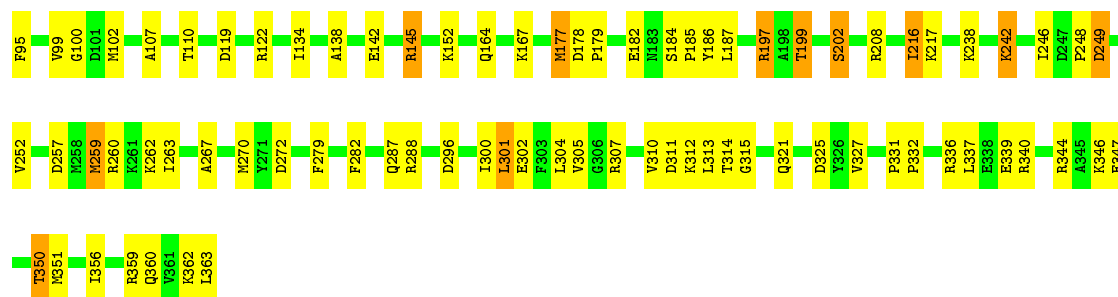
Chain B: 



- Molecule 1: Acyl-[acyl-carrier protein] desaturase

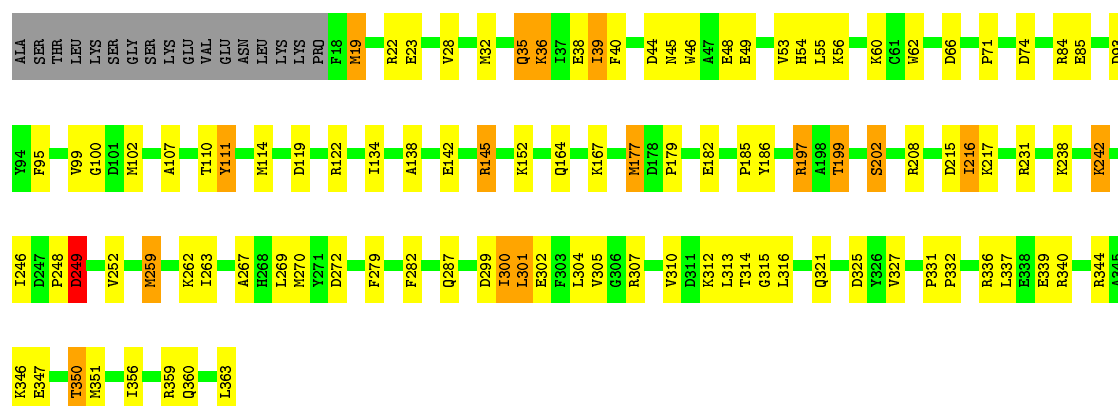
Chain C: 





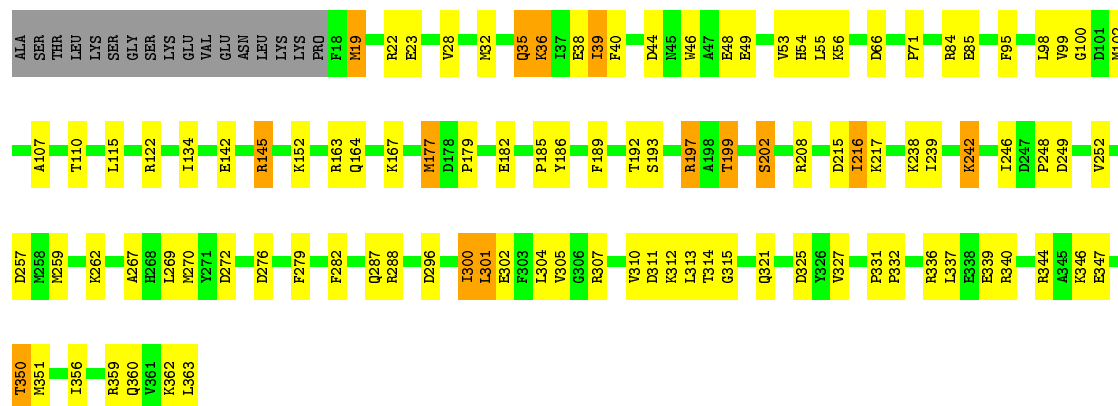
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain D: 67% 24% 5%



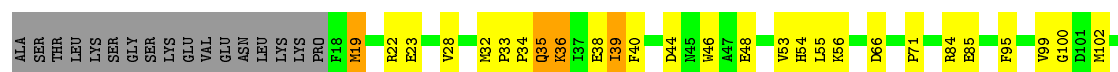
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

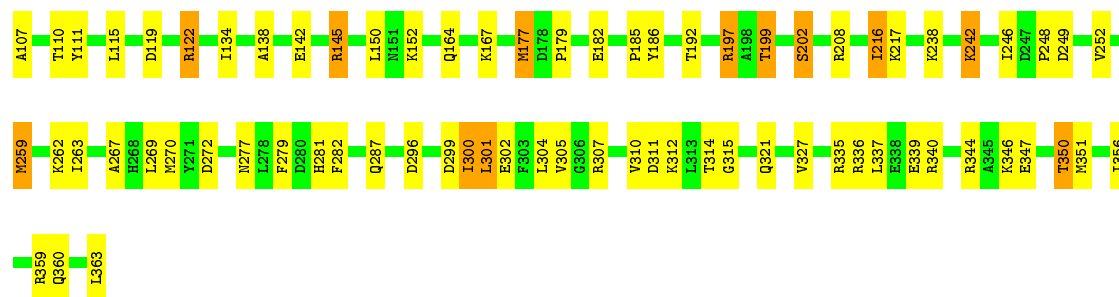
Chain E: 67% 25% 5%



• Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain F: 68% 23% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.91Å 145.79Å 192.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	79.3 (20.00-2.80) 79.3 (19.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.224 , 0.248 (Not available) , (Not available)	Depositor DCC
R_{free} test set	935 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	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	0.88	EDS
Total number of atoms	16847	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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	0.59	0/2874	0.80	12/3892 (0.3%)
1	B	0.63	0/2874	0.80	5/3892 (0.1%)
1	C	0.59	0/2874	0.81	13/3892 (0.3%)
1	D	0.62	0/2874	0.81	10/3892 (0.3%)
1	E	0.57	0/2874	0.79	9/3892 (0.2%)
1	F	0.56	0/2874	0.78	5/3892 (0.1%)
All	All	0.59	0/17244	0.80	54/23352 (0.2%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	44	ASP	CB-CG-OD2	6.62	124.25	118.30
1	A	44	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	74	ASP	CB-CG-OD2	6.45	124.10	118.30
1	D	272	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	74	ASP	CB-CG-OD2	6.14	123.83	118.30
1	F	272	ASP	CB-CG-OD2	6.13	123.81	118.30
1	C	178	ASP	CB-CG-OD2	6.09	123.78	118.30
1	F	296	ASP	CB-CG-OD2	6.02	123.71	118.30
1	E	66	ASP	CB-CG-OD2	5.97	123.67	118.30
1	E	215	ASP	CB-CG-OD2	5.88	123.59	118.30
1	E	44	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	161	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	119	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	74	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	249	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	178	ASP	CB-CG-OD2	5.62	123.36	118.30
1	F	44	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	296	ASP	CB-CG-OD2	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	272	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	311	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	92	ASP	CB-CG-OD2	5.48	123.23	118.30
1	F	66	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	119	ASP	CB-CG-OD2	5.45	123.21	118.30
1	D	299	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	66	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	296	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	93	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	119	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	325	ASP	CB-CG-OD2	5.34	123.10	118.30
1	C	44	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	311	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	44	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	249	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	101	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	74	ASP	CB-CG-OD2	5.25	123.02	118.30
1	E	311	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	84	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	280	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	325	ASP	CB-CG-OD2	5.23	123.00	118.30
1	C	325	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	311	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	247	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	272	ASP	CB-CG-OD2	5.18	122.96	118.30
1	F	311	ASP	CB-CG-OD2	5.16	122.95	118.30
1	D	215	ASP	CB-CG-OD2	5.16	122.94	118.30
1	E	325	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	92	ASP	CB-CG-OD2	5.15	122.94	118.30
1	C	257	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	249	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	257	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	299	ASP	CB-CG-OD2	5.09	122.88	118.30
1	E	257	ASP	CB-CG-OD2	5.07	122.86	118.30
1	E	276	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	66	ASP	CB-CG-OD2	5.02	122.82	118.30

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	2806	0	2748	45	0
1	B	2806	0	2748	50	1
1	C	2806	0	2748	43	0
1	D	2806	0	2748	43	1
1	E	2806	0	2748	44	0
1	F	2806	0	2748	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
All	All	16847	0	16488	263	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 8.

All (263) 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:32:MET:HE1	1:F:185:PRO:HD2	1.56	0.88
1:D:32:MET:HE1	1:D:185:PRO:HD2	1.57	0.85
1:C:270:MET:HE1	1:C:279:PHE:HA	1.60	0.83
1:E:32:MET:HE1	1:E:185:PRO:HD2	1.62	0.82
1:A:32:MET:HE1	1:A:185:PRO:HD2	1.63	0.80
1:A:145:ARG:HG3	1:A:145:ARG:HH11	1.48	0.79
1:A:84:ARG:NH2	1:B:71:PRO:O	2.14	0.79
1:A:270:MET:HE1	1:A:279:PHE:HA	1.63	0.78
1:C:145:ARG:HG3	1:C:145:ARG:HH11	1.49	0.78
1:C:71:PRO:O	1:D:84:ARG:NH2	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:MET:HE1	1:E:279:PHE:HA	1.66	0.77
1:C:84:ARG:NH2	1:D:71:PRO:O	2.17	0.77
1:C:32:MET:HE1	1:C:185:PRO:HD2	1.69	0.75
1:E:216:ILE:HD12	1:E:216:ILE:H	1.54	0.73
1:E:84:ARG:NH2	1:F:71:PRO:O	2.20	0.73
1:A:71:PRO:O	1:B:84:ARG:NH2	2.21	0.73
1:F:32:MET:CE	1:F:185:PRO:HD2	2.19	0.73
1:A:216:ILE:HD12	1:A:216:ILE:H	1.52	0.72
1:E:145:ARG:HG3	1:E:145:ARG:HH11	1.55	0.72
1:B:270:MET:HE2	1:B:279:PHE:HA	1.72	0.71
1:E:270:MET:CE	1:E:279:PHE:HA	2.19	0.71
1:E:71:PRO:O	1:F:84:ARG:NH2	2.23	0.71
1:B:32:MET:HE1	1:B:185:PRO:HD2	1.72	0.70
1:C:216:ILE:H	1:C:216:ILE:HD12	1.56	0.70
1:D:145:ARG:HG3	1:D:145:ARG:HH11	1.55	0.69
1:C:270:MET:CE	1:C:279:PHE:HA	2.21	0.69
1:B:216:ILE:H	1:B:216:ILE:HD12	1.58	0.69
1:C:36:LYS:O	1:C:39:ILE:HG23	1.93	0.69
1:F:145:ARG:HG3	1:F:145:ARG:HH11	1.57	0.68
1:F:216:ILE:HD12	1:F:216:ILE:H	1.58	0.68
1:F:270:MET:HE1	1:F:279:PHE:HA	1.75	0.68
1:D:270:MET:HE1	1:D:279:PHE:HA	1.76	0.68
1:B:270:MET:CE	1:B:279:PHE:HA	2.25	0.67
1:B:32:MET:CE	1:B:185:PRO:HD2	2.25	0.67
1:D:32:MET:CE	1:D:185:PRO:HD2	2.25	0.67
1:D:270:MET:CE	1:D:279:PHE:HA	2.26	0.66
1:A:36:LYS:O	1:A:39:ILE:HG23	1.95	0.66
1:A:270:MET:CE	1:A:279:PHE:HA	2.25	0.65
1:D:36:LYS:O	1:D:39:ILE:HG23	1.96	0.65
1:B:145:ARG:HH11	1:B:145:ARG:HG3	1.60	0.65
1:F:270:MET:CE	1:F:279:PHE:HA	2.27	0.64
1:E:32:MET:CE	1:E:185:PRO:HD2	2.27	0.64
1:E:36:LYS:O	1:E:39:ILE:HG23	1.97	0.64
1:B:36:LYS:O	1:B:39:ILE:HG23	1.97	0.63
1:C:145:ARG:NH1	1:C:145:ARG:HG3	2.14	0.63
1:A:95:PHE:O	1:A:99:VAL:HG23	1.98	0.63
1:E:248:PRO:O	1:E:252:VAL:HG23	1.98	0.63
1:A:32:MET:CE	1:A:185:PRO:HD2	2.27	0.63
1:A:145:ARG:NH1	1:A:145:ARG:HG3	2.14	0.63
1:F:36:LYS:O	1:F:39:ILE:HG23	1.99	0.63
1:D:216:ILE:HD12	1:D:216:ILE:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PRO:O	1:A:252:VAL:HG23	2.01	0.61
1:C:32:MET:CE	1:C:185:PRO:HD2	2.29	0.60
1:F:46:TRP:CE2	1:F:242:LYS:HG3	2.37	0.60
1:F:248:PRO:O	1:F:252:VAL:HG23	2.01	0.60
1:A:199:THR:HA	1:A:202:SER:HB2	1.83	0.60
1:B:248:PRO:O	1:B:252:VAL:HG23	2.01	0.60
1:B:164:GLN:OE1	1:B:167:LYS:HE2	2.02	0.60
1:B:46:TRP:CE2	1:B:242:LYS:HG3	2.36	0.60
1:C:248:PRO:O	1:C:252:VAL:HG23	2.03	0.58
1:D:248:PRO:O	1:D:252:VAL:HG23	2.03	0.58
1:B:199:THR:HA	1:B:202:SER:HB2	1.86	0.58
1:B:19:MET:CE	1:B:22:ARG:HH21	2.17	0.57
1:C:199:THR:HA	1:C:202:SER:HB2	1.87	0.57
1:E:199:THR:HA	1:E:202:SER:HB2	1.85	0.57
1:F:95:PHE:O	1:F:99:VAL:HG23	2.04	0.56
1:D:199:THR:HA	1:D:202:SER:HB2	1.86	0.56
1:D:19:MET:CE	1:D:22:ARG:HH21	2.17	0.56
1:C:95:PHE:O	1:C:99:VAL:HG23	2.05	0.56
1:C:164:GLN:OE1	1:C:167:LYS:HE2	2.06	0.56
1:A:164:GLN:OE1	1:A:167:LYS:HE2	2.06	0.56
1:B:95:PHE:O	1:B:99:VAL:HG23	2.06	0.56
1:F:199:THR:HA	1:F:202:SER:HB2	1.86	0.56
1:C:46:TRP:CE2	1:C:242:LYS:HG3	2.41	0.56
1:A:197:ARG:HG2	1:A:300:ILE:HD13	1.88	0.55
1:D:301:LEU:O	1:D:305:VAL:HG23	2.06	0.55
1:A:46:TRP:CE2	1:A:242:LYS:HG3	2.42	0.55
1:D:145:ARG:NH1	1:D:145:ARG:HG3	2.21	0.55
1:B:301:LEU:O	1:B:305:VAL:HG23	2.07	0.54
1:C:301:LEU:O	1:C:305:VAL:HG23	2.07	0.54
1:E:95:PHE:O	1:E:99:VAL:HG23	2.08	0.54
1:D:53:VAL:C	1:D:55:LEU:H	2.11	0.54
1:E:356:ILE:HD12	1:E:359:ARG:HB2	1.90	0.53
1:B:53:VAL:C	1:B:55:LEU:H	2.11	0.53
1:E:164:GLN:OE1	1:E:167:LYS:HE2	2.08	0.53
1:C:53:VAL:C	1:C:55:LEU:H	2.13	0.52
1:D:46:TRP:CE2	1:D:242:LYS:HG3	2.44	0.52
1:F:164:GLN:OE1	1:F:167:LYS:HE2	2.08	0.52
1:E:46:TRP:CE2	1:E:242:LYS:HG3	2.45	0.52
1:D:95:PHE:O	1:D:99:VAL:HG23	2.09	0.52
1:C:100:GLY:HA3	1:C:282:PHE:CE1	2.45	0.52
1:A:19:MET:CE	1:A:22:ARG:HH21	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HB	1:A:182:GLU:HG2	1.92	0.52
1:A:301:LEU:O	1:A:305:VAL:HG23	2.09	0.52
1:B:145:ARG:HG3	1:B:145:ARG:NH1	2.25	0.51
1:A:350:THR:HG23	1:A:360:GLN:HB3	1.91	0.51
1:C:19:MET:CE	1:C:22:ARG:HH21	2.23	0.51
1:F:19:MET:CE	1:F:22:ARG:HH21	2.22	0.51
1:F:53:VAL:C	1:F:55:LEU:H	2.13	0.51
1:E:145:ARG:NH1	1:E:145:ARG:HG3	2.21	0.51
1:E:53:VAL:C	1:E:55:LEU:H	2.14	0.51
1:F:267:ALA:O	1:F:270:MET:HB2	2.10	0.51
1:F:46:TRP:CD1	1:F:242:LYS:HE2	2.46	0.51
1:E:305:VAL:HG13	1:E:310:VAL:HB	1.93	0.50
1:F:100:GLY:HA3	1:F:282:PHE:CE1	2.47	0.50
1:D:356:ILE:HD12	1:D:359:ARG:HB2	1.93	0.50
1:A:19:MET:HE1	1:A:22:ARG:HH21	1.76	0.50
1:A:100:GLY:HA3	1:A:282:PHE:CE1	2.47	0.50
1:E:267:ALA:O	1:E:270:MET:HB2	2.12	0.50
1:F:305:VAL:HG13	1:F:310:VAL:HB	1.94	0.50
1:B:32:MET:HE2	1:B:186:TYR:CE1	2.47	0.49
1:D:331:PRO:HB2	1:D:332:PRO:HD3	1.95	0.49
1:A:53:VAL:C	1:A:55:LEU:H	2.15	0.49
1:C:305:VAL:HG13	1:C:310:VAL:HB	1.95	0.49
1:B:356:ILE:HD12	1:B:359:ARG:HB2	1.94	0.48
1:D:197:ARG:HG2	1:D:300:ILE:HD13	1.95	0.48
1:E:100:GLY:HA3	1:E:282:PHE:CE1	2.49	0.48
1:B:197:ARG:HG2	1:B:300:ILE:HD13	1.94	0.48
1:C:177:MET:HG2	1:C:179:PRO:HD3	1.95	0.48
1:C:28:VAL:HB	1:C:182:GLU:HG2	1.94	0.48
1:A:356:ILE:HD12	1:A:359:ARG:HB2	1.94	0.48
1:A:32:MET:HE2	1:A:186:TYR:CE1	2.49	0.48
1:B:305:VAL:HG13	1:B:310:VAL:HB	1.95	0.48
1:B:46:TRP:CD1	1:B:242:LYS:HE2	2.48	0.48
1:C:35:GLN:H	1:C:35:GLN:HG3	1.36	0.48
1:C:197:ARG:HG2	1:C:300:ILE:HD13	1.95	0.48
1:A:267:ALA:O	1:A:270:MET:HB2	2.14	0.48
1:C:39:ILE:HD13	1:C:246:ILE:HG21	1.94	0.48
1:F:145:ARG:HG3	1:F:145:ARG:NH1	2.27	0.48
1:E:301:LEU:HA	1:E:304:LEU:HB2	1.96	0.47
1:F:28:VAL:HB	1:F:182:GLU:HG2	1.95	0.47
1:F:356:ILE:HD12	1:F:359:ARG:HB2	1.96	0.47
1:A:40:PHE:CZ	1:A:185:PRO:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:TRP:CD1	1:C:242:LYS:HE2	2.48	0.47
1:E:197:ARG:HG2	1:E:300:ILE:HD13	1.96	0.47
1:B:28:VAL:HB	1:B:182:GLU:HG2	1.97	0.47
1:E:216:ILE:H	1:E:216:ILE:CD1	2.19	0.47
1:E:19:MET:CE	1:E:22:ARG:HH21	2.27	0.47
1:F:301:LEU:O	1:F:305:VAL:HG23	2.14	0.47
1:A:39:ILE:HD13	1:A:246:ILE:HG21	1.96	0.47
1:B:80:VAL:O	1:B:84:ARG:HG3	2.15	0.47
1:A:310:VAL:HA	1:A:313:LEU:HD12	1.97	0.47
1:B:301:LEU:HA	1:B:304:LEU:HB2	1.97	0.47
1:D:111:TYR:CE2	1:D:114:MET:CE	2.98	0.47
1:C:216:ILE:CD1	1:C:216:ILE:H	2.23	0.47
1:D:142:GLU:O	1:D:145:ARG:HG3	2.15	0.47
1:C:301:LEU:HA	1:C:304:LEU:HB2	1.97	0.47
1:B:267:ALA:O	1:B:270:MET:HB2	2.15	0.46
1:C:142:GLU:O	1:C:145:ARG:HG3	2.15	0.46
1:D:164:GLN:OE1	1:D:167:LYS:HE2	2.15	0.46
1:E:301:LEU:O	1:E:305:VAL:HG23	2.15	0.46
1:F:39:ILE:HD13	1:F:246:ILE:HG21	1.96	0.46
1:F:177:MET:HG2	1:F:179:PRO:HD3	1.96	0.46
1:C:267:ALA:O	1:C:270:MET:HB2	2.16	0.46
1:D:32:MET:HE2	1:D:186:TYR:CE1	2.51	0.46
1:E:142:GLU:O	1:E:145:ARG:HG3	2.15	0.46
1:F:197:ARG:HG2	1:F:300:ILE:HD13	1.97	0.46
1:B:331:PRO:HB2	1:B:332:PRO:HD3	1.97	0.46
1:D:39:ILE:HD13	1:D:246:ILE:HG21	1.97	0.46
1:D:350:THR:HG23	1:D:360:GLN:HB3	1.98	0.46
1:B:142:GLU:O	1:B:145:ARG:HG3	2.16	0.45
1:F:301:LEU:HA	1:F:304:LEU:HB2	1.97	0.45
1:B:195:GLN:HE22	1:B:265:MET:CE	2.30	0.45
1:C:107:ALA:O	1:C:110:THR:HB	2.16	0.45
1:D:259:MET:HE1	1:D:263:ILE:HD13	1.97	0.45
1:F:107:ALA:O	1:F:110:THR:HB	2.16	0.45
1:D:35:GLN:H	1:D:35:GLN:HG3	1.31	0.45
1:E:35:GLN:HG3	1:E:35:GLN:H	1.35	0.45
1:D:267:ALA:O	1:D:270:MET:HB2	2.17	0.45
1:A:32:MET:HE2	1:A:186:TYR:CD1	2.52	0.45
1:D:301:LEU:HA	1:D:304:LEU:HB2	1.99	0.45
1:A:331:PRO:HB2	1:A:332:PRO:HD3	1.99	0.45
1:C:356:ILE:HD12	1:C:359:ARG:HB2	1.99	0.44
1:D:60:LYS:HA	1:D:60:LYS:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:PHE:CD2	1:E:239:ILE:HG21	2.52	0.44
1:D:305:VAL:HG13	1:D:310:VAL:HB	1.99	0.44
1:E:331:PRO:HB2	1:E:332:PRO:HD3	1.98	0.44
1:D:32:MET:HE2	1:D:186:TYR:CD1	2.53	0.44
1:E:177:MET:HG2	1:E:179:PRO:HD3	2.00	0.44
1:A:305:VAL:HG13	1:A:310:VAL:HB	1.98	0.44
1:B:60:LYS:HD3	1:B:60:LYS:HA	1.83	0.44
1:D:28:VAL:HB	1:D:182:GLU:HG2	2.00	0.44
1:E:28:VAL:HB	1:E:182:GLU:HG2	2.00	0.44
1:F:32:MET:HE2	1:F:186:TYR:CD1	2.52	0.44
1:B:350:THR:HG23	1:B:360:GLN:HB3	2.00	0.44
1:B:32:MET:HE2	1:B:186:TYR:CD1	2.53	0.44
1:C:60:LYS:HA	1:C:60:LYS:HD3	1.80	0.44
1:E:288:ARG:NH1	1:E:362:LYS:HB3	2.32	0.44
1:A:107:ALA:O	1:A:110:THR:HB	2.18	0.43
1:A:46:TRP:CD1	1:A:242:LYS:HE2	2.53	0.43
1:B:150:LEU:HA	1:B:150:LEU:HD23	1.86	0.43
1:E:23:GLU:HG2	1:E:269:LEU:HD11	2.00	0.43
1:B:184:SER:HB3	1:B:187:LEU:HD12	2.01	0.43
1:B:107:ALA:O	1:B:110:THR:HB	2.18	0.43
1:A:142:GLU:O	1:A:145:ARG:HG3	2.18	0.43
1:D:310:VAL:HA	1:D:313:LEU:HD12	1.99	0.43
1:C:259:MET:HE1	1:C:263:ILE:HD13	1.99	0.43
1:D:46:TRP:CD1	1:D:242:LYS:HE2	2.54	0.43
1:A:62:TRP:CE2	1:A:145:ARG:NH2	2.87	0.43
1:C:288:ARG:HD2	1:C:362:LYS:HD3	2.01	0.43
1:D:177:MET:HG2	1:D:179:PRO:HD3	2.00	0.43
1:D:62:TRP:CE2	1:D:145:ARG:NH2	2.87	0.43
1:F:350:THR:HG23	1:F:360:GLN:HB3	2.00	0.43
1:A:301:LEU:HA	1:A:304:LEU:HB2	1.99	0.43
1:B:288:ARG:NH1	1:B:362:LYS:HB3	2.34	0.43
1:C:350:THR:HG23	1:C:360:GLN:HB3	2.01	0.43
1:F:32:MET:HE2	1:F:186:TYR:CE1	2.54	0.43
1:A:60:LYS:HD3	1:A:60:LYS:HA	1.82	0.43
1:E:40:PHE:CZ	1:E:185:PRO:HB2	2.53	0.43
1:A:189:PHE:CD2	1:A:239:ILE:HG21	2.54	0.42
1:D:40:PHE:CZ	1:D:185:PRO:HB2	2.55	0.42
1:E:32:MET:HE2	1:E:186:TYR:CE1	2.54	0.42
1:A:216:ILE:CD1	1:A:216:ILE:H	2.20	0.42
1:C:310:VAL:HA	1:C:313:LEU:HD12	2.01	0.42
1:E:107:ALA:O	1:E:110:THR:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:PHE:CZ	1:F:185:PRO:HB2	2.55	0.42
1:B:115:LEU:HD21	1:B:192:THR:HG21	2.01	0.42
1:B:19:MET:HE1	1:B:22:ARG:HH21	1.84	0.42
1:D:23:GLU:HG2	1:D:269:LEU:HD11	2.00	0.42
1:E:46:TRP:CD1	1:E:242:LYS:HE2	2.55	0.42
1:E:310:VAL:HA	1:E:313:LEU:HD12	2.01	0.42
1:F:115:LEU:HD21	1:F:192:THR:HG21	2.02	0.42
1:B:32:MET:HE3	1:B:185:PRO:HD2	2.02	0.42
1:C:184:SER:HB3	1:C:187:LEU:HD12	2.01	0.42
1:B:177:MET:SD	1:B:266:PRO:HA	2.60	0.42
1:C:331:PRO:HB2	1:C:332:PRO:HD3	2.01	0.42
1:E:39:ILE:HD13	1:E:246:ILE:HG21	2.02	0.42
1:F:138:ALA:O	1:F:142:GLU:HG3	2.19	0.42
1:A:177:MET:HG2	1:A:179:PRO:HD3	2.01	0.42
1:A:23:GLU:HG2	1:A:269:LEU:HD11	2.02	0.42
1:C:138:ALA:O	1:C:142:GLU:HG3	2.20	0.42
1:C:33:PRO:HA	1:C:34:PRO:HD3	1.95	0.41
1:F:259:MET:HE1	1:F:263:ILE:HD13	2.02	0.41
1:B:119:ASP:HA	1:B:122:ARG:NH1	2.36	0.41
1:C:32:MET:HE2	1:C:186:TYR:CE1	2.55	0.41
1:F:33:PRO:HA	1:F:34:PRO:HD3	1.92	0.41
1:B:103:ILE:HG12	1:B:169:ILE:HG13	2.01	0.41
1:E:350:THR:HG23	1:E:360:GLN:HB3	2.02	0.41
1:B:177:MET:HG2	1:B:179:PRO:HD3	2.03	0.41
1:C:40:PHE:CZ	1:C:185:PRO:HB2	2.55	0.41
1:F:23:GLU:HG2	1:F:269:LEU:HD11	2.01	0.41
1:A:108:LEU:O	1:A:111:TYR:N	2.52	0.41
1:B:221:ILE:O	1:B:225:ILE:HG13	2.20	0.41
1:D:100:GLY:HA3	1:D:282:PHE:CE1	2.55	0.41
1:E:115:LEU:HD21	1:E:192:THR:HG21	2.02	0.41
1:E:98:LEU:HD12	1:E:98:LEU:HA	1.87	0.41
1:F:142:GLU:O	1:F:145:ARG:HG3	2.21	0.41
1:B:39:ILE:HD13	1:B:246:ILE:HG21	2.02	0.41
1:B:33:PRO:HA	1:B:34:PRO:HD3	1.92	0.41
1:F:277:ASN:HB2	1:F:281:HIS:CE1	2.56	0.41
1:B:299:ASP:OD1	1:B:335:ARG:NH1	2.54	0.41
1:B:118:LEU:O	1:B:122:ARG:HB3	2.21	0.41
1:D:138:ALA:O	1:D:142:GLU:HG3	2.21	0.41
1:E:32:MET:HE2	1:E:186:TYR:CD1	2.55	0.41
1:F:119:ASP:HA	1:F:122:ARG:NH1	2.36	0.41
1:A:108:LEU:O	1:A:109:PRO:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:ASP:OD1	1:F:335:ARG:NH1	2.54	0.40
1:B:35:GLN:HG3	1:B:35:GLN:H	1.31	0.40
1:E:288:ARG:HD2	1:E:362:LYS:HD3	2.03	0.40
1:F:35:GLN:HG3	1:F:35:GLN:H	1.32	0.40
1:F:150:LEU:HA	1:F:150:LEU:HD23	1.92	0.40
1:A:288:ARG:NH1	1:A:362:LYS:O	2.54	0.40
1:D:107:ALA:O	1:D:110:THR:HB	2.22	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:B:45:ASN:ND2	1:D:45:ASN:ND2[3_555]	2.00	0.20

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	344/363 (95%)	315 (92%)	26 (8%)	3 (1%)	17	46
1	B	344/363 (95%)	317 (92%)	23 (7%)	4 (1%)	13	39
1	C	344/363 (95%)	319 (93%)	22 (6%)	3 (1%)	17	46
1	D	344/363 (95%)	315 (92%)	25 (7%)	4 (1%)	13	39
1	E	344/363 (95%)	317 (92%)	24 (7%)	3 (1%)	17	46
1	F	344/363 (95%)	317 (92%)	24 (7%)	3 (1%)	17	46
All	All	2064/2178 (95%)	1900 (92%)	144 (7%)	20 (1%)	15	44

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	HIS

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Mol	Chain	Res	Type
1	B	315	GLY
1	D	315	GLY
1	E	315	GLY
1	A	262	LYS
1	A	315	GLY
1	B	262	LYS
1	C	262	LYS
1	C	315	GLY
1	D	54	HIS
1	E	262	LYS
1	F	262	LYS
1	F	315	GLY
1	A	54	HIS
1	C	54	HIS
1	D	262	LYS
1	E	54	HIS
1	B	249	ASP
1	D	249	ASP
1	F	54	HIS

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	300/315 (95%)	254 (85%)	46 (15%)	2	8
1	B	300/315 (95%)	253 (84%)	47 (16%)	2	8
1	C	300/315 (95%)	254 (85%)	46 (15%)	2	8
1	D	300/315 (95%)	253 (84%)	47 (16%)	2	8
1	E	300/315 (95%)	254 (85%)	46 (15%)	2	8
1	F	300/315 (95%)	256 (85%)	44 (15%)	3	9
All	All	1800/1890 (95%)	1524 (85%)	276 (15%)	2	8

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	MET
1	A	32	MET
1	A	35	GLN
1	A	36	LYS
1	A	38	GLU
1	A	39	ILE
1	A	48	GLU
1	A	56	LYS
1	A	85	GLU
1	A	102	MET
1	A	122	ARG
1	A	134	ILE
1	A	145	ARG
1	A	152	LYS
1	A	177	MET
1	A	197	ARG
1	A	199	THR
1	A	202	SER
1	A	208	ARG
1	A	216	ILE
1	A	217	LYS
1	A	231	ARG
1	A	238	LYS
1	A	242	LYS
1	A	249	ASP
1	A	259	MET
1	A	260	ARG
1	A	287	GLN
1	A	300	ILE
1	A	301	LEU
1	A	302	GLU
1	A	307	ARG
1	A	312	LYS
1	A	314	THR
1	A	321	GLN
1	A	327	VAL
1	A	336	ARG
1	A	337	LEU
1	A	339	GLU
1	A	340	ARG
1	A	344	ARG
1	A	346	LYS
1	A	347	GLU

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Mol	Chain	Res	Type
1	A	350	THR
1	A	351	MET
1	A	363	LEU
1	B	19	MET
1	B	32	MET
1	B	35	GLN
1	B	36	LYS
1	B	38	GLU
1	B	39	ILE
1	B	48	GLU
1	B	49	GLU
1	B	56	LYS
1	B	85	GLU
1	B	102	MET
1	B	111	TYR
1	B	122	ARG
1	B	134	ILE
1	B	145	ARG
1	B	152	LYS
1	B	177	MET
1	B	197	ARG
1	B	199	THR
1	B	202	SER
1	B	208	ARG
1	B	216	ILE
1	B	217	LYS
1	B	238	LYS
1	B	242	LYS
1	B	249	ASP
1	B	259	MET
1	B	287	GLN
1	B	300	ILE
1	B	301	LEU
1	B	302	GLU
1	B	307	ARG
1	B	312	LYS
1	B	314	THR
1	B	321	GLN
1	B	327	VAL
1	B	333	ARG
1	B	336	ARG
1	B	337	LEU

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Mol	Chain	Res	Type
1	B	339	GLU
1	B	340	ARG
1	B	344	ARG
1	B	346	LYS
1	B	347	GLU
1	B	350	THR
1	B	351	MET
1	B	363	LEU
1	C	19	MET
1	C	32	MET
1	C	35	GLN
1	C	36	LYS
1	C	38	GLU
1	C	39	ILE
1	C	48	GLU
1	C	49	GLU
1	C	56	LYS
1	C	85	GLU
1	C	93	ASP
1	C	102	MET
1	C	122	ARG
1	C	134	ILE
1	C	145	ARG
1	C	152	LYS
1	C	177	MET
1	C	197	ARG
1	C	199	THR
1	C	202	SER
1	C	208	ARG
1	C	216	ILE
1	C	217	LYS
1	C	238	LYS
1	C	242	LYS
1	C	249	ASP
1	C	259	MET
1	C	260	ARG
1	C	287	GLN
1	C	301	LEU
1	C	302	GLU
1	C	307	ARG
1	C	312	LYS
1	C	314	THR

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Mol	Chain	Res	Type
1	C	321	GLN
1	C	327	VAL
1	C	336	ARG
1	C	337	LEU
1	C	339	GLU
1	C	340	ARG
1	C	344	ARG
1	C	346	LYS
1	C	347	GLU
1	C	350	THR
1	C	351	MET
1	C	363	LEU
1	D	19	MET
1	D	35	GLN
1	D	36	LYS
1	D	38	GLU
1	D	39	ILE
1	D	48	GLU
1	D	49	GLU
1	D	56	LYS
1	D	85	GLU
1	D	102	MET
1	D	111	TYR
1	D	122	ARG
1	D	134	ILE
1	D	145	ARG
1	D	152	LYS
1	D	177	MET
1	D	197	ARG
1	D	199	THR
1	D	202	SER
1	D	208	ARG
1	D	216	ILE
1	D	217	LYS
1	D	231	ARG
1	D	238	LYS
1	D	242	LYS
1	D	249	ASP
1	D	259	MET
1	D	287	GLN
1	D	300	ILE
1	D	301	LEU

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Mol	Chain	Res	Type
1	D	302	GLU
1	D	307	ARG
1	D	312	LYS
1	D	314	THR
1	D	316	LEU
1	D	321	GLN
1	D	327	VAL
1	D	336	ARG
1	D	337	LEU
1	D	339	GLU
1	D	340	ARG
1	D	344	ARG
1	D	346	LYS
1	D	347	GLU
1	D	350	THR
1	D	351	MET
1	D	363	LEU
1	E	19	MET
1	E	35	GLN
1	E	36	LYS
1	E	38	GLU
1	E	39	ILE
1	E	48	GLU
1	E	49	GLU
1	E	56	LYS
1	E	85	GLU
1	E	102	MET
1	E	122	ARG
1	E	134	ILE
1	E	145	ARG
1	E	152	LYS
1	E	163	ARG
1	E	177	MET
1	E	193	SER
1	E	197	ARG
1	E	199	THR
1	E	202	SER
1	E	208	ARG
1	E	216	ILE
1	E	217	LYS
1	E	238	LYS
1	E	242	LYS

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Mol	Chain	Res	Type
1	E	249	ASP
1	E	259	MET
1	E	287	GLN
1	E	300	ILE
1	E	301	LEU
1	E	302	GLU
1	E	307	ARG
1	E	312	LYS
1	E	314	THR
1	E	321	GLN
1	E	327	VAL
1	E	336	ARG
1	E	337	LEU
1	E	339	GLU
1	E	340	ARG
1	E	344	ARG
1	E	346	LYS
1	E	347	GLU
1	E	350	THR
1	E	351	MET
1	E	363	LEU
1	F	19	MET
1	F	35	GLN
1	F	36	LYS
1	F	38	GLU
1	F	39	ILE
1	F	48	GLU
1	F	56	LYS
1	F	85	GLU
1	F	102	MET
1	F	111	TYR
1	F	122	ARG
1	F	134	ILE
1	F	145	ARG
1	F	152	LYS
1	F	177	MET
1	F	197	ARG
1	F	199	THR
1	F	202	SER
1	F	208	ARG
1	F	216	ILE
1	F	217	LYS

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Mol	Chain	Res	Type
1	F	238	LYS
1	F	242	LYS
1	F	249	ASP
1	F	259	MET
1	F	287	GLN
1	F	300	ILE
1	F	301	LEU
1	F	302	GLU
1	F	307	ARG
1	F	312	LYS
1	F	314	THR
1	F	321	GLN
1	F	327	VAL
1	F	336	ARG
1	F	337	LEU
1	F	339	GLU
1	F	340	ARG
1	F	344	ARG
1	F	346	LYS
1	F	347	GLU
1	F	350	THR
1	F	351	MET
1	F	363	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	195	GLN
1	A	268	HIS
1	B	54	HIS
1	B	195	GLN
1	B	268	HIS
1	C	54	HIS
1	C	195	GLN
1	C	268	HIS
1	D	54	HIS
1	D	195	GLN
1	D	268	HIS
1	E	54	HIS
1	E	195	GLN
1	E	268	HIS

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Mol	Chain	Res	Type
1	F	195	GLN
1	F	268	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.