



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:04 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

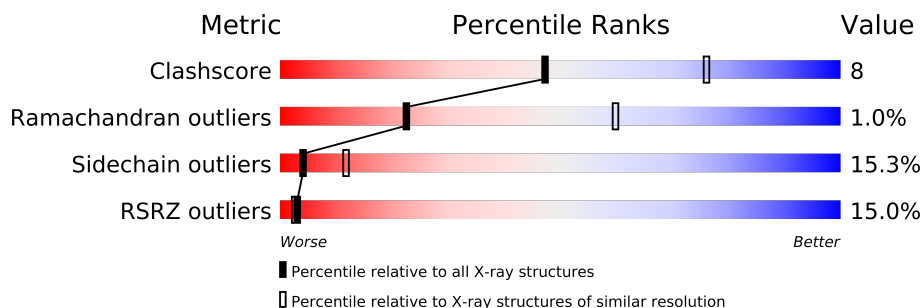
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance







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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	363	
1	B	363	
1	C	363	
1	D	363	
1	E	363	
1	F	363	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16847 atoms, of which 0 are hydrogen and 0 are deuterium.

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		

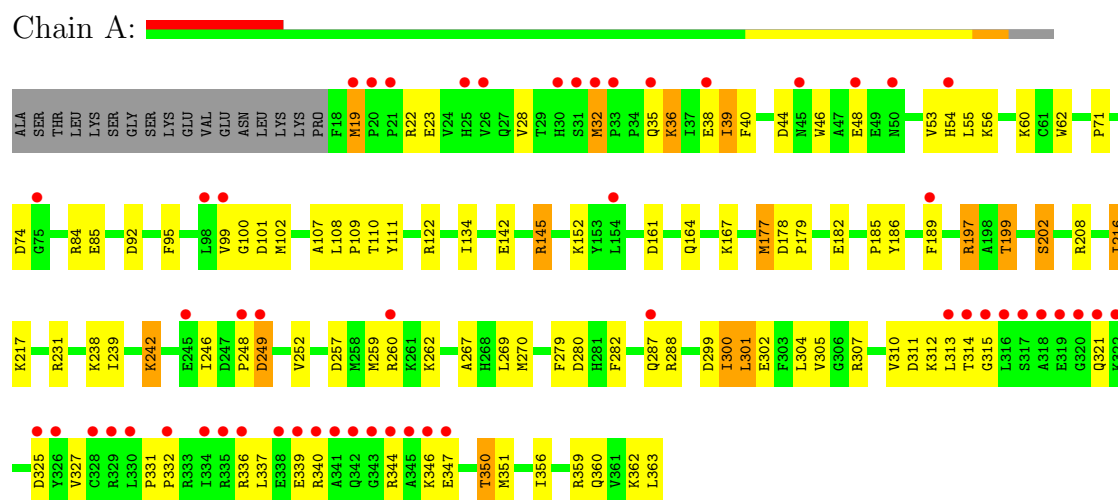
- Molecule 3 is water.

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

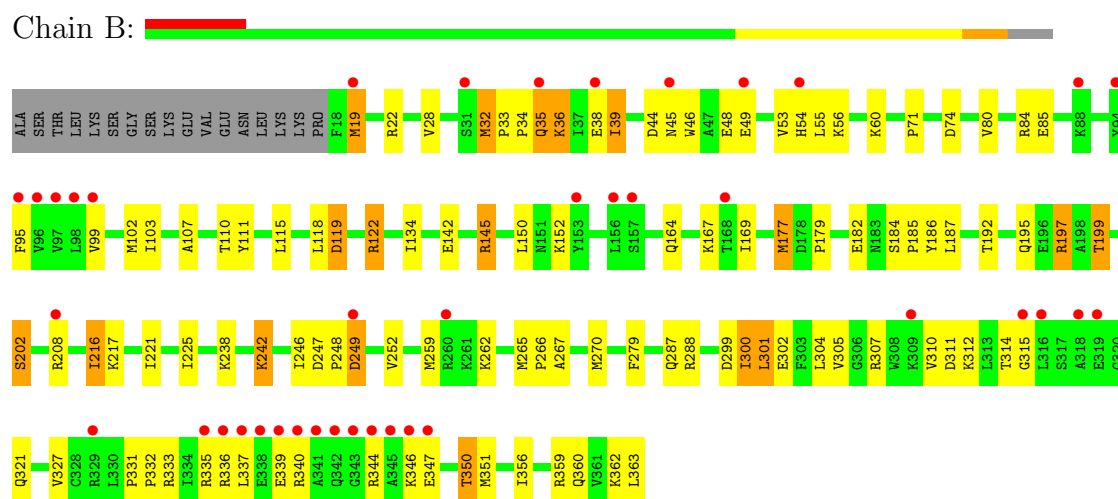
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

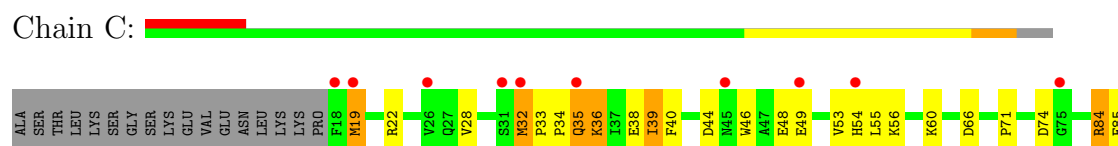
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

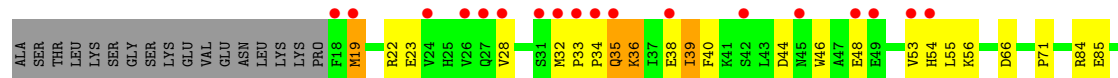


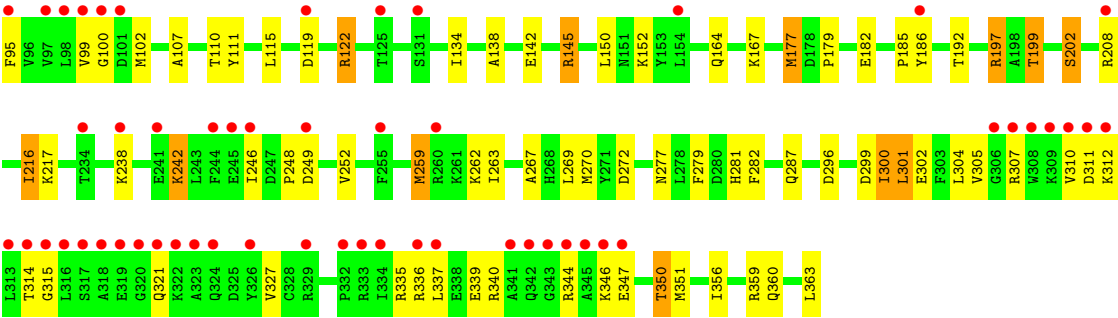
- Molecule 1: Acyl-[acyl-carrier protein] desaturase



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







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	NotAvailable	DCC
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 0.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 45472 reflections	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (263) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:E:270:MET:HE1	1:E:279:PHE:HA	1.66	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:71:PRO:O	1:D:84:ARG:NH2	2.17	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:84:ARG:NH2	1:F:71:PRO:O	2.20	0.73
1:E:216:ILE:HD12	1:E:216:ILE:H	1.54	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:E:270:MET:CE	1:E:279:PHE:HA	2.19	0.71
1:B:270:MET:HE2	1:B:279:PHE:HA	1.72	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:D:32:MET:CE	1:D:185:PRO:HD2	2.25	0.67
1:B:32:MET:CE	1:B: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
1:A:248:PRO:O	1:A:252:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:32:MET:CE	1:C:185:PRO:HD2	2.29	0.60
1:F:248:PRO:O	1:F:252:VAL:HG23	2.01	0.60
1:F:46:TRP:CE2	1:F:242:LYS:HG3	2.37	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:46:TRP:CE2	1:B:242:LYS:HG3	2.36	0.60
1:B:164:GLN:OE1	1:B:167:LYS:HE2	2.02	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:B:95:PHE:O	1:B:99:VAL:HG23	2.06	0.56
1:A:164:GLN:OE1	1:A:167:LYS:HE2	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:D:145:ARG:NH1	1:D:145:ARG:HG3	2.21	0.55
1:A:46:TRP:CE2	1:A:242:LYS:HG3	2.42	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:F:267:ALA:O	1:F:270:MET:HB2	2.10	0.51
1:E:53:VAL:C	1:E:55:LEU:H	2.14	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:46:TRP:CD1	1:B:242:LYS:HE2	2.48	0.48
1:B:305:VAL:HG13	1:B:310:VAL:HB	1.95	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:356:ILE:HD12	1:F:359:ARG:HB2	1.96	0.47
1:F:28:VAL:HB	1:F:182:GLU:HG2	1.95	0.47
1:A:40:PHE:CZ	1:A:185:PRO:HB2	2.49	0.47
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:E:216:ILE:H	1:E:216:ILE:CD1	2.19	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:28:VAL:HB	1:B:182:GLU:HG2	1.97	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:B:80:VAL:O	1:B:84:ARG:HG3	2.15	0.47
1:A:39:ILE:HD13	1:A:246:ILE:HG21	1.96	0.47
1:B:301:LEU:HA	1:B:304:LEU:HB2	1.97	0.47
1:A:310:VAL:HA	1:A:313:LEU:HD12	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:C:142:GLU:O	1:C:145:ARG:HG3	2.15	0.46
1:B:267:ALA:O	1:B:270:MET:HB2	2.15	0.46
1:D:164:GLN:OE1	1:D:167:LYS:HE2	2.15	0.46
1:F:39:ILE:HD13	1:F:246:ILE:HG21	1.96	0.46
1:E:301:LEU:O	1:E:305:VAL:HG23	2.15	0.46
1:F:177:MET:HG2	1:F:179:PRO:HD3	1.96	0.46
1:D:32:MET:HE2	1:D:186:TYR:CE1	2.51	0.46
1:C:267:ALA:O	1:C:270:MET:HB2	2.16	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:D:259:MET:HE1	1:D:263:ILE:HD13	1.97	0.45
1:C:107:ALA:O	1:C:110:THR:HB	2.16	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:F:32:MET:HE2	1:F:186:TYR:CD1	2.52	0.44
1:B:60:LYS:HD3	1:B:60:LYS:HA	1.83	0.44
1:E:28:VAL:HB	1:E:182:GLU:HG2	2.00	0.44
1:D:28:VAL:HB	1:D:182:GLU:HG2	2.00	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:46:TRP:CD1	1:A:242:LYS:HE2	2.53	0.43
1:A:107:ALA:O	1:A:110:THR:HB	2.18	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:D:46:TRP:CD1	1:D:242:LYS:HE2	2.54	0.43
1:C:259:MET:HE1	1:C:263:ILE:HD13	1.99	0.43
1:A:62:TRP:CE2	1:A:145:ARG:NH2	2.87	0.43
1:D:62:TRP:CE2	1:D: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: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:E:40:PHE:CZ	1:E:185:PRO:HB2	2.53	0.43
1:A:60:LYS:HD3	1:A:60:LYS:HA	1.82	0.43
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:189:PHE:CD2	1:A:239:ILE:HG21	2.54	0.42
1:F:40:PHE:CZ	1:F:185:PRO:HB2	2.55	0.42
1:A:216:ILE:H	1:A:216:ILE:CD1	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
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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:115:LEU:HD21	1:F:192:THR:HG21	2.02	0.42
1:D:23:GLU:HG2	1:D:269:LEU:HD11	2.00	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:F:138:ALA:O	1:F:142:GLU:HG3	2.19	0.42
1:E:39:ILE:HD13	1:E:246:ILE:HG21	2.02	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:C:138:ALA:O	1:C:142:GLU:HG3	2.20	0.42
1:A:23:GLU:HG2	1:A:269:LEU:HD11	2.02	0.42
1:A:177:MET:HG2	1:A:179:PRO:HD3	2.01	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:C:32:MET:HE2	1:C:186:TYR:CE1	2.55	0.41
1:B:119:ASP:HA	1:B:122:ARG:NH1	2.36	0.41
1:F:33:PRO:HA	1:F:34:PRO:HD3	1.92	0.41
1:E:350:THR:HG23	1:E:360:GLN:HB3	2.02	0.41
1:B:103:ILE:HG12	1:B:169:ILE:HG13	2.01	0.41
1:C:40:PHE:CZ	1:C:185:PRO:HB2	2.55	0.41
1:B:177:MET:HG2	1:B:179:PRO:HD3	2.03	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:F:142:GLU:O	1:F:145:ARG:HG3	2.21	0.41
1:E:98:LEU:HD12	1:E:98:LEU:HA	1.87	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:E:32:MET:HE2	1:E:186:TYR:CD1	2.55	0.41
1:D:138:ALA:O	1:D:142:GLU:HG3	2.21	0.41
1:B:118:LEU:O	1:B:122:ARG:HB3	2.21	0.41
1:B:299:ASP:OD1	1:B:335:ARG:NH1	2.54	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
1:F:299:ASP:OD1	1:F:335:ARG:NH1	2.54	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:B:35:GLN:HG3	1:B:35:GLN:H	1.31	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	Distance(Å)	Clash(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%)	25	63
1	B	344/363 (95%)	317 (92%)	23 (7%)	4 (1%)	19	54
1	C	344/363 (95%)	319 (93%)	22 (6%)	3 (1%)	25	63
1	D	344/363 (95%)	315 (92%)	25 (7%)	4 (1%)	19	54
1	E	344/363 (95%)	317 (92%)	24 (7%)	3 (1%)	25	63
1	F	344/363 (95%)	317 (92%)	24 (7%)	3 (1%)	25	63
All	All	2064/2178 (95%)	1900 (92%)	144 (7%)	20 (1%)	22	60

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	HIS
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

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Mol	Chain	Res	Type
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%)	4	12
1	B	300/315 (95%)	253 (84%)	47 (16%)	4	11
1	C	300/315 (95%)	254 (85%)	46 (15%)	4	12
1	D	300/315 (95%)	253 (84%)	47 (16%)	4	11
1	E	300/315 (95%)	254 (85%)	46 (15%)	4	12
1	F	300/315 (95%)	256 (85%)	44 (15%)	4	13
All	All	1800/1890 (95%)	1524 (85%)	276 (15%)	4	12

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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.

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	346/363 (95%)	0.83	54 (15%)	3 2	22, 27, 31, 35	8 (2%)
1	B	346/363 (95%)	0.66	40 (11%)	5 4	22, 27, 31, 36	8 (2%)
1	C	346/363 (95%)	0.68	40 (11%)	5 4	22, 27, 31, 36	8 (2%)
1	D	346/363 (95%)	0.77	43 (12%)	5 4	22, 27, 31, 36	8 (2%)
1	E	346/363 (95%)	0.94	64 (18%)	2 2	22, 27, 31, 35	8 (2%)
1	F	346/363 (95%)	1.12	72 (20%)	1 1	22, 27, 31, 35	8 (2%)
All	All	2076/2178 (95%)	0.83	313 (15%)	3 2	22, 27, 32, 36	48 (2%)

All (313) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	ARG	11.2
1	A	341	ALA	10.6
1	B	345	ALA	10.4
1	F	344	ARG	9.7
1	F	345	ALA	9.7
1	D	344	ARG	9.4
1	D	343	GLY	8.3
1	F	317	SER	8.2
1	E	318	ALA	7.6
1	F	19	MET	7.6
1	A	345	ALA	7.3
1	F	318	ALA	7.0
1	F	322	LYS	6.9
1	E	337	LEU	6.6
1	B	341	ALA	6.4
1	A	318	ALA	6.4
1	C	316	LEU	6.3
1	A	346	LYS	6.3
1	A	316	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	316	LEU	5.9
1	E	315	GLY	5.8
1	F	35	GLN	5.8
1	B	318	ALA	5.5
1	C	19	MET	5.5
1	B	342	GLN	5.5
1	D	341	ALA	5.4
1	F	321	GLN	5.4
1	F	337	LEU	5.3
1	F	319	GLU	5.3
1	F	343	GLY	5.2
1	E	35	GLN	5.2
1	F	341	ALA	5.2
1	C	18	PHE	5.1
1	F	245	GLU	5.1
1	D	318	ALA	5.1
1	B	45	ASN	5.0
1	F	260	ARG	5.0
1	C	321	GLN	4.9
1	A	332	PRO	4.9
1	F	54	HIS	4.9
1	B	344	ARG	4.9
1	F	336	ARG	4.8
1	F	329	ARG	4.7
1	D	337	LEU	4.7
1	F	32	MET	4.7
1	D	35	GLN	4.7
1	F	249	ASP	4.7
1	B	340	ARG	4.6
1	C	45	ASN	4.6
1	A	322	LYS	4.6
1	E	45	ASN	4.6
1	F	45	ASN	4.5
1	A	329	ARG	4.5
1	D	347	GLU	4.5
1	C	54	HIS	4.4
1	D	45	ASN	4.4
1	E	309	LYS	4.3
1	A	35	GLN	4.3
1	C	343	GLY	4.3
1	E	321	GLN	4.3
1	A	336	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	343	GLY	4.2
1	A	338	GLU	4.2
1	E	54	HIS	4.2
1	B	343	GLY	4.2
1	A	334	ILE	4.2
1	D	19	MET	4.2
1	F	98	LEU	4.1
1	A	319	GLU	4.1
1	E	42	SER	4.1
1	F	347	GLU	4.1
1	E	329	ARG	4.1
1	F	186	TYR	4.1
1	D	345	ALA	4.1
1	D	340	ARG	4.1
1	E	249	ASP	4.1
1	A	343	GLY	4.0
1	E	208	ARG	4.0
1	D	342	GLN	4.0
1	A	19	MET	4.0
1	B	338	GLU	4.0
1	E	32	MET	4.0
1	A	342	GLN	3.9
1	F	26	VAL	3.9
1	D	307	ARG	3.9
1	D	249	ASP	3.9
1	E	336	ARG	3.8
1	E	317	SER	3.8
1	C	287	GLN	3.8
1	F	346	LYS	3.8
1	A	335	ARG	3.8
1	D	319	GLU	3.8
1	E	306	GLY	3.8
1	F	314	THR	3.8
1	F	332	PRO	3.8
1	E	340	ARG	3.7
1	C	32	MET	3.7
1	A	314	THR	3.7
1	D	329	ARG	3.7
1	E	30	HIS	3.7
1	A	347	GLU	3.7
1	A	313	LEU	3.7
1	C	318	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	314	THR	3.6
1	F	306	GLY	3.6
1	B	347	GLU	3.6
1	B	337	LEU	3.6
1	B	309	LYS	3.6
1	F	28	VAL	3.6
1	E	339	GLU	3.6
1	F	309	LYS	3.6
1	E	18	PHE	3.6
1	A	260	ARG	3.6
1	B	35	GLN	3.6
1	E	98	LEU	3.5
1	F	33	PRO	3.5
1	D	315	GLY	3.5
1	D	316	LEU	3.5
1	D	98	LEU	3.5
1	C	307	ARG	3.5
1	E	245	GLU	3.4
1	B	98	LEU	3.4
1	F	131	SER	3.4
1	C	345	ALA	3.4
1	A	321	GLN	3.4
1	E	333	ARG	3.3
1	B	339	GLU	3.3
1	C	329	ARG	3.3
1	B	31	SER	3.3
1	E	325	ASP	3.3
1	E	307	ARG	3.3
1	F	34	PRO	3.3
1	B	38	GLU	3.3
1	E	319	GLU	3.3
1	E	322	LYS	3.3
1	F	208	ARG	3.3
1	C	49	GLU	3.3
1	D	338	GLU	3.3
1	E	338	GLU	3.3
1	E	19	MET	3.3
1	C	35	GLN	3.3
1	A	339	GLU	3.3
1	A	326	TYR	3.2
1	E	260	ARG	3.2
1	B	319	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	153	TYR	3.2
1	A	32	MET	3.2
1	C	347	GLU	3.2
1	D	96	VAL	3.2
1	C	98	LEU	3.1
1	A	26	VAL	3.1
1	B	97	VAL	3.1
1	A	248	PRO	3.1
1	B	346	LYS	3.1
1	F	244	PHE	3.1
1	A	340	ARG	3.1
1	E	29	THR	3.1
1	F	320	GLY	3.0
1	F	342	GLN	3.0
1	A	317	SER	3.0
1	E	20	PRO	3.0
1	E	119	ASP	3.0
1	E	342	GLN	3.0
1	B	336	ARG	3.0
1	D	95	PHE	3.0
1	D	317	SER	3.0
1	E	326	TYR	3.0
1	A	54	HIS	2.9
1	F	315	GLY	2.9
1	D	99	VAL	2.9
1	E	38	GLU	2.9
1	B	95	PHE	2.9
1	F	99	VAL	2.9
1	F	323	ALA	2.9
1	C	208	ARG	2.9
1	F	241	GLU	2.9
1	F	119	ASP	2.9
1	E	34	PRO	2.8
1	E	294	ALA	2.8
1	D	322	LYS	2.8
1	F	313	LEU	2.8
1	F	238	LYS	2.8
1	B	94	TYR	2.8
1	D	309	LYS	2.8
1	D	334	ILE	2.8
1	E	344	ARG	2.8
1	F	27	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	125	THR	2.8
1	A	50	ASN	2.8
1	F	95	PHE	2.8
1	C	180	ARG	2.8
1	E	180	ARG	2.8
1	D	339	GLU	2.8
1	C	337	LEU	2.8
1	F	316	LEU	2.8
1	B	208	ARG	2.7
1	E	341	ALA	2.7
1	E	248	PRO	2.7
1	E	345	ALA	2.7
1	D	321	GLN	2.7
1	D	38	GLU	2.7
1	F	334	ILE	2.7
1	F	307	ARG	2.7
1	D	346	LYS	2.7
1	E	212	GLU	2.7
1	B	96	VAL	2.6
1	E	31	SER	2.6
1	E	128	SER	2.6
1	B	49	GLU	2.6
1	F	49	GLU	2.6
1	A	320	GLY	2.6
1	E	313	LEU	2.6
1	E	335	ARG	2.6
1	D	238	LYS	2.6
1	C	325	ASP	2.6
1	A	315	GLY	2.6
1	B	315	GLY	2.6
1	A	325	ASP	2.6
1	C	26	VAL	2.6
1	F	308	TRP	2.5
1	D	314	THR	2.5
1	E	41	LYS	2.5
1	A	245	GLU	2.5
1	C	319	GLU	2.5
1	F	31	SER	2.5
1	C	314	THR	2.5
1	F	234	THR	2.5
1	A	154	LEU	2.5
1	C	312	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	157	SER	2.5
1	A	249	ASP	2.5
1	C	211	LYS	2.5
1	F	312	LYS	2.5
1	E	33	PRO	2.4
1	C	322	LYS	2.4
1	C	338	GLU	2.4
1	A	45	ASN	2.4
1	F	53	VAL	2.4
1	E	37	ILE	2.4
1	A	98	LEU	2.4
1	A	30	HIS	2.4
1	C	154	LEU	2.4
1	F	97	VAL	2.4
1	F	324	GLN	2.4
1	D	37	ILE	2.4
1	A	330	LEU	2.4
1	C	313	LEU	2.4
1	B	153	TYR	2.4
1	F	42	SER	2.4
1	A	33	PRO	2.4
1	A	287	GLN	2.3
1	B	168	THR	2.3
1	F	310	VAL	2.3
1	F	333	ARG	2.3
1	A	189	PHE	2.3
1	E	264	SER	2.3
1	A	25	HIS	2.3
1	E	154	LEU	2.3
1	C	168	THR	2.3
1	E	181	THR	2.3
1	A	31	SER	2.3
1	E	211	LYS	2.3
1	B	156	LEU	2.3
1	E	28	VAL	2.3
1	F	24	VAL	2.3
1	D	94	TYR	2.2
1	C	331	PRO	2.2
1	A	48	GLU	2.2
1	F	326	TYR	2.2
1	D	54	HIS	2.2
1	F	48	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	99	VAL	2.2
1	E	168	THR	2.2
1	F	311	ASP	2.2
1	D	193	SER	2.2
1	F	100	GLY	2.2
1	E	99	VAL	2.2
1	F	246	ILE	2.2
1	B	54	HIS	2.2
1	D	97	VAL	2.2
1	B	249	ASP	2.2
1	C	95	PHE	2.1
1	E	246	ILE	2.1
1	D	49	GLU	2.1
1	F	18	PHE	2.1
1	E	311	ASP	2.1
1	C	262	LYS	2.1
1	F	255	PHE	2.1
1	A	20	PRO	2.1
1	B	329	ARG	2.1
1	A	328	CYS	2.1
1	C	302	GLU	2.1
1	B	335	ARG	2.1
1	C	75	GLY	2.1
1	C	156	LEU	2.1
1	B	260	ARG	2.1
1	B	19	MET	2.1
1	E	88	LYS	2.1
1	A	21	PRO	2.1
1	B	88	LYS	2.1
1	B	316	LEU	2.1
1	D	336	ARG	2.0
1	B	99	VAL	2.0
1	F	101	ASP	2.0
1	A	38	GLU	2.0
1	F	38	GLU	2.0
1	C	315	GLY	2.0
1	F	154	LEU	2.0
1	C	31	SER	2.0
1	D	168	THR	2.0
1	A	75	GLY	2.0
1	D	308	TRP	2.0
1	D	190	ILE	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FE2	E	364	1/1	0.19	-0.12	53,53,53,53	0
2	FE2	C	364	1/1	0.12	-1.81	53,53,53,53	0
2	FE2	F	364	1/1	0.08	-2.57	53,53,53,53	0
2	FE2	A	364	1/1	0.07	-2.63	53,53,53,53	0
2	FE2	B	364	1/1	0.08	-3.22	53,53,53,53	0
2	FE2	D	364	1/1	0.07	-5.73	54,54,54,54	0

6.5 Other polymers

There are no such residues in this entry.