



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:16 am GMT

PDB ID : 1OQ4
Title : The Crystal Structure of the Complex between Stearoyl Acyl Carrier Protein Desaturase from Ricinus Communis (Castor Bean) and Azide.
Authors : Moche, M.; Ghoshal, A.K.; Shanklin, J.; Lindqvist, Y.
Deposited on : 2003-03-07
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

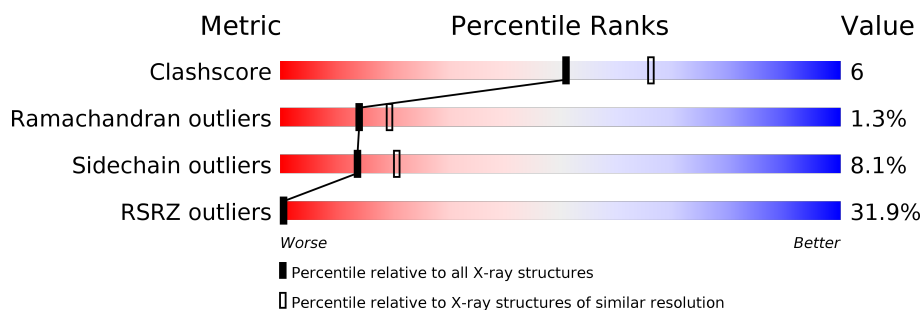
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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. 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	363	<div> <div>33%</div> <div>74%</div> <div>20%</div> <div>• 5%</div> </div>
1	B	363	<div> <div>29%</div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div>
1	C	363	<div> <div>36%</div> <div>74%</div> <div>20%</div> <div>• 5%</div> </div>
1	D	363	<div> <div>12%</div> <div>74%</div> <div>19%</div> <div>• 5%</div> </div>
1	E	363	<div> <div>36%</div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div>
1	F	363	<div> <div>36%</div> <div>74%</div> <div>20%</div> <div>• 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FE	F	365	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17235 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.

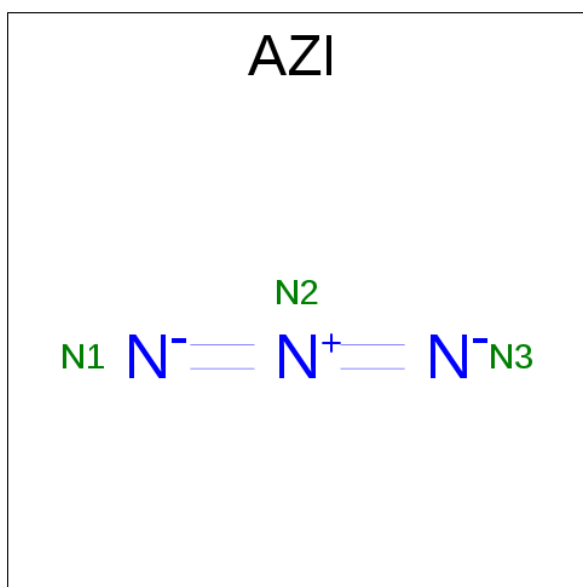
- Molecule 1 is a protein called Acyl-[acyl-carrier protein] desaturase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	26	0	0
			2806	1780	487	525	14			
1	B	346	Total	C	N	O	S	26	0	0
			2806	1780	487	525	14			
1	C	346	Total	C	N	O	S	26	1	0
			2807	1780	487	526	14			
1	D	346	Total	C	N	O	S	26	0	0
			2806	1780	487	525	14			
1	E	346	Total	C	N	O	S	26	0	0
			2806	1780	487	525	14			
1	F	346	Total	C	N	O	S	26	0	0
			2806	1780	487	525	14			

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

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

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N₃).



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

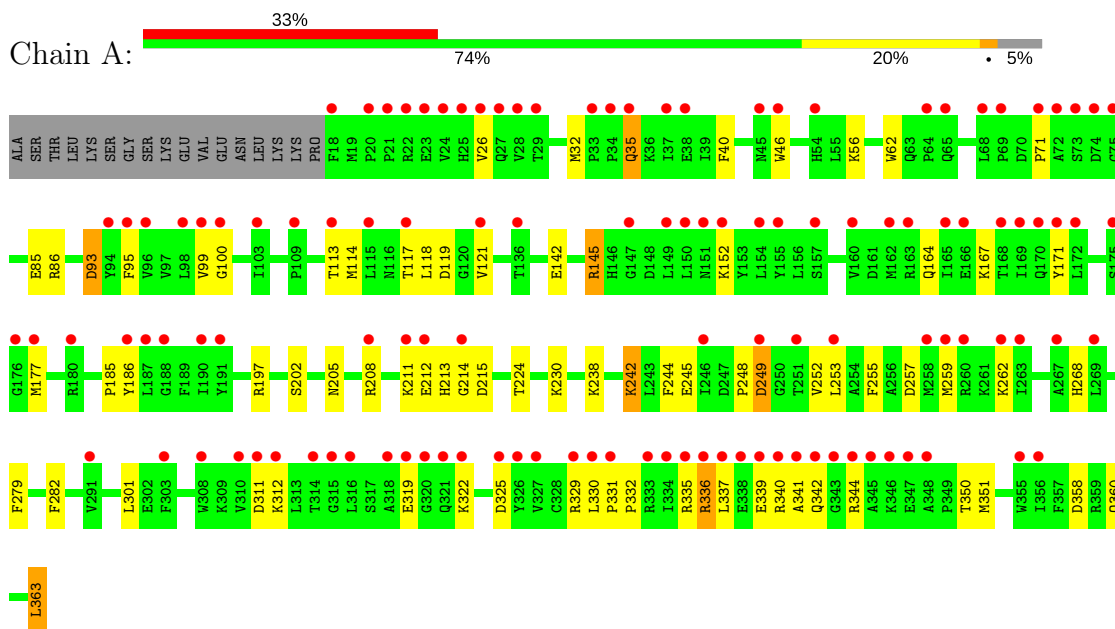
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	60	Total O 60 60	0	0
4	B	64	Total O 64 64	0	0
4	C	60	Total O 60 60	0	0
4	D	65	Total O 65 65	0	0
4	E	66	Total O 66 66	0	0
4	F	53	Total O 53 53	0	0

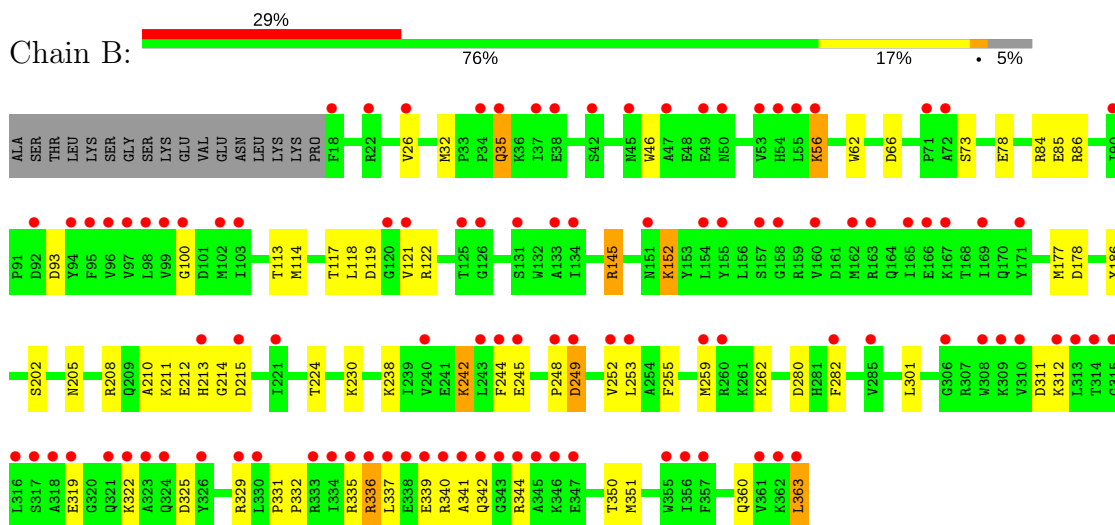
3 Residue-property plots

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 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.

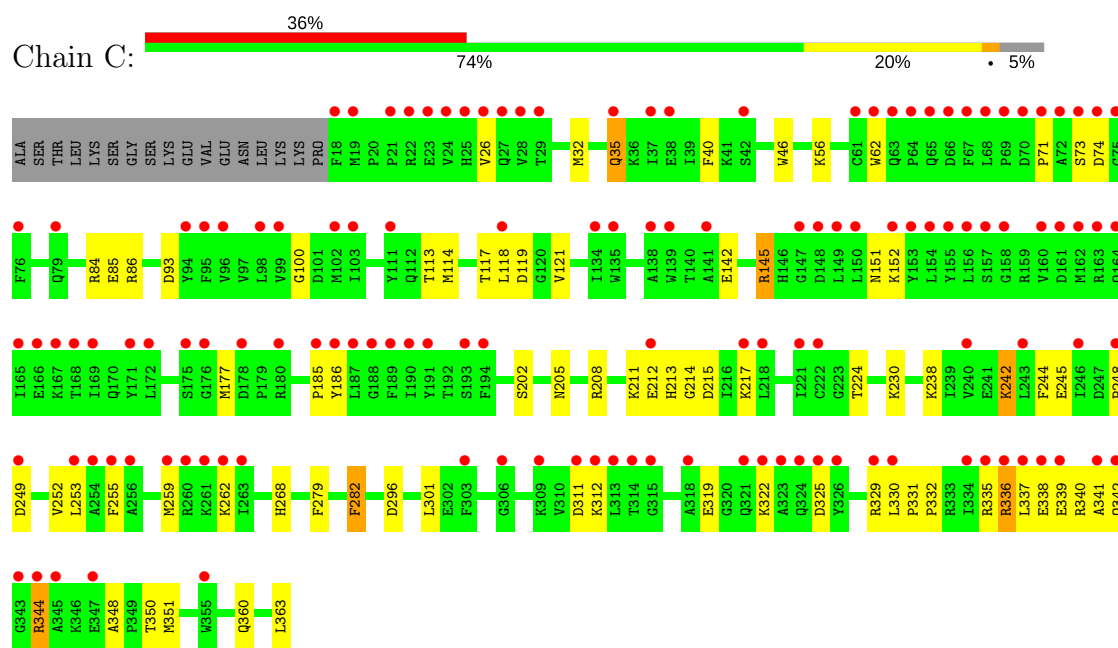
• Molecule 1: Acyl-[acyl-carrier protein] desaturase



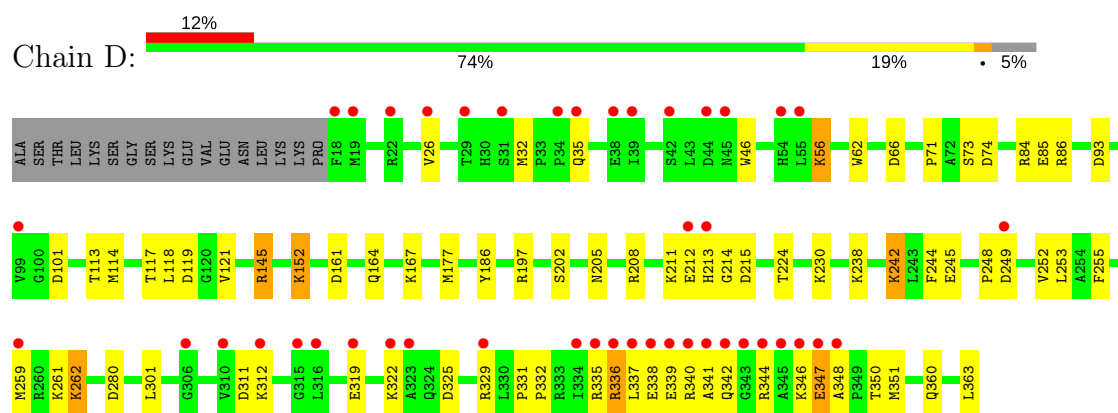
• Molecule 1: Acyl-[acyl-carrier protein] desaturase



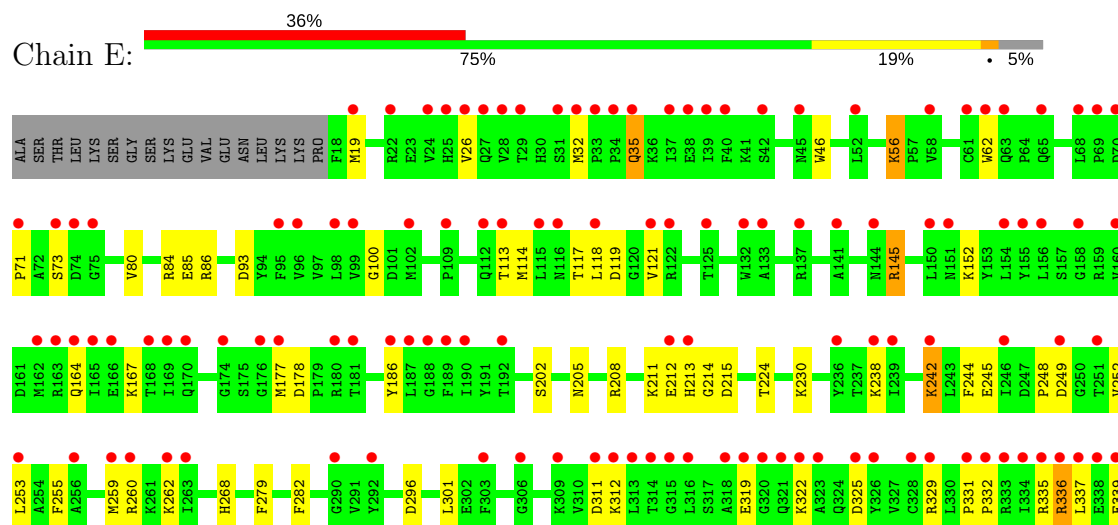
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

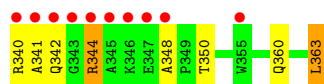


• Molecule 1: Acyl-[acyl-carrier protein] desaturase

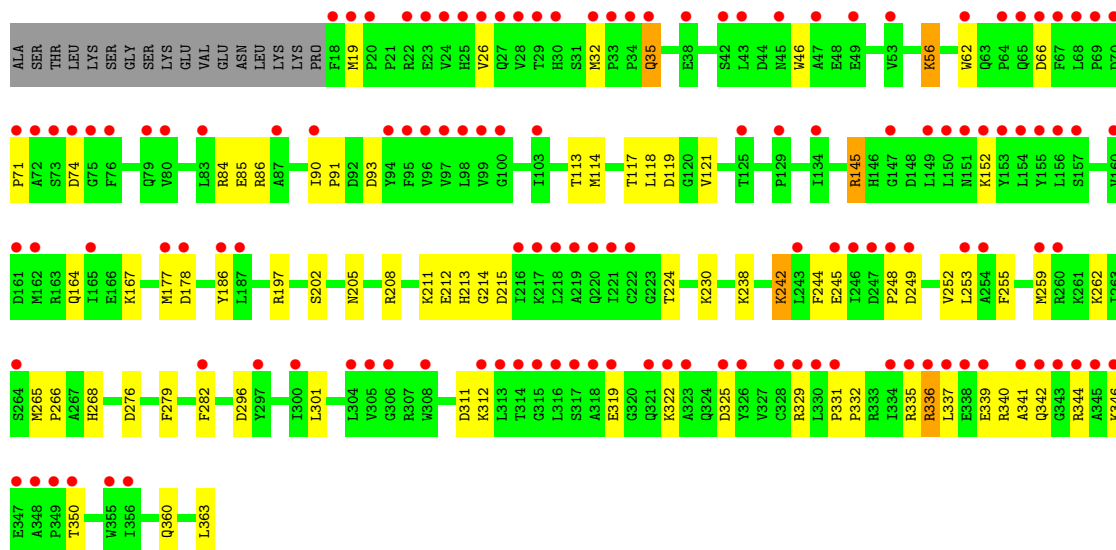


• Molecule 1: Acyl-[acyl-carrier protein] desaturase





- 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	81.77Å 145.21Å 192.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.92 – 2.40 24.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (24.92-2.40) 99.3 (24.90-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.242 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.1	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	0.84	EDS
Total number of atoms	17235	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.96% 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: AZI, FE

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	0.45	0/2874	0.76	7/3892 (0.2%)
1	B	0.49	0/2874	0.78	9/3892 (0.2%)
1	C	0.47	0/2883	0.76	6/3903 (0.2%)
1	D	0.51	0/2874	0.78	8/3892 (0.2%)
1	E	0.50	0/2874	0.77	6/3892 (0.2%)
1	F	0.48	0/2874	0.76	9/3892 (0.2%)
All	All	0.48	0/17253	0.77	45/23363 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	D	86	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	F	119	ASP	CB-CG-OD2	6.76	124.38	118.30
1	D	66	ASP	CB-CG-OD2	6.72	124.35	118.30
1	C	74	ASP	CB-CG-OD2	6.52	124.17	118.30
1	F	86	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	119	ASP	CB-CG-OD2	6.25	123.93	118.30
1	B	66	ASP	CB-CG-OD2	6.13	123.82	118.30
1	C	119	ASP	CB-CG-OD2	6.10	123.79	118.30
1	E	119	ASP	CB-CG-OD2	6.06	123.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	119	ASP	CB-CG-OD2	6.04	123.74	118.30
1	E	296	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	311	ASP	CB-CG-OD2	6.01	123.71	118.30
1	F	325	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	358	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	86	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	C	296	ASP	CB-CG-OD2	5.75	123.47	118.30
1	E	311	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	86	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	119	ASP	CB-CG-OD2	5.73	123.45	118.30
1	F	66	ASP	CB-CG-OD2	5.66	123.39	118.30
1	F	178	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	311	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	311	ASP	CB-CG-OD2	5.58	123.32	118.30
1	E	178	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	249	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	311	ASP	CB-CG-OD2	5.46	123.21	118.30
1	F	296	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	311	ASP	CB-CG-OD2	5.40	123.16	118.30
1	F	276	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	325	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	152	LYS	CD-CE-NZ	-5.30	99.50	111.70
1	A	257	ASP	CB-CG-OD2	5.29	123.06	118.30
1	E	325	ASP	CB-CG-OD2	5.23	123.01	118.30
1	F	74	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	178	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	325	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	325	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	249	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	325	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	101	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	280	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	74	ASP	CB-CG-OD2	5.03	122.83	118.30
1	E	86	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	280	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	217[B]	LYS	Mainchain

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	38	2
1	B	2806	0	2748	35	0
1	C	2807	0	2735	40	2
1	D	2806	0	2748	38	0
1	E	2806	0	2748	39	0
1	F	2806	0	2748	35	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	60	0	0	2	0
4	B	64	0	0	1	0
4	C	60	0	0	1	0
4	D	65	0	0	1	0
4	E	66	0	0	1	0
4	F	53	0	0	1	0
All	All	17235	0	16475	214	2

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 6.

All (214) 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:145:ARG:HG3	1:A:145:ARG:HH11	1.54	0.72
1:B:73:SER:HB3	1:C:73:SER:HB3	1.72	0.70
1:D:73:SER:HB3	1:E:73:SER:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ARG:HG3	1:F:145:ARG:HH11	1.57	0.70
1:B:145:ARG:HH11	1:B:145:ARG:HG3	1.59	0.67
1:C:253:LEU:HD21	1:C:319:GLU:HG3	1.77	0.66
1:D:253:LEU:HD21	1:D:319:GLU:HG3	1.78	0.66
1:A:253:LEU:HD21	1:A:319:GLU:HG3	1.77	0.66
1:C:350:THR:HG22	1:C:360:GLN:HB3	1.77	0.66
1:F:253:LEU:HD21	1:F:319:GLU:HG3	1.78	0.66
1:B:253:LEU:HD21	1:B:319:GLU:HG3	1.78	0.65
1:E:253:LEU:HD21	1:E:319:GLU:HG3	1.77	0.65
1:D:145:ARG:HG3	1:D:145:ARG:HH11	1.61	0.65
1:C:145:ARG:HG3	1:C:145:ARG:HH11	1.61	0.64
1:C:259:MET:SD	1:C:301:LEU:HD22	2.37	0.64
1:A:350:THR:HG22	1:A:360:GLN:HB3	1.81	0.63
1:F:350:THR:HG22	1:F:360:GLN:HB3	1.80	0.63
1:E:350:THR:HG22	1:E:360:GLN:HB3	1.78	0.63
1:E:145:ARG:HG3	1:E:145:ARG:HH11	1.64	0.63
1:B:339:GLU:O	1:B:341:ALA:N	2.33	0.62
1:D:350:THR:HG22	1:D:360:GLN:HB3	1.81	0.62
1:B:350:THR:HG22	1:B:360:GLN:HB3	1.82	0.61
1:C:339:GLU:O	1:C:341:ALA:N	2.34	0.61
1:B:336:ARG:HE	1:B:336:ARG:HA	1.65	0.61
1:A:336:ARG:HE	1:A:336:ARG:HA	1.66	0.61
1:A:339:GLU:O	1:A:341:ALA:N	2.33	0.61
1:D:339:GLU:O	1:D:341:ALA:N	2.33	0.61
1:C:331:PRO:HB2	1:C:332:PRO:HD3	1.83	0.61
1:E:259:MET:SD	1:E:301:LEU:HD22	2.41	0.61
1:E:339:GLU:O	1:E:341:ALA:N	2.34	0.61
1:E:46:TRP:CZ2	1:E:242:LYS:HG3	2.36	0.60
1:B:213:HIS:HB2	1:B:215:ASP:OD2	2.02	0.60
1:D:336:ARG:HE	1:D:336:ARG:HA	1.66	0.60
1:D:213:HIS:HB2	1:D:215:ASP:OD2	2.03	0.59
1:D:46:TRP:CZ2	1:D:242:LYS:HG3	2.37	0.59
1:B:46:TRP:CZ2	1:B:242:LYS:HG3	2.37	0.59
1:F:336:ARG:HA	1:F:336:ARG:HE	1.65	0.59
1:F:339:GLU:O	1:F:341:ALA:N	2.34	0.59
1:E:336:ARG:HE	1:E:336:ARG:HA	1.67	0.59
1:C:336:ARG:HE	1:C:336:ARG:HA	1.67	0.59
1:A:259:MET:SD	1:A:301:LEU:HD22	2.43	0.58
1:E:213:HIS:HB2	1:E:215:ASP:OD2	2.03	0.58
1:E:335:ARG:O	1:E:339:GLU:HB3	2.03	0.58
1:C:335:ARG:O	1:C:339:GLU:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:TRP:CZ2	1:A:242:LYS:HG3	2.39	0.57
1:C:213:HIS:HB2	1:C:215:ASP:OD2	2.03	0.57
1:A:335:ARG:O	1:A:339:GLU:HB3	2.04	0.57
1:D:335:ARG:O	1:D:339:GLU:HB3	2.05	0.57
1:B:335:ARG:O	1:B:339:GLU:HB3	2.05	0.57
1:C:46:TRP:CZ2	1:C:242:LYS:HG3	2.40	0.57
1:B:248:PRO:O	1:B:252:VAL:HG23	2.05	0.57
1:F:46:TRP:CZ2	1:F:242:LYS:HG3	2.40	0.56
1:E:248:PRO:O	1:E:252:VAL:HG23	2.05	0.56
1:D:248:PRO:O	1:D:252:VAL:HG23	2.06	0.56
1:F:335:ARG:O	1:F:339:GLU:HB3	2.06	0.56
1:E:331:PRO:HB2	1:E:332:PRO:HD3	1.88	0.56
1:B:255:PHE:O	1:B:259:MET:HG2	2.06	0.55
1:D:145:ARG:NH1	1:D:145:ARG:HG3	2.20	0.55
1:B:145:ARG:HG3	1:B:145:ARG:NH1	2.19	0.55
1:A:331:PRO:HB2	1:A:332:PRO:HD3	1.87	0.55
1:A:248:PRO:O	1:A:252:VAL:HG23	2.07	0.55
1:C:248:PRO:O	1:C:252:VAL:HG23	2.07	0.55
1:F:248:PRO:O	1:F:252:VAL:HG23	2.07	0.55
1:E:212:GLU:C	1:E:214:GLY:H	2.10	0.54
1:E:84:ARG:NH2	1:F:71:PRO:O	2.41	0.54
1:A:213:HIS:HB2	1:A:215:ASP:OD2	2.07	0.54
1:F:259:MET:SD	1:F:301:LEU:HD22	2.48	0.54
1:F:213:HIS:HB2	1:F:215:ASP:OD2	2.07	0.53
1:F:145:ARG:HG3	1:F:145:ARG:NH1	2.19	0.53
1:F:336:ARG:NE	1:F:336:ARG:HA	2.24	0.53
1:E:32:MET:CE	1:E:186:TYR:CD1	2.92	0.52
1:A:212:GLU:C	1:A:214:GLY:H	2.13	0.52
1:C:212:GLU:C	1:C:214:GLY:H	2.12	0.52
1:D:255:PHE:O	1:D:259:MET:HG2	2.09	0.52
1:E:71:PRO:O	1:F:84:ARG:NH2	2.41	0.52
1:C:32:MET:CE	1:C:186:TYR:CD1	2.92	0.52
1:D:336:ARG:NE	1:D:336:ARG:HA	2.25	0.52
1:C:113:THR:O	1:C:117:THR:HG23	2.10	0.52
1:D:212:GLU:C	1:D:214:GLY:H	2.13	0.52
1:D:32:MET:CE	1:D:186:TYR:CD1	2.93	0.51
1:A:336:ARG:NE	1:A:336:ARG:HA	2.25	0.51
1:A:118:LEU:HB2	1:A:121:VAL:HG23	1.92	0.51
1:B:259:MET:SD	1:B:301:LEU:HD22	2.50	0.51
1:B:336:ARG:HA	1:B:336:ARG:NE	2.24	0.51
1:F:32:MET:CE	1:F:186:TYR:CD1	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:PHE:O	1:F:259:MET:HG2	2.11	0.51
1:A:113:THR:O	1:A:117:THR:HG23	2.11	0.51
1:F:113:THR:O	1:F:117:THR:HG23	2.10	0.51
1:A:71:PRO:O	1:B:84:ARG:NH2	2.44	0.51
1:A:32:MET:CE	1:A:186:TYR:CD1	2.94	0.51
1:F:212:GLU:C	1:F:214:GLY:H	2.13	0.50
1:C:336:ARG:NE	1:C:336:ARG:HA	2.26	0.50
1:B:32:MET:CE	1:B:186:TYR:CD1	2.94	0.50
1:C:255:PHE:O	1:C:259:MET:HG2	2.10	0.50
1:E:255:PHE:O	1:E:259:MET:HG2	2.11	0.50
1:F:331:PRO:HB2	1:F:332:PRO:HD3	1.92	0.50
1:E:336:ARG:HA	1:E:336:ARG:NE	2.26	0.50
1:B:212:GLU:C	1:B:214:GLY:H	2.13	0.50
1:E:113:THR:O	1:E:117:THR:HG23	2.12	0.49
1:A:145:ARG:NH1	1:A:145:ARG:HG3	2.21	0.49
1:E:32:MET:CE	1:E:186:TYR:HD1	2.26	0.49
1:B:331:PRO:HB2	1:B:332:PRO:HD3	1.95	0.48
1:C:336:ARG:O	1:C:339:GLU:N	2.41	0.48
1:D:331:PRO:HB2	1:D:332:PRO:HD3	1.95	0.48
1:A:35:GLN:HG3	1:A:35:GLN:H	1.42	0.48
1:F:215:ASP:HB3	4:F:5423:HOH:O	2.12	0.48
1:A:255:PHE:O	1:A:259:MET:HG2	2.13	0.48
1:E:118:LEU:HB2	1:E:121:VAL:CG2	2.44	0.48
1:E:205:ASN:OD1	1:E:208:ARG:NH1	2.46	0.48
1:D:205:ASN:OD1	1:D:208:ARG:NH1	2.47	0.48
1:D:259:MET:SD	1:D:301:LEU:HD22	2.53	0.48
1:A:118:LEU:HB2	1:A:121:VAL:CG2	2.44	0.47
1:C:32:MET:CE	1:C:186:TYR:HD1	2.27	0.47
1:D:32:MET:CE	1:D:186:TYR:HD1	2.28	0.47
1:E:118:LEU:HB2	1:E:121:VAL:HG23	1.97	0.47
1:B:118:LEU:HB2	1:B:121:VAL:CG2	2.44	0.47
1:E:46:TRP:CE2	1:E:242:LYS:HG3	2.50	0.47
1:B:244:PHE:HE1	1:B:252:VAL:HG22	1.80	0.47
1:D:215:ASP:HB3	4:D:3423:HOH:O	2.15	0.47
1:F:118:LEU:HB2	1:F:121:VAL:HG23	1.96	0.47
1:A:100:GLY:HA3	1:A:282:PHE:CE1	2.50	0.47
1:F:118:LEU:HB2	1:F:121:VAL:CG2	2.45	0.47
1:A:205:ASN:OD1	1:A:208:ARG:NH1	2.48	0.46
1:C:118:LEU:HB2	1:C:121:VAL:CG2	2.44	0.46
1:C:118:LEU:HB2	1:C:121:VAL:HG23	1.97	0.46
1:D:118:LEU:HB2	1:D:121:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:MET:CE	1:A:186:TYR:HD1	2.29	0.46
1:B:215:ASP:HB3	4:B:1423:HOH:O	2.15	0.46
1:F:336:ARG:O	1:F:339:GLU:N	2.44	0.46
1:E:145:ARG:NH1	1:E:145:ARG:HG3	2.27	0.46
1:A:93:ASP:N	1:A:93:ASP:OD1	2.48	0.46
1:C:244:PHE:HE1	1:C:252:VAL:HG22	1.81	0.46
1:D:336:ARG:O	1:D:339:GLU:N	2.43	0.46
1:D:244:PHE:HE1	1:D:252:VAL:HG22	1.81	0.45
1:A:336:ARG:O	1:A:339:GLU:N	2.45	0.45
1:D:118:LEU:HB2	1:D:121:VAL:CG2	2.46	0.45
1:F:32:MET:CE	1:F:186:TYR:HD1	2.29	0.45
1:D:113:THR:O	1:D:117:THR:HG23	2.17	0.45
1:D:46:TRP:CE2	1:D:242:LYS:HG3	2.51	0.45
1:C:100:GLY:HA3	1:C:282:PHE:CE1	2.52	0.45
1:C:142:GLU:O	1:C:145:ARG:HG3	2.16	0.45
1:F:244:PHE:HE1	1:F:252:VAL:HG22	1.82	0.45
1:B:100:GLY:HA3	1:B:282:PHE:CE1	2.52	0.44
1:A:142:GLU:O	1:A:145:ARG:HG3	2.16	0.44
1:E:35:GLN:HG3	1:E:35:GLN:H	1.39	0.44
1:A:95:PHE:O	1:A:99:VAL:HG23	2.18	0.44
1:B:32:MET:CE	1:B:186:TYR:HD1	2.30	0.44
1:C:344:ARG:O	1:C:348:ALA:HB2	2.17	0.44
1:C:46:TRP:CE2	1:C:242:LYS:HG3	2.52	0.44
1:B:46:TRP:CE2	1:B:242:LYS:HG3	2.53	0.44
1:C:215:ASP:HB3	4:C:2423:HOH:O	2.17	0.44
1:D:56:LYS:HA	1:D:56:LYS:HD2	1.81	0.44
1:A:46:TRP:CE2	1:A:242:LYS:HG3	2.53	0.44
1:C:84:ARG:NH2	1:D:71:PRO:O	2.50	0.44
1:E:164:GLN:OE1	1:E:167:LYS:HE2	2.18	0.44
1:A:244:PHE:HE1	1:A:252:VAL:HG22	1.83	0.44
1:F:56:LYS:HD2	1:F:56:LYS:HA	1.81	0.44
1:C:268:HIS:HA	1:C:279:PHE:CG	2.53	0.43
1:E:363:LEU:HA	1:E:363:LEU:HD12	1.89	0.43
1:F:46:TRP:CE2	1:F:242:LYS:HG3	2.53	0.43
1:B:205:ASN:OD1	1:B:208:ARG:NH1	2.51	0.43
1:B:56:LYS:HD2	1:B:56:LYS:HA	1.78	0.43
1:C:151:ASN:OD1	1:D:152:LYS:HE2	2.18	0.43
1:C:205:ASN:OD1	1:C:208:ARG:NH1	2.51	0.43
1:B:118:LEU:HB2	1:B:121:VAL:HG23	1.99	0.43
1:F:35:GLN:HG3	1:F:35:GLN:H	1.38	0.43
1:F:205:ASN:OD1	1:F:208:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ARG:NH1	1:C:145:ARG:HG3	2.27	0.43
1:D:73:SER:HA	1:E:73:SER:HA	2.00	0.43
1:B:113:THR:O	1:B:117:THR:HG23	2.19	0.43
1:A:164:GLN:OE1	1:A:167:LYS:HE2	2.19	0.42
1:F:62:TRP:CD1	1:F:224:THR:HG22	2.55	0.42
1:A:363:LEU:HA	1:A:363:LEU:HD12	1.89	0.42
1:C:71:PRO:O	1:D:84:ARG:NH2	2.52	0.42
1:E:344:ARG:O	1:E:348:ALA:HB2	2.19	0.42
1:E:56:LYS:HD2	1:E:56:LYS:HA	1.83	0.42
1:A:40:PHE:CZ	1:A:185:PRO:HB2	2.55	0.42
1:A:215:ASP:HB3	4:A:423:HOH:O	2.19	0.42
1:B:78:GLU:OE2	1:D:161:ASP:OD2	2.38	0.42
1:D:261:LYS:O	1:D:262:LYS:HB2	2.20	0.42
1:E:100:GLY:HA3	1:E:282:PHE:CE1	2.53	0.42
1:E:244:PHE:HE1	1:E:252:VAL:HG22	1.83	0.42
1:B:35:GLN:HG3	1:B:35:GLN:H	1.40	0.42
1:F:164:GLN:OE1	1:F:167:LYS:HE2	2.20	0.42
1:D:32:MET:CE	1:D:186:TYR:CE1	3.03	0.41
1:B:62:TRP:CD1	1:B:224:THR:HG22	2.55	0.41
1:C:259:MET:HB3	1:C:330:LEU:HD22	2.01	0.41
1:E:215:ASP:HB3	4:E:4423:HOH:O	2.19	0.41
1:A:62:TRP:CD1	1:A:224:THR:HG22	2.55	0.41
1:C:35:GLN:H	1:C:35:GLN:HG3	1.35	0.41
1:F:32:MET:CE	1:F:186:TYR:CE1	3.03	0.41
1:A:268:HIS:HA	1:A:279:PHE:CG	2.56	0.41
1:E:62:TRP:CD1	1:E:224:THR:HG22	2.55	0.41
1:F:268:HIS:HA	1:F:279:PHE:CG	2.55	0.41
1:B:73:SER:HA	1:C:73:SER:HA	2.02	0.41
1:D:336:ARG:O	1:D:338:GLU:N	2.53	0.41
1:E:336:ARG:O	1:E:339:GLU:N	2.43	0.41
1:A:171:TYR:HB3	4:A:512:HOH:O	2.20	0.41
1:F:90:ILE:HA	1:F:91:PRO:HD3	1.93	0.41
1:D:164:GLN:OE1	1:D:167:LYS:HE2	2.21	0.41
1:C:40:PHE:CZ	1:C:185:PRO:HB2	2.56	0.41
1:C:62:TRP:CD1	1:C:224:THR:HG22	2.55	0.41
1:C:32:MET:CE	1:C:186:TYR:CE1	3.04	0.40
1:E:212:GLU:C	1:E:214:GLY:N	2.74	0.40
1:F:265:MET:HA	1:F:266:PRO:HD3	1.95	0.40
1:D:62:TRP:CD1	1:D:224:THR:HG22	2.56	0.40
1:E:80:VAL:O	1:E:84:ARG:HG3	2.21	0.40
1:A:259:MET:HB3	1:A:330:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ARG:O	1:C:338:GLU:N	2.54	0.40
1:E:268:HIS:HA	1:E:279:PHE:CG	2.56	0.40
1:B:336:ARG:O	1:B:339:GLU:N	2.45	0.40
1:B:210:ALA:C	1:B:212:GLU:H	2.24	0.40
1:B:363:LEU:HA	1:B:363:LEU:HD12	1.88	0.40
1:D:347:GLU:O	1:D:348:ALA:C	2.60	0.40

All (2) 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:A:339:GLU:OE2	1:C:35:GLN:NE2[2_464]	1.32	0.88
1:A:339:GLU:CD	1:C:35:GLN:NE2[2_464]	2.02	0.18

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%)	328 (95%)	12 (4%)	4 (1%)	15	21
1	B	344/363 (95%)	328 (95%)	12 (4%)	4 (1%)	15	21
1	C	345/363 (95%)	329 (95%)	12 (4%)	4 (1%)	15	21
1	D	344/363 (95%)	327 (95%)	11 (3%)	6 (2%)	11	13
1	E	344/363 (95%)	325 (94%)	15 (4%)	4 (1%)	15	21
1	F	344/363 (95%)	328 (95%)	11 (3%)	5 (2%)	12	16
All	All	2065/2178 (95%)	1965 (95%)	73 (4%)	27 (1%)	14	19

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ARG

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Mol	Chain	Res	Type
1	B	340	ARG
1	C	337	LEU
1	C	340	ARG
1	D	337	LEU
1	D	340	ARG
1	E	340	ARG
1	F	340	ARG
1	A	337	LEU
1	B	337	LEU
1	E	337	LEU
1	F	337	LEU
1	D	336	ARG
1	A	262	LYS
1	B	336	ARG
1	C	262	LYS
1	C	336	ARG
1	D	346	LYS
1	D	347	GLU
1	E	262	LYS
1	E	336	ARG
1	F	262	LYS
1	A	336	ARG
1	B	262	LYS
1	D	262	LYS
1	F	336	ARG
1	F	346	LYS

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%)	276 (92%)	24 (8%)	14	21
1	B	300/315 (95%)	276 (92%)	24 (8%)	14	21
1	C	301/315 (96%)	277 (92%)	24 (8%)	14	21
1	D	300/315 (95%)	276 (92%)	24 (8%)	14	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	300/315 (95%)	276 (92%)	24 (8%)	14	21
1	F	300/315 (95%)	275 (92%)	25 (8%)	13	20
All	All	1801/1890 (95%)	1656 (92%)	145 (8%)	14	21

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	35	GLN
1	A	56	LYS
1	A	85	GLU
1	A	93	ASP
1	A	114	MET
1	A	145	ARG
1	A	152	LYS
1	A	177	MET
1	A	197	ARG
1	A	202	SER
1	A	211	LYS
1	A	230	LYS
1	A	238	LYS
1	A	242	LYS
1	A	245	GLU
1	A	249	ASP
1	A	312	LYS
1	A	322	LYS
1	A	329	ARG
1	A	342	GLN
1	A	344	ARG
1	A	351	MET
1	A	363	LEU
1	B	26	VAL
1	B	35	GLN
1	B	56	LYS
1	B	85	GLU
1	B	93	ASP
1	B	114	MET
1	B	122	ARG
1	B	145	ARG
1	B	152	LYS
1	B	177	MET

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Mol	Chain	Res	Type
1	B	202	SER
1	B	211	LYS
1	B	230	LYS
1	B	238	LYS
1	B	242	LYS
1	B	245	GLU
1	B	249	ASP
1	B	312	LYS
1	B	322	LYS
1	B	329	ARG
1	B	342	GLN
1	B	344	ARG
1	B	351	MET
1	B	363	LEU
1	C	26	VAL
1	C	35	GLN
1	C	56	LYS
1	C	85	GLU
1	C	93	ASP
1	C	114	MET
1	C	145	ARG
1	C	152	LYS
1	C	177	MET
1	C	202	SER
1	C	211	LYS
1	C	230	LYS
1	C	238	LYS
1	C	242	LYS
1	C	245	GLU
1	C	249	ASP
1	C	282	PHE
1	C	312	LYS
1	C	322	LYS
1	C	329	ARG
1	C	342	GLN
1	C	344	ARG
1	C	351	MET
1	C	363	LEU
1	D	26	VAL
1	D	35	GLN
1	D	56	LYS
1	D	85	GLU

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Mol	Chain	Res	Type
1	D	93	ASP
1	D	114	MET
1	D	145	ARG
1	D	152	LYS
1	D	177	MET
1	D	197	ARG
1	D	202	SER
1	D	211	LYS
1	D	230	LYS
1	D	238	LYS
1	D	242	LYS
1	D	245	GLU
1	D	249	ASP
1	D	312	LYS
1	D	322	LYS
1	D	329	ARG
1	D	342	GLN
1	D	344	ARG
1	D	351	MET
1	D	363	LEU
1	E	19	MET
1	E	26	VAL
1	E	35	GLN
1	E	56	LYS
1	E	85	GLU
1	E	93	ASP
1	E	114	MET
1	E	145	ARG
1	E	152	LYS
1	E	177	MET
1	E	202	SER
1	E	211	LYS
1	E	230	LYS
1	E	238	LYS
1	E	242	LYS
1	E	245	GLU
1	E	249	ASP
1	E	260	ARG
1	E	312	LYS
1	E	322	LYS
1	E	329	ARG
1	E	342	GLN

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Mol	Chain	Res	Type
1	E	344	ARG
1	E	363	LEU
1	F	19	MET
1	F	26	VAL
1	F	35	GLN
1	F	56	LYS
1	F	85	GLU
1	F	93	ASP
1	F	114	MET
1	F	145	ARG
1	F	152	LYS
1	F	177	MET
1	F	197	ARG
1	F	202	SER
1	F	211	LYS
1	F	230	LYS
1	F	238	LYS
1	F	242	LYS
1	F	245	GLU
1	F	249	ASP
1	F	282	PHE
1	F	312	LYS
1	F	322	LYS
1	F	329	ARG
1	F	342	GLN
1	F	344	ARG
1	F	363	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	B	268	HIS
1	C	268	HIS
1	D	268	HIS
1	E	268	HIS
1	F	268	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AZI	A	366	2	0,2,2	0.00	-	0,1,1	0.00	-
3	AZI	B	1366	2	0,2,2	0.00	-	0,1,1	0.00	-
3	AZI	C	2366	2	0,2,2	0.00	-	0,1,1	0.00	-
3	AZI	D	3366	2	0,2,2	0.00	-	0,1,1	0.00	-
3	AZI	E	4366	2	0,2,2	0.00	-	0,1,1	0.00	-
3	AZI	F	5366	2	0,2,2	0.00	-	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AZI	A	366	2	-	0/0/0/0	0/0/0/0
3	AZI	B	1366	2	-	0/0/0/0	0/0/0/0
3	AZI	C	2366	2	-	0/0/0/0	0/0/0/0
3	AZI	D	3366	2	-	0/0/0/0	0/0/0/0
3	AZI	E	4366	2	-	0/0/0/0	0/0/0/0
3	AZI	F	5366	2	-	0/0/0/0	0/0/0/0

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

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%)	1.80	121 (34%) 0 0	5, 12, 21, 25	6 (1%)
1	B	346/363 (95%)	1.62	104 (30%) 1 1	4, 11, 21, 25	6 (1%)
1	C	346/363 (95%)	1.79	131 (37%) 0 0	4, 11, 20, 25	6 (1%)
1	D	346/363 (95%)	0.82	44 (12%) 4 4	5, 12, 21, 25	6 (1%)
1	E	346/363 (95%)	1.67	132 (38%) 0 0	5, 12, 21, 25	6 (1%)
1	F	346/363 (95%)	1.81	131 (37%) 0 0	4, 11, 21, 25	6 (1%)
All	All	2076/2178 (95%)	1.59	663 (31%) 0 0	4, 12, 21, 25	36 (1%)

All (663) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	ALA	14.8
1	D	343	GLY	14.5
1	B	345	ALA	14.0
1	A	345	ALA	14.0
1	D	342	GLN	12.4
1	D	344	ARG	11.8
1	D	345	ALA	11.8
1	D	341	ALA	10.6
1	A	344	ARG	10.6
1	F	344	ARG	10.0
1	F	343	GLY	9.8
1	B	316	LEU	9.0
1	F	345	ALA	8.5
1	A	343	GLY	8.0
1	B	344	ARG	7.8
1	B	315	GLY	7.4
1	B	337	LEU	7.2
1	A	338	GLU	7.1
1	A	329	ARG	6.9

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Mol	Chain	Res	Type	RSRZ
1	C	249	ASP	6.7
1	E	35	GLN	6.6
1	B	249	ASP	6.5
1	E	340	ARG	6.4
1	B	96	VAL	6.4
1	C	343	GLY	6.4
1	D	42	SER	6.4
1	F	330	LEU	6.2
1	B	338	GLU	6.2
1	A	24	VAL	6.2
1	F	29	THR	6.1
1	F	94	TYR	6.0
1	C	336	ARG	6.0
1	C	338	GLU	6.0
1	B	341	ALA	5.8
1	C	69	PRO	5.8
1	E	336	ARG	5.8
1	D	340	ARG	5.8
1	B	343	GLY	5.7
1	C	347	GLU	5.7
1	D	338	GLU	5.7
1	A	165	ILE	5.7
1	F	42	SER	5.7
1	C	344	ARG	5.7
1	F	334	ILE	5.7
1	A	355	TRP	5.5
1	E	338	GLU	5.5
1	A	314	THR	5.4
1	B	355	TRP	5.4
1	C	74	ASP	5.4
1	F	341	ALA	5.4
1	B	322	LYS	5.3
1	F	322	LYS	5.3
1	F	99	VAL	5.3
1	C	18	PHE	5.3
1	F	160	VAL	5.2
1	F	26	VAL	5.2
1	C	325	ASP	5.1
1	B	42	SER	5.1
1	C	342	GLN	5.1
1	B	336	ARG	5.0
1	C	329	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	26	VAL	5.0
1	E	42	SER	5.0
1	C	35	GLN	5.0
1	B	313	LEU	4.9
1	C	314	THR	4.9
1	A	321	GLN	4.8
1	A	320	GLY	4.8
1	C	318	ALA	4.8
1	F	337	LEU	4.8
1	B	53	VAL	4.8
1	A	339	GLU	4.8
1	B	330	LEU	4.8
1	C	68	LEU	4.8
1	F	346	LYS	4.8
1	C	345	ALA	4.7
1	D	315	GLY	4.7
1	D	249	ASP	4.7
1	E	322	LYS	4.7
1	E	344	ARG	4.7
1	B	99	VAL	4.7
1	A	342	GLN	4.6
1	A	327	VAL	4.6
1	C	75	GLY	4.6
1	A	35	GLN	4.6
1	D	347	GLU	4.6
1	E	345	ALA	4.6
1	F	96	VAL	4.6
1	F	316	LEU	4.6
1	F	28	VAL	4.5
1	C	28	VAL	4.5
1	A	311	ASP	4.5
1	F	154	LEU	4.4
1	F	218	LEU	4.4
1	B	165	ILE	4.4
1	F	165	ILE	4.4
1	B	35	GLN	4.4
1	C	312	LYS	4.4
1	C	72	ALA	4.4
1	A	28	VAL	4.4
1	E	189	PHE	4.4
1	E	318	ALA	4.4
1	C	155	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	331	PRO	4.4
1	F	95	PHE	4.4
1	F	306	GLY	4.3
1	C	70	ASP	4.3
1	B	317	SER	4.3
1	A	318	ALA	4.3
1	C	262	LYS	4.3
1	A	330	LEU	4.3
1	A	99	VAL	4.3
1	F	98	LEU	4.3
1	A	260	ARG	4.2
1	B	326	TYR	4.2
1	E	315	GLY	4.2
1	C	162	MET	4.2
1	F	253	LEU	4.1
1	F	313	LEU	4.1
1	A	155	TYR	4.1
1	F	329	ARG	4.1
1	F	23	GLU	4.1
1	F	71	PRO	4.1
1	D	336	ARG	4.1
1	D	35	GLN	4.1
1	F	68	LEU	4.1
1	F	83	LEU	4.1
1	F	38	GLU	4.0
1	E	155	TYR	4.0
1	F	32	MET	4.0
1	F	156	LEU	4.0
1	E	25	HIS	4.0
1	E	186	TYR	4.0
1	B	97	VAL	4.0
1	C	25	HIS	4.0
1	A	26	VAL	4.0
1	F	347	GLU	4.0
1	A	336	ARG	4.0
1	A	346	LYS	4.0
1	F	24	VAL	4.0
1	C	311	ASP	3.9
1	F	45	ASN	3.9
1	E	262	LYS	3.9
1	F	153	TYR	3.9
1	D	339	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	177	MET	3.9
1	C	248	PRO	3.9
1	C	154	LEU	3.9
1	F	25	HIS	3.9
1	C	313	LEU	3.9
1	E	40	PHE	3.9
1	C	29	THR	3.9
1	F	221	ILE	3.9
1	C	156	LEU	3.9
1	F	76	PHE	3.8
1	F	72	ALA	3.8
1	A	121	VAL	3.8
1	D	337	LEU	3.8
1	E	323	ALA	3.8
1	A	316	LEU	3.8
1	E	37	ILE	3.8
1	F	314	THR	3.8
1	B	49	GLU	3.8
1	E	154	LEU	3.8
1	E	337	LEU	3.8
1	E	68	LEU	3.8
1	B	347	GLU	3.8
1	A	262	LYS	3.8
1	C	160	VAL	3.8
1	E	238	LYS	3.7
1	F	318	ALA	3.7
1	A	334	ILE	3.7
1	A	246	ILE	3.7
1	F	355	TRP	3.7
1	B	319	GLU	3.7
1	E	19	MET	3.7
1	E	61	CYS	3.7
1	A	154	LEU	3.7
1	A	312	LYS	3.7
1	E	99	VAL	3.7
1	A	340	ARG	3.7
1	B	154	LEU	3.7
1	D	39	ILE	3.7
1	B	98	LEU	3.7
1	C	212	GLU	3.7
1	E	180	ARG	3.6
1	C	158	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	55	LEU	3.6
1	C	339	GLU	3.6
1	E	325	ASP	3.6
1	E	28	VAL	3.6
1	F	19	MET	3.6
1	B	309	LYS	3.6
1	C	337	LEU	3.6
1	F	149	LEU	3.6
1	C	24	VAL	3.6
1	B	333	ARG	3.6
1	C	153	TYR	3.6
1	E	133	ALA	3.6
1	E	236	TYR	3.6
1	F	325	ASP	3.5
1	A	190	ILE	3.5
1	D	322	LYS	3.5
1	E	309	LYS	3.5
1	F	326	TYR	3.5
1	B	50	ASN	3.5
1	F	73	SER	3.5
1	A	103	ILE	3.5
1	C	189	PHE	3.5
1	F	162	MET	3.5
1	F	34	PRO	3.5
1	A	319	GLU	3.5
1	B	34	PRO	3.5
1	B	329	ARG	3.5
1	C	321	GLN	3.5
1	B	45	ASN	3.5
1	B	314	THR	3.5
1	A	315	GLY	3.5
1	C	67	PHE	3.4
1	F	74	ASP	3.4
1	F	64	PRO	3.4
1	B	160	VAL	3.4
1	B	155	TYR	3.4
1	C	186	TYR	3.4
1	F	186	TYR	3.4
1	D	348	ALA	3.4
1	E	69	PRO	3.4
1	E	162	MET	3.4
1	C	150	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	155	TYR	3.4
1	A	188	GLY	3.4
1	E	187	LEU	3.4
1	A	211	LYS	3.4
1	F	323	ALA	3.4
1	F	259	MET	3.4
1	F	216	ILE	3.4
1	D	31	SER	3.4
1	D	346	LYS	3.4
1	E	312	LYS	3.4
1	F	100	GLY	3.3
1	C	263	ILE	3.3
1	F	222	CYS	3.3
1	A	160	VAL	3.3
1	E	116	ASN	3.3
1	B	253	LEU	3.3
1	D	29	THR	3.3
1	E	341	ALA	3.3
1	B	346	LYS	3.3
1	A	172	LEU	3.3
1	D	335	ARG	3.3
1	B	321	GLN	3.3
1	B	103	ILE	3.3
1	C	341	ALA	3.3
1	C	217[A]	LYS	3.3
1	E	249	ASP	3.3
1	C	306	GLY	3.3
1	D	259	MET	3.3
1	E	24	VAL	3.3
1	A	54	HIS	3.2
1	B	120	GLY	3.2
1	E	39	ILE	3.2
1	E	38	GLU	3.2
1	A	136	THR	3.2
1	C	19	MET	3.2
1	F	342	GLN	3.2
1	A	94	TYR	3.2
1	A	180	ARG	3.2
1	B	282	PHE	3.2
1	E	212	GLU	3.2
1	A	176	GLY	3.2
1	A	170	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	260	ARG	3.2
1	B	306	GLY	3.2
1	C	66	ASP	3.2
1	B	342	GLN	3.2
1	C	79	GLN	3.2
1	C	94	TYR	3.2
1	C	169	ILE	3.2
1	E	334	ILE	3.2
1	E	333	ARG	3.2
1	E	121	VAL	3.2
1	A	337	LEU	3.2
1	E	190	ILE	3.2
1	E	347	GLU	3.2
1	C	221	ILE	3.1
1	C	152	LYS	3.1
1	E	332	PRO	3.1
1	E	329	ARG	3.1
1	A	168	THR	3.1
1	A	23	GLU	3.1
1	A	18	PHE	3.1
1	E	29	THR	3.1
1	A	347	GLU	3.1
1	E	263	ILE	3.1
1	C	166	GLU	3.1
1	C	61	CYS	3.1
1	A	191	TYR	3.1
1	F	338	GLU	3.1
1	B	100	GLY	3.1
1	B	126	GLY	3.1
1	A	25	HIS	3.1
1	C	42	SER	3.1
1	F	69	PRO	3.1
1	F	319	GLU	3.1
1	C	22	ARG	3.1
1	A	27	GLN	3.0
1	C	164	GLN	3.0
1	C	246	ILE	3.0
1	C	191	TYR	3.0
1	B	245	GLU	3.0
1	A	310	VAL	3.0
1	C	167	LYS	3.0
1	A	186	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	308	TRP	3.0
1	A	335	ARG	3.0
1	C	71	PRO	3.0
1	A	73	SER	3.0
1	E	239	ILE	3.0
1	F	336	ARG	3.0
1	B	318	ALA	3.0
1	B	38	GLU	3.0
1	E	259	MET	3.0
1	B	95	PHE	3.0
1	A	348	ALA	3.0
1	B	248	PRO	3.0
1	D	316	LEU	3.0
1	C	335	ARG	3.0
1	C	37	ILE	2.9
1	A	187	LEU	2.9
1	B	158	GLY	2.9
1	D	319	GLU	2.9
1	B	56	LYS	2.9
1	F	312	LYS	2.9
1	B	134	ILE	2.9
1	D	45	ASN	2.9
1	E	316	LEU	2.9
1	E	292	TYR	2.9
1	A	22	ARG	2.9
1	F	35	GLN	2.9
1	C	62	TRP	2.9
1	A	100	GLY	2.9
1	A	29	THR	2.9
1	A	117	THR	2.9
1	B	340	ARG	2.9
1	C	168	THR	2.9
1	C	27	GLN	2.9
1	D	54	HIS	2.9
1	B	259	MET	2.9
1	F	317	SER	2.9
1	A	37	ILE	2.9
1	B	90	ILE	2.9
1	C	38	GLU	2.9
1	F	248	PRO	2.9
1	C	253	LEU	2.9
1	F	27	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	87	ALA	2.9
1	E	45	ASN	2.8
1	F	243	LEU	2.8
1	A	151	ASN	2.8
1	F	304	LEU	2.8
1	C	148	ASP	2.8
1	C	355	TRP	2.8
1	E	122	ARG	2.8
1	E	321	GLN	2.8
1	B	37	ILE	2.8
1	B	244	PHE	2.8
1	D	212	GLU	2.8
1	C	323	ALA	2.8
1	E	166	GLU	2.8
1	E	163	ARG	2.8
1	A	69	PRO	2.8
1	E	71	PRO	2.8
1	C	95	PHE	2.8
1	C	102	MET	2.8
1	A	96	VAL	2.8
1	F	125	THR	2.8
1	F	348	ALA	2.8
1	E	74	ASP	2.8
1	F	220	GLN	2.7
1	C	222	CYS	2.7
1	A	326	TYR	2.7
1	F	75	GLY	2.7
1	F	308	TRP	2.7
1	A	325	ASP	2.7
1	E	311	ASP	2.7
1	F	339	GLU	2.7
1	C	259	MET	2.7
1	E	102	MET	2.7
1	C	256	ALA	2.7
1	A	150	LEU	2.7
1	A	162	MET	2.7
1	F	20	PRO	2.7
1	F	97	VAL	2.7
1	E	348	ALA	2.7
1	F	260	ARG	2.7
1	C	73	SER	2.7
1	B	308	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	355	TRP	2.7
1	A	38	GLU	2.7
1	B	102	MET	2.7
1	E	343	GLY	2.7
1	F	247	ASP	2.7
1	C	157	SER	2.7
1	A	169	ILE	2.7
1	A	21	PRO	2.7
1	C	139	TRP	2.7
1	B	166	GLU	2.6
1	F	282	PHE	2.6
1	C	326	TYR	2.6
1	A	163	ARG	2.6
1	A	333	ARG	2.6
1	E	314	THR	2.6
1	B	363	LEU	2.6
1	A	249	ASP	2.6
1	A	113	THR	2.6
1	C	303	PHE	2.6
1	F	217	LYS	2.6
1	A	166	GLU	2.6
1	A	291	VAL	2.6
1	A	74	ASP	2.6
1	E	98	LEU	2.6
1	E	137	ARG	2.6
1	E	331	PRO	2.6
1	E	335	ARG	2.6
1	E	164	GLN	2.6
1	B	356	ILE	2.6
1	C	165	ILE	2.6
1	D	38	GLU	2.6
1	B	324	GLN	2.6
1	F	328	CYS	2.6
1	B	133	ALA	2.6
1	C	64	PRO	2.6
1	F	129	PRO	2.6
1	A	45	ASN	2.6
1	E	165	ILE	2.5
1	E	342	GLN	2.5
1	F	70	ASP	2.5
1	A	253	LEU	2.5
1	C	149	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	55	LEU	2.5
1	F	43	LEU	2.5
1	E	319	GLU	2.5
1	F	18	PHE	2.5
1	A	33	PRO	2.5
1	A	109	PRO	2.5
1	E	115	LEU	2.5
1	E	313	LEU	2.5
1	B	54	HIS	2.5
1	E	242	LYS	2.5
1	F	254	ALA	2.5
1	E	96	VAL	2.5
1	A	147	GLY	2.5
1	A	258	MET	2.5
1	D	19	MET	2.5
1	A	212	GLU	2.5
1	C	138	ALA	2.5
1	E	346	LYS	2.5
1	D	99	VAL	2.5
1	A	303	PHE	2.5
1	C	65	GLN	2.5
1	C	175	SER	2.5
1	F	65	GLN	2.5
1	C	260	ARG	2.5
1	F	245	GLU	2.5
1	E	32	MET	2.5
1	A	72	ALA	2.5
1	B	323	ALA	2.5
1	E	118	LEU	2.5
1	F	80	VAL	2.5
1	F	150	LEU	2.5
1	A	64	PRO	2.5
1	E	181	THR	2.5
1	C	187	LEU	2.4
1	B	285	VAL	2.4
1	B	310	VAL	2.4
1	F	49	GLU	2.4
1	E	168	THR	2.4
1	E	251	THR	2.4
1	F	350	THR	2.4
1	C	118	LEU	2.4
1	C	171	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	339	GLU	2.4
1	F	161	ASP	2.4
1	C	176	GLY	2.4
1	C	185	PRO	2.4
1	D	22	ARG	2.4
1	B	47	ALA	2.4
1	E	125	THR	2.4
1	A	269	LEU	2.4
1	C	103	ILE	2.4
1	F	321	GLN	2.4
1	A	20	PRO	2.4
1	A	331	PRO	2.4
1	E	33	PRO	2.4
1	E	141	ALA	2.4
1	E	144	ASN	2.4
1	E	246	ILE	2.4
1	E	34	PRO	2.4
1	E	132	TRP	2.4
1	C	330	LEU	2.4
1	A	356	ILE	2.4
1	B	169	ILE	2.4
1	B	171	TYR	2.4
1	C	76	PHE	2.4
1	F	79	GLN	2.4
1	B	151	ASN	2.4
1	F	53	VAL	2.4
1	A	152	LYS	2.4
1	C	322	LYS	2.4
1	C	190	ILE	2.4
1	C	111	TYR	2.4
1	D	44	ASP	2.4
1	E	256	ALA	2.4
1	C	63	GLN	2.4
1	E	65	GLN	2.4
1	B	362	LYS	2.3
1	B	213	HIS	2.3
1	C	21	PRO	2.3
1	F	246	ILE	2.3
1	C	23	GLU	2.3
1	F	47	ALA	2.3
1	E	113	THR	2.3
1	B	121	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	58	VAL	2.3
1	E	160	VAL	2.3
1	B	71	PRO	2.3
1	F	249	ASP	2.3
1	B	334	ILE	2.3
1	E	177	MET	2.3
1	A	322	LYS	2.3
1	B	167	LYS	2.3
1	C	193	SER	2.3
1	E	290	GLY	2.3
1	F	335	ARG	2.3
1	F	178	ASP	2.3
1	A	71	PRO	2.3
1	E	70	ASP	2.3
1	E	170	GLN	2.3
1	C	134	ILE	2.3
1	F	90	ILE	2.3
1	E	75	GLY	2.3
1	E	188	GLY	2.3
1	E	306	GLY	2.3
1	A	68	LEU	2.3
1	A	98	LEU	2.3
1	E	52	LEU	2.3
1	D	213	HIS	2.3
1	E	213	HIS	2.3
1	F	151	ASN	2.3
1	F	315	GLY	2.3
1	C	141	ALA	2.3
1	D	323	ALA	2.3
1	E	253	LEU	2.3
1	F	187	LEU	2.3
1	B	361	VAL	2.3
1	F	22	ARG	2.3
1	B	157	SER	2.3
1	D	334	ILE	2.3
1	F	356	ILE	2.3
1	A	149	LEU	2.3
1	C	172	LEU	2.3
1	C	178	ASP	2.2
1	E	169	ILE	2.2
1	F	219	ALA	2.2
1	B	312	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	297	TYR	2.2
1	C	188	GLY	2.2
1	B	252	VAL	2.2
1	D	26	VAL	2.2
1	A	175	SER	2.2
1	A	263	ILE	2.2
1	A	267	ALA	2.2
1	E	26	VAL	2.2
1	B	260	ARG	2.2
1	A	65	GLN	2.2
1	A	214	GLY	2.2
1	E	326	TYR	2.2
1	C	96	VAL	2.2
1	C	163	ARG	2.2
1	C	180	ARG	2.2
1	C	194	PHE	2.2
1	A	34	PRO	2.2
1	D	306	GLY	2.2
1	B	163	ARG	2.2
1	A	157	SER	2.2
1	A	115	LEU	2.2
1	C	218	LEU	2.2
1	E	328	CYS	2.2
1	F	62	TRP	2.2
1	A	251	THR	2.2
1	B	221	ILE	2.2
1	C	147	GLY	2.2
1	C	261	LYS	2.1
1	F	157	SER	2.2
1	B	26	VAL	2.1
1	F	147	GLY	2.1
1	C	243	LEU	2.1
1	D	312	LYS	2.1
1	A	171	TYR	2.1
1	C	334	ILE	2.1
1	F	103	ILE	2.1
1	F	349	PRO	2.1
1	B	357	PHE	2.1
1	C	255	PHE	2.1
1	E	150	LEU	2.1
1	B	339	GLU	2.1
1	E	158	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	63	GLN	2.1
1	F	33	PRO	2.1
1	B	243	LEU	2.1
1	E	73	SER	2.1
1	B	92	ASP	2.1
1	B	215	ASP	2.1
1	E	151	ASN	2.1
1	E	176	GLY	2.1
1	E	320	GLY	2.1
1	C	324	GLN	2.1
1	D	34	PRO	2.1
1	B	18	PHE	2.1
1	B	335	ARG	2.1
1	C	161	ASP	2.1
1	F	30	HIS	2.1
1	A	259	MET	2.1
1	B	162	MET	2.1
1	E	27	GLN	2.1
1	E	112	GLN	2.1
1	E	109	PRO	2.1
1	F	305	VAL	2.1
1	E	22	ARG	2.1
1	F	134	ILE	2.1
1	E	31	SER	2.1
1	E	303	PHE	2.1
1	A	46	TRP	2.1
1	E	62	TRP	2.1
1	C	309	LYS	2.1
1	F	152	LYS	2.1
1	F	300	ILE	2.1
1	F	67	PHE	2.1
1	C	315	GLY	2.1
1	A	208	ARG	2.1
1	B	22	ARG	2.1
1	B	125	THR	2.0
1	C	240	VAL	2.0
1	D	310	VAL	2.0
1	E	192	THR	2.0
1	B	94	TYR	2.0
1	B	131	SER	2.0
1	F	264	SER	2.0
1	E	156	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	174	GLY	2.0
1	D	329	ARG	2.0
1	B	240	VAL	2.0
1	C	99	VAL	2.0
1	A	75	GLY	2.0
1	A	95	PHE	2.0
1	D	18	PHE	2.0
1	F	177	MET	2.0
1	B	72	ALA	2.0
1	C	135	TRP	2.0
1	C	254	ALA	2.0
1	C	98	LEU	2.0
1	E	95	PHE	2.0
1	F	66	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FE	F	365	1/1	0.95	0.29	2.24	23,23,23,23	0
2	FE	D	365	1/1	0.99	0.15	0.65	23,23,23,23	0
3	AZI	F	5366	3/3	0.90	0.20	0.28	2,2,4,5	0
2	FE	C	365	1/1	0.96	0.20	-0.11	23,23,23,23	0
3	AZI	C	2366	3/3	0.91	0.20	-0.12	2,2,4,6	0
2	FE	C	364	1/1	0.96	0.20	-0.17	31,31,31,31	0
2	FE	D	364	1/1	0.96	0.14	-0.20	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	AZI	D	3366	3/3	0.94	0.12	-0.62	2,2,4,6	0
2	FE	A	365	1/1	0.98	0.17	-1.09	22,22,22,22	0
3	AZI	A	366	3/3	0.94	0.15	-1.55	2,2,4,6	0
2	FE	E	364	1/1	0.98	0.15	-1.72	32,32,32,32	0
2	FE	B	364	1/1	0.97	0.13	-1.85	31,31,31,31	0
2	FE	A	364	1/1	0.97	0.15	-2.01	32,32,32,32	0
2	FE	E	365	1/1	0.93	0.16	-2.11	22,22,22,22	0
2	FE	F	364	1/1	0.97	0.13	-2.43	32,32,32,32	0
3	AZI	E	4366	3/3	0.92	0.15	-2.69	2,2,4,5	0
3	AZI	B	1366	3/3	0.94	0.12	-2.90	2,2,4,5	0
2	FE	B	365	1/1	0.98	0.11	-3.45	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.