Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:23 PM 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

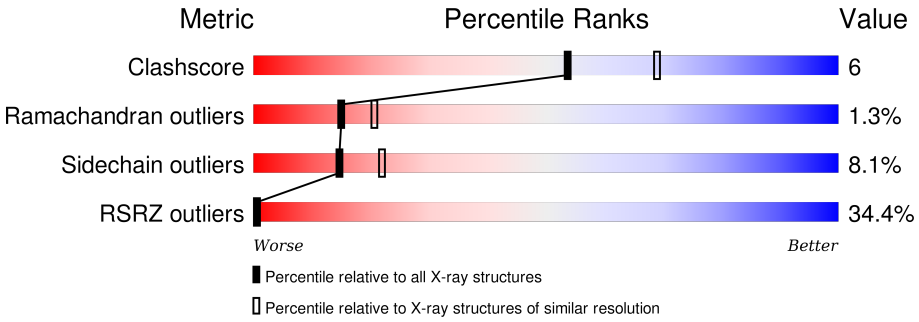
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 <=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	37% 74% 20% • 5%
1	B	363	30% 76% 17% • 5%
1	C	363	39% 74% 20% • 5%
1	D	363	14% 74% 19% • 5%
1	E	363	39% 75% 19% • 5%
1	F	363	39% 74% 20% • 5%

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.

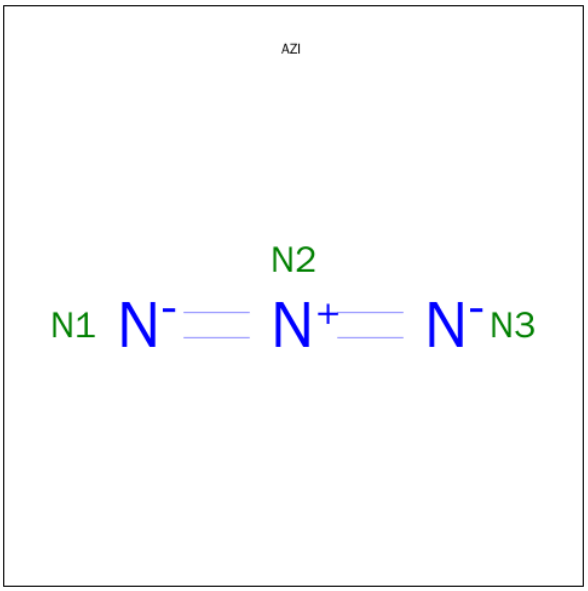
- Molecule 1 is a protein called Acyl-[acyl-carrier protein] desaturase.

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: N_3).



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.

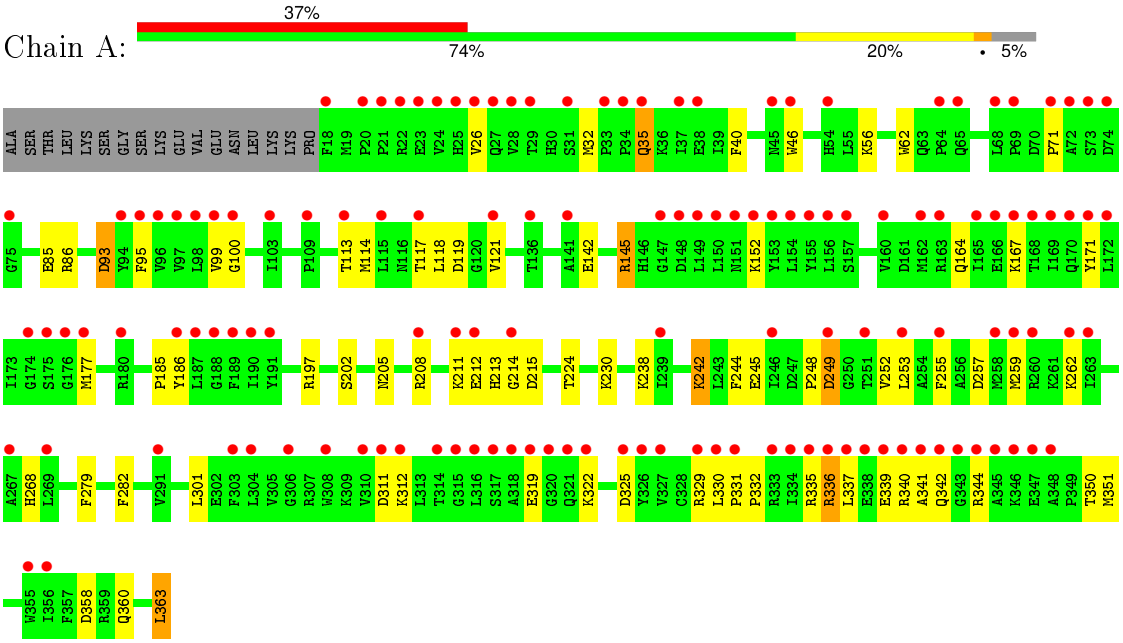
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	60	Total O 60 60	0	0
4	B	64	Total O 64 64	0	0
4	C	60	Total O 60 60	0	0
4	D	65	Total O 65 65	0	0
4	E	66	Total O 66 66	0	0
4	F	53	Total O 53 53	0	0

3 Residue-property plots (i)

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.

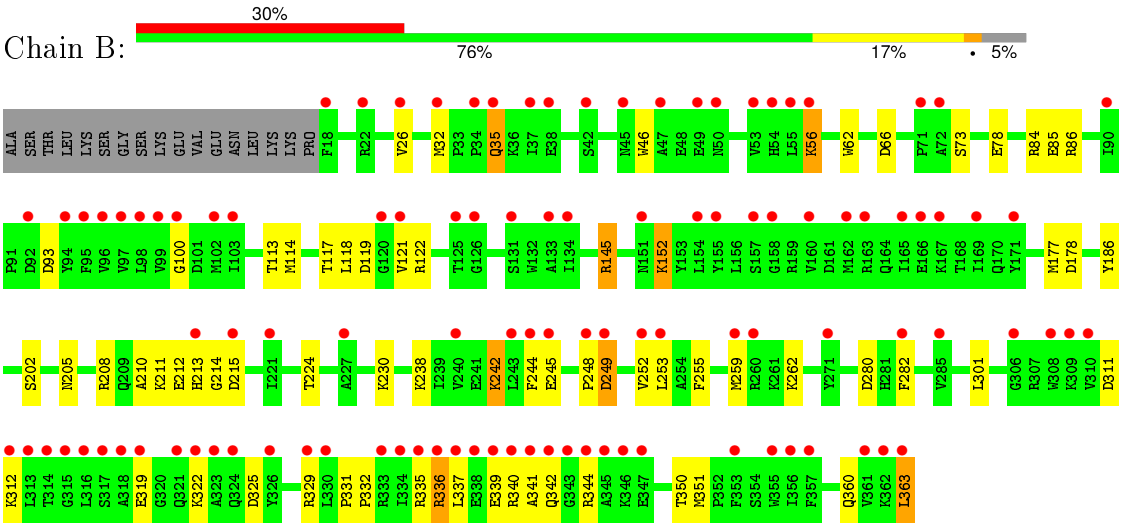
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain A:



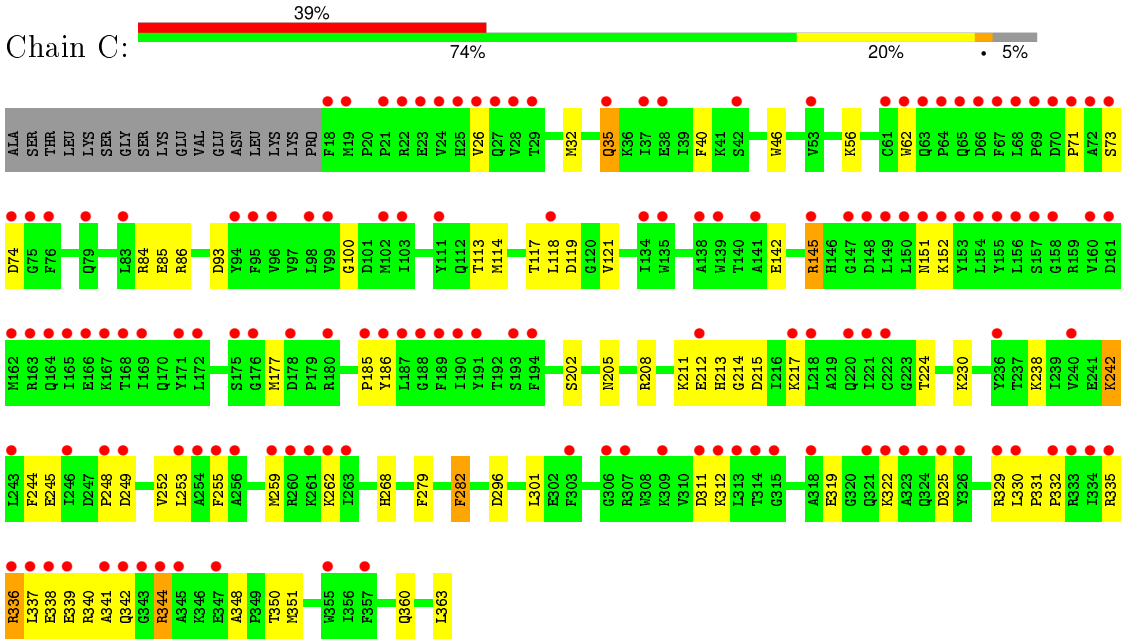
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain B:



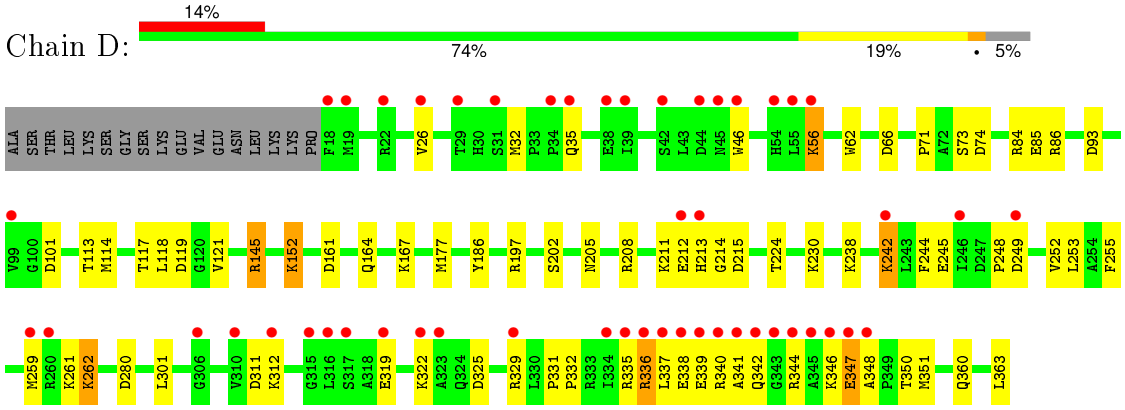
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain C:



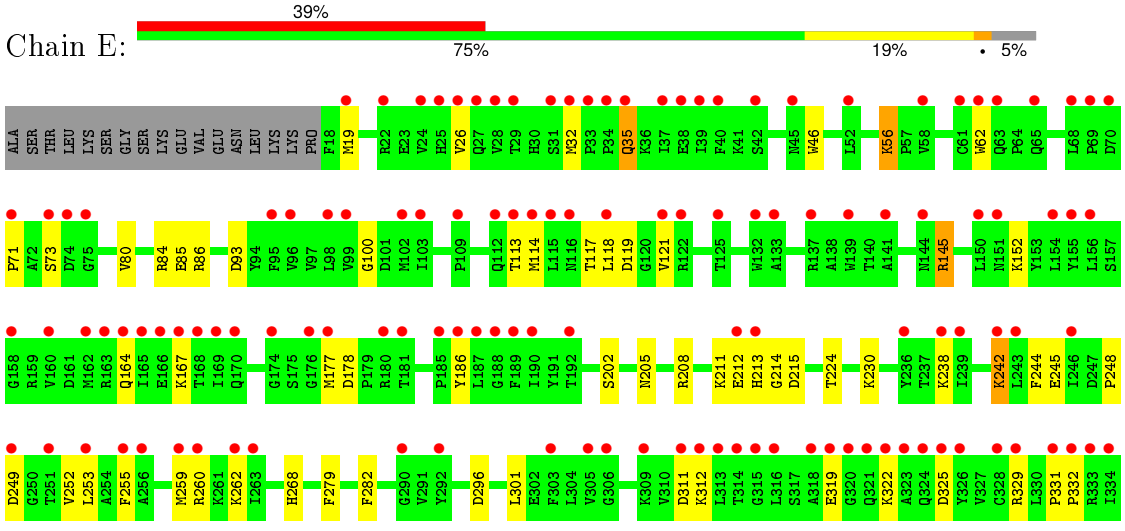
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

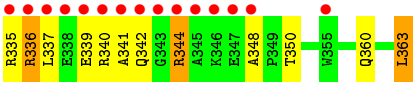
Chain D:



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

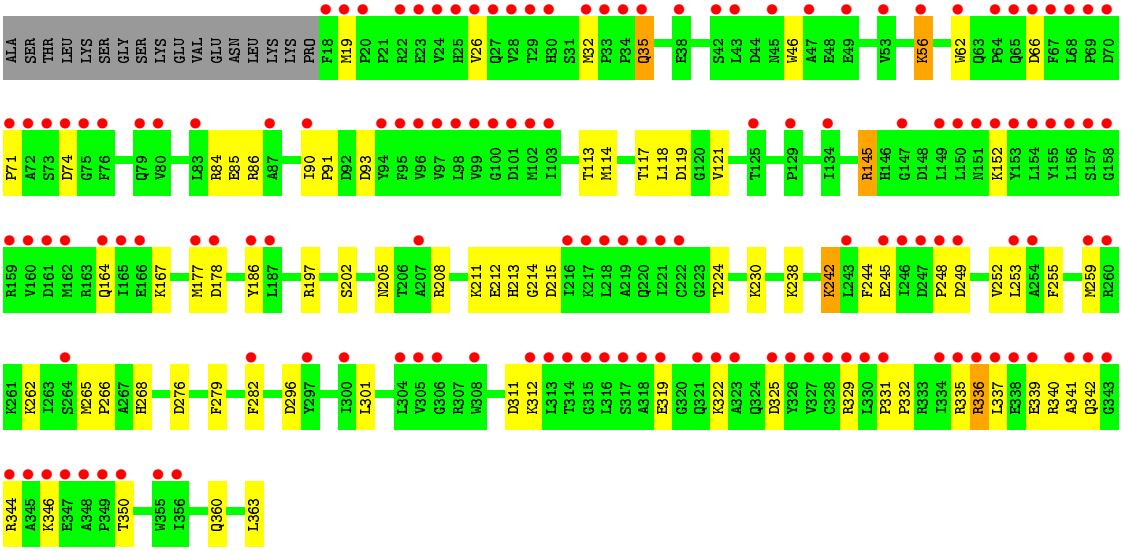
Chain E:





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

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 90115 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:F:350:THR:HG22	1:F:360:GLN:HB3	1.80	0.63
1:A:350:THR:HG22	1:A:360:GLN:HB3	1.81	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:D:339:GLU:O	1:D:341:ALA:N	2.33	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:C:331:PRO:HB2	1:C:332:PRO:HD3	1.83	0.61
1:E:339:GLU:O	1:E:341:ALA:N	2.34	0.61
1:E:259:MET:SD	1:E:301:LEU:HD22	2.41	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:F:248:PRO:O	1:F:252:VAL:HG23	2.07	0.55
1:C:248:PRO:O	1:C: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:D:255:PHE:O	1:D:259:MET:HG2	2.09	0.52
1:C:212:GLU:C	1:C:214:GLY:H	2.12	0.52
1:E:71:PRO:O	1:F:84:ARG:NH2	2.41	0.52
1:D:336:ARG:NE	1:D:336:ARG:HA	2.25	0.52
1:C:32:MET:CE	1:C:186:TYR:CD1	2.92	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:336:ARG:HA	1:B:336:ARG:NE	2.24	0.51
1:B:259:MET:SD	1:B:301:LEU:HD22	2.50	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: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:B:32:MET:CE	1:B:186:TYR:CD1	2.94	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:C:336:ARG:O	1:C:339:GLU:N	2.41	0.48
1:B:331:PRO:HB2	1:B:332:PRO:HD3	1.95	0.48
1:D:331:PRO:HB2	1:D:332:PRO:HD3	1.95	0.48
1:F:215:ASP:HB3	4:F:5423:HOH:O	2.12	0.48
1:A:35:GLN:H	1:A:35:GLN:HG3	1.42	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:C:32:MET:CE	1:C:186:TYR:HD1	2.27	0.47
1:A:118:LEU:HB2	1:A:121:VAL:CG2	2.44	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:E:46:TRP:CE2	1:E:242:LYS:HG3	2.50	0.47
1:B:118:LEU:HB2	1:B:121:VAL:CG2	2.44	0.47
1:D:215:ASP:HB3	4:D:3423:HOH:O	2.15	0.47
1:B:244:PHE:HE1	1:B:252:VAL:HG22	1.80	0.47
1:F:118:LEU:HB2	1:F:121:VAL:HG23	1.96	0.47
1:F:118:LEU:HB2	1:F:121:VAL:CG2	2.45	0.47
1:A:100:GLY:HA3	1:A:282:PHE:CE1	2.50	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:D:336:ARG:O	1:D:339:GLU:N	2.43	0.46
1:C:244:PHE:HE1	1:C:252:VAL:HG22	1.81	0.46
1:A:93:ASP:N	1:A:93:ASP:OD1	2.48	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: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:C:100:GLY:HA3	1:C:282:PHE:CE1	2.52	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:C:46:TRP:CE2	1:C:242:LYS:HG3	2.52	0.44
1:B:32:MET:CE	1:B:186:TYR:HD1	2.30	0.44
1:A:95:PHE:O	1:A:99:VAL:HG23	2.18	0.44
1:C:344:ARG:O	1:C:348:ALA:HB2	2.17	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:E:164:GLN:OE1	1:E:167:LYS:HE2	2.18	0.44
1:C:84:ARG:NH2	1:D:71:PRO:O	2.50	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:F:46:TRP:CE2	1:F:242:LYS:HG3	2.53	0.43
1:E:363:LEU:HA	1:E:363:LEU:HD12	1.89	0.43
1:C:268:HIS:HA	1:C:279:PHE:CG	2.53	0.43
1:B:56:LYS:HD2	1:B:56:LYS:HA	1.78	0.43
1:B:205:ASN:OD1	1:B:208:ARG:NH1	2.51	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: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:A:40:PHE:CZ	1:A:185:PRO:HB2	2.55	0.42
1:E:244:PHE:HE1	1:E:252:VAL:HG22	1.83	0.42
1:E:100:GLY:HA3	1:E:282:PHE:CE1	2.53	0.42
1:B:35:GLN:H	1:B:35:GLN:HG3	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: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:B:62:TRP:CD1	1:B:224:THR:HG22	2.55	0.41
1:F:32:MET:CE	1:F:186:TYR:CE1	3.03	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:268:HIS:HA	1:F:279:PHE:CG	2.55	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: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:F:90:ILE:HA	1:F:91:PRO:HD3	1.93	0.41
1:A:171:TYR:HB3	4:A:512:HOH:O	2.20	0.41
1:D:164:GLN:OE1	1:D:167:LYS:HE2	2.21	0.41
1:C:62:TRP:CD1	1:C:224:THR:HG22	2.55	0.41
1:C:40:PHE:CZ	1:C:185:PRO:HB2	2.56	0.41
1:E:212:GLU:C	1:E:214:GLY:N	2.74	0.40
1:C:32:MET:CE	1:C:186:TYR:CE1	3.04	0.40
1:F:265:MET:HA	1:F:266:PRO:HD3	1.95	0.40
1:E:80:VAL:O	1:E:84:ARG:HG3	2.21	0.40
1:D:62:TRP:CD1	1:D:224:THR:HG22	2.56	0.40
1:C:336:ARG:O	1:C:338:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:MET:HB3	1:A:330:LEU:HD22	2.02	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:D:347:GLU:O	1:D:348:ALA:C	2.60	0.40
1:B:363:LEU:HA	1:B:363:LEU:HD12	1.88	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	344/363 (95%)	328 (95%)	12 (4%)	4 (1%)	16	23
1	B	344/363 (95%)	328 (95%)	12 (4%)	4 (1%)	16	23
1	C	345/363 (95%)	329 (95%)	12 (4%)	4 (1%)	16	23
1	D	344/363 (95%)	327 (95%)	11 (3%)	6 (2%)	11	14
1	E	344/363 (95%)	325 (94%)	15 (4%)	4 (1%)	16	23
1	F	344/363 (95%)	328 (95%)	11 (3%)	5 (2%)	13	17
All	All	2065/2178 (95%)	1965 (95%)	73 (4%)	27 (1%)	15	21

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	300/315 (95%)	276 (92%)	24 (8%)	15 23
1	B	300/315 (95%)	276 (92%)	24 (8%)	15 23
1	C	301/315 (96%)	277 (92%)	24 (8%)	15 23
1	D	300/315 (95%)	276 (92%)	24 (8%)	15 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	300/315 (95%)	276 (92%)	24 (8%)	15 23
1	F	300/315 (95%)	275 (92%)	25 (8%)	14 21
All	All	1801/1890 (95%)	1656 (92%)	145 (8%)	15 22

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	346/363 (95%)	1.92	135 (39%)	0	0	5, 12, 21, 25	6 (1%)
1	B	346/363 (95%)	1.72	108 (31%)	1	1	4, 11, 21, 25	6 (1%)
1	C	346/363 (95%)	1.90	141 (40%)	0	0	4, 11, 20, 25	6 (1%)
1	D	346/363 (95%)	0.90	50 (14%)	3	3	5, 12, 21, 25	6 (1%)
1	E	346/363 (95%)	1.78	141 (40%)	0	0	5, 12, 21, 25	6 (1%)
1	F	346/363 (95%)	1.93	140 (40%)	0	0	4, 11, 21, 25	6 (1%)
All	All	2076/2178 (95%)	1.69	715 (34%)	0	0	4, 12, 21, 25	36 (1%)

All (715) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	ALA	15.4
1	D	343	GLY	15.1
1	B	345	ALA	14.6
1	A	345	ALA	14.6
1	D	342	GLN	12.8
1	D	345	ALA	12.3
1	D	344	ARG	12.1
1	D	341	ALA	11.1
1	A	344	ARG	10.9
1	F	344	ARG	10.3
1	F	343	GLY	10.2
1	B	316	LEU	9.3
1	F	345	ALA	8.9
1	A	343	GLY	8.4
1	B	344	ARG	8.1
1	B	315	GLY	7.7
1	B	337	LEU	7.5
1	A	338	GLU	7.4
1	A	329	ARG	7.1

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Mol	Chain	Res	Type	RSRZ
1	C	249	ASP	7.0
1	E	35	GLN	6.8
1	B	249	ASP	6.8
1	C	343	GLY	6.7
1	B	96	VAL	6.7
1	E	340	ARG	6.6
1	D	42	SER	6.6
1	F	330	LEU	6.5
1	A	24	VAL	6.5
1	B	338	GLU	6.5
1	F	29	THR	6.4
1	C	336	ARG	6.2
1	F	94	TYR	6.2
1	C	338	GLU	6.2
1	B	341	ALA	6.1
1	C	69	PRO	6.1
1	E	336	ARG	6.0
1	B	343	GLY	6.0
1	D	340	ARG	6.0
1	C	347	GLU	5.9
1	A	165	ILE	5.9
1	D	338	GLU	5.9
1	F	334	ILE	5.9
1	C	344	ARG	5.9
1	F	42	SER	5.8
1	A	314	THR	5.7
1	E	338	GLU	5.7
1	A	355	TRP	5.7
1	F	341	ALA	5.6
1	C	74	ASP	5.6
1	B	355	TRP	5.6
1	F	99	VAL	5.5
1	B	322	LYS	5.5
1	F	322	LYS	5.5
1	F	160	VAL	5.5
1	C	18	PHE	5.5
1	F	26	VAL	5.4
1	C	325	ASP	5.4
1	B	42	SER	5.3
1	C	342	GLN	5.3
1	C	26	VAL	5.2
1	B	336	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	329	ARG	5.2
1	E	42	SER	5.1
1	C	35	GLN	5.1
1	B	313	LEU	5.1
1	A	320	GLY	5.1
1	C	314	THR	5.1
1	C	318	ALA	5.1
1	B	53	VAL	5.0
1	A	321	GLN	5.0
1	F	337	LEU	5.0
1	C	345	ALA	5.0
1	D	315	GLY	5.0
1	C	68	LEU	5.0
1	A	339	GLU	5.0
1	B	330	LEU	4.9
1	D	249	ASP	4.9
1	F	346	LYS	4.9
1	B	99	VAL	4.9
1	A	327	VAL	4.8
1	C	75	GLY	4.8
1	E	344	ARG	4.8
1	E	322	LYS	4.8
1	E	345	ALA	4.8
1	F	96	VAL	4.8
1	A	342	GLN	4.8
1	A	35	GLN	4.8
1	F	28	VAL	4.8
1	D	347	GLU	4.8
1	F	316	LEU	4.7
1	C	28	VAL	4.7
1	A	311	ASP	4.7
1	B	165	ILE	4.6
1	F	154	LEU	4.6
1	F	165	ILE	4.6
1	F	218	LEU	4.6
1	C	72	ALA	4.6
1	A	28	VAL	4.6
1	F	331	PRO	4.6
1	E	318	ALA	4.6
1	B	35	GLN	4.6
1	F	306	GLY	4.6
1	C	70	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	318	ALA	4.6
1	C	312	LYS	4.6
1	C	155	TYR	4.5
1	E	189	PHE	4.5
1	A	99	VAL	4.5
1	A	330	LEU	4.5
1	B	317	SER	4.5
1	F	95	PHE	4.5
1	C	262	LYS	4.5
1	F	98	LEU	4.5
1	C	162	MET	4.4
1	E	315	GLY	4.4
1	A	260	ARG	4.4
1	B	326	TYR	4.4
1	F	71	PRO	4.3
1	F	253	LEU	4.3
1	F	313	LEU	4.3
1	A	155	TYR	4.3
1	F	23	GLU	4.3
1	F	329	ARG	4.3
1	F	32	MET	4.3
1	F	68	LEU	4.3
1	D	336	ARG	4.3
1	D	35	GLN	4.2
1	F	83	LEU	4.2
1	B	97	VAL	4.2
1	F	38	GLU	4.2
1	A	26	VAL	4.2
1	F	156	LEU	4.2
1	E	155	TYR	4.2
1	E	25	HIS	4.2
1	F	24	VAL	4.2
1	E	186	TYR	4.2
1	C	25	HIS	4.2
1	C	311	ASP	4.2
1	A	177	MET	4.1
1	F	347	GLU	4.1
1	A	336	ARG	4.1
1	C	248	PRO	4.1
1	A	346	LYS	4.1
1	F	45	ASN	4.1
1	D	339	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	154	LEU	4.1
1	E	262	LYS	4.1
1	F	153	TYR	4.1
1	C	29	THR	4.1
1	F	72	ALA	4.1
1	F	25	HIS	4.0
1	A	121	VAL	4.0
1	F	221	ILE	4.0
1	C	313	LEU	4.0
1	E	323	ALA	4.0
1	C	156	LEU	4.0
1	E	40	PHE	4.0
1	D	337	LEU	4.0
1	F	314	THR	4.0
1	E	37	ILE	4.0
1	F	76	PHE	4.0
1	A	316	LEU	4.0
1	C	160	VAL	4.0
1	E	154	LEU	4.0
1	E	337	LEU	4.0
1	F	318	ALA	3.9
1	B	49	GLU	3.9
1	E	68	LEU	3.9
1	B	347	GLU	3.9
1	A	334	ILE	3.9
1	E	19	MET	3.9
1	A	246	ILE	3.9
1	E	61	CYS	3.9
1	A	262	LYS	3.9
1	E	99	VAL	3.9
1	E	238	LYS	3.9
1	B	319	GLU	3.9
1	F	355	TRP	3.9
1	A	154	LEU	3.9
1	C	158	GLY	3.8
1	B	154	LEU	3.8
1	D	39	ILE	3.8
1	A	340	ARG	3.8
1	B	98	LEU	3.8
1	A	312	LYS	3.8
1	F	19	MET	3.8
1	C	212	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	325	ASP	3.8
1	E	28	VAL	3.8
1	E	180	ARG	3.8
1	B	55	LEU	3.8
1	C	24	VAL	3.8
1	C	337	LEU	3.8
1	C	339	GLU	3.8
1	E	133	ALA	3.8
1	F	149	LEU	3.8
1	B	309	LYS	3.7
1	F	325	ASP	3.7
1	B	333	ARG	3.7
1	C	153	TYR	3.7
1	A	190	ILE	3.7
1	F	162	MET	3.7
1	E	236	TYR	3.7
1	B	34	PRO	3.7
1	F	34	PRO	3.7
1	A	103	ILE	3.7
1	B	50	ASN	3.7
1	F	326	TYR	3.7
1	D	322	LYS	3.7
1	E	309	LYS	3.7
1	A	315	GLY	3.6
1	F	73	SER	3.6
1	B	314	THR	3.6
1	C	189	PHE	3.6
1	F	74	ASP	3.6
1	F	64	PRO	3.6
1	A	319	GLU	3.6
1	B	45	ASN	3.6
1	C	321	GLN	3.6
1	B	160	VAL	3.6
1	B	329	ARG	3.6
1	E	162	MET	3.6
1	E	69	PRO	3.6
1	D	348	ALA	3.6
1	C	67	PHE	3.6
1	F	259	MET	3.6
1	A	188	GLY	3.6
1	F	323	ALA	3.6
1	B	155	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	150	LEU	3.6
1	C	186	TYR	3.6
1	F	100	GLY	3.5
1	E	187	LEU	3.5
1	F	222	CYS	3.5
1	F	155	TYR	3.5
1	F	186	TYR	3.5
1	A	160	VAL	3.5
1	F	216	ILE	3.5
1	E	341	ALA	3.5
1	C	263	ILE	3.5
1	A	211	LYS	3.5
1	D	31	SER	3.5
1	D	29	THR	3.5
1	B	253	LEU	3.5
1	E	116	ASN	3.5
1	C	341	ALA	3.5
1	D	346	LYS	3.5
1	E	312	LYS	3.5
1	A	172	LEU	3.5
1	D	259	MET	3.5
1	B	103	ILE	3.5
1	E	249	ASP	3.5
1	B	321	GLN	3.4
1	C	306	GLY	3.4
1	D	335	ARG	3.4
1	B	346	LYS	3.4
1	E	24	VAL	3.4
1	B	120	GLY	3.4
1	C	19	MET	3.4
1	C	217[A]	LYS	3.4
1	E	39	ILE	3.4
1	A	136	THR	3.4
1	A	176	GLY	3.4
1	B	306	GLY	3.4
1	A	54	HIS	3.4
1	E	38	GLU	3.4
1	A	94	TYR	3.4
1	C	66	ASP	3.4
1	F	342	GLN	3.4
1	A	180	ARG	3.4
1	E	121	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	212	GLU	3.3
1	B	282	PHE	3.3
1	A	170	GLN	3.3
1	C	169	ILE	3.3
1	E	334	ILE	3.3
1	E	260	ARG	3.3
1	E	332	PRO	3.3
1	B	342	GLN	3.3
1	C	79	GLN	3.3
1	A	337	LEU	3.3
1	C	94	TYR	3.3
1	E	190	ILE	3.3
1	E	333	ARG	3.3
1	C	221	ILE	3.3
1	A	168	THR	3.3
1	E	347	GLU	3.3
1	E	329	ARG	3.3
1	C	61	CYS	3.3
1	B	126	GLY	3.3
1	E	29	THR	3.3
1	C	152	LYS	3.3
1	A	23	GLU	3.3
1	B	100	GLY	3.2
1	E	263	ILE	3.2
1	F	69	PRO	3.2
1	A	18	PHE	3.2
1	A	347	GLU	3.2
1	C	166	GLU	3.2
1	A	310	VAL	3.2
1	A	191	TYR	3.2
1	F	338	GLU	3.2
1	A	25	HIS	3.2
1	C	42	SER	3.2
1	C	246	ILE	3.2
1	C	71	PRO	3.2
1	F	319	GLU	3.2
1	C	22	ARG	3.2
1	A	27	GLN	3.2
1	C	191	TYR	3.2
1	B	245	GLU	3.2
1	C	164	GLN	3.2
1	E	259	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	318	ALA	3.2
1	A	186	TYR	3.2
1	A	308	TRP	3.2
1	A	335	ARG	3.1
1	B	248	PRO	3.1
1	C	167	LYS	3.1
1	E	239	ILE	3.1
1	A	348	ALA	3.1
1	A	73	SER	3.1
1	F	336	ARG	3.1
1	B	38	GLU	3.1
1	B	158	GLY	3.1
1	B	95	PHE	3.1
1	D	316	LEU	3.1
1	C	37	ILE	3.1
1	A	187	LEU	3.1
1	B	134	ILE	3.1
1	A	100	GLY	3.1
1	C	335	ARG	3.1
1	D	319	GLU	3.1
1	B	259	MET	3.0
1	E	316	LEU	3.0
1	A	29	THR	3.0
1	B	56	LYS	3.0
1	F	312	LYS	3.0
1	D	45	ASN	3.0
1	F	248	PRO	3.0
1	E	292	TYR	3.0
1	F	35	GLN	3.0
1	A	22	ARG	3.0
1	A	117	THR	3.0
1	C	168	THR	3.0
1	F	87	ALA	3.0
1	C	62	TRP	3.0
1	B	340	ARG	3.0
1	A	37	ILE	3.0
1	B	90	ILE	3.0
1	C	27	GLN	3.0
1	D	54	HIS	3.0
1	C	253	LEU	3.0
1	F	317	SER	3.0
1	C	38	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	148	ASP	3.0
1	F	27	GLN	3.0
1	E	45	ASN	3.0
1	F	243	LEU	3.0
1	C	323	ALA	3.0
1	A	151	ASN	3.0
1	F	304	LEU	3.0
1	B	37	ILE	3.0
1	A	69	PRO	3.0
1	E	71	PRO	3.0
1	C	102	MET	2.9
1	E	122	ARG	2.9
1	E	321	GLN	2.9
1	C	355	TRP	2.9
1	D	212	GLU	2.9
1	A	96	VAL	2.9
1	B	244	PHE	2.9
1	E	166	GLU	2.9
1	F	348	ALA	2.9
1	C	222	CYS	2.9
1	E	163	ARG	2.9
1	C	259	MET	2.9
1	E	74	ASP	2.9
1	E	102	MET	2.9
1	E	311	ASP	2.9
1	F	75	GLY	2.9
1	F	125	THR	2.9
1	A	325	ASP	2.9
1	A	162	MET	2.9
1	C	95	PHE	2.9
1	C	256	ALA	2.9
1	F	20	PRO	2.9
1	F	97	VAL	2.9
1	F	220	GLN	2.9
1	E	348	ALA	2.9
1	A	326	TYR	2.9
1	F	308	TRP	2.9
1	A	150	LEU	2.9
1	B	102	MET	2.9
1	F	339	GLU	2.9
1	E	343	GLY	2.9
1	F	247	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	21	PRO	2.8
1	F	260	ARG	2.8
1	A	169	ILE	2.8
1	C	73	SER	2.8
1	A	38	GLU	2.8
1	B	308	TRP	2.8
1	E	355	TRP	2.8
1	C	157	SER	2.8
1	A	249	ASP	2.8
1	E	314	THR	2.8
1	B	166	GLU	2.8
1	C	139	TRP	2.8
1	B	363	LEU	2.8
1	A	113	THR	2.8
1	A	291	VAL	2.8
1	C	326	TYR	2.8
1	F	282	PHE	2.8
1	E	331	PRO	2.8
1	A	163	ARG	2.8
1	A	333	ARG	2.8
1	A	74	ASP	2.8
1	F	328	CYS	2.7
1	E	98	LEU	2.7
1	C	64	PRO	2.7
1	C	303	PHE	2.7
1	A	166	GLU	2.7
1	B	133	ALA	2.7
1	B	356	ILE	2.7
1	C	165	ILE	2.7
1	F	217	LYS	2.7
1	E	137	ARG	2.7
1	E	335	ARG	2.7
1	E	164	GLN	2.7
1	F	129	PRO	2.7
1	D	38	GLU	2.7
1	F	70	ASP	2.7
1	B	324	GLN	2.7
1	A	45	ASN	2.7
1	E	165	ILE	2.7
1	A	33	PRO	2.7
1	A	109	PRO	2.7
1	E	342	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	253	LEU	2.7
1	C	149	LEU	2.7
1	D	55	LEU	2.7
1	F	43	LEU	2.7
1	A	258	MET	2.7
1	D	19	MET	2.7
1	E	96	VAL	2.7
1	A	147	GLY	2.7
1	F	254	ALA	2.7
1	E	319	GLU	2.6
1	E	115	LEU	2.6
1	E	313	LEU	2.6
1	E	32	MET	2.6
1	C	138	ALA	2.6
1	D	99	VAL	2.6
1	F	18	PHE	2.6
1	B	54	HIS	2.6
1	A	72	ALA	2.6
1	B	323	ALA	2.6
1	F	80	VAL	2.6
1	E	242	LYS	2.6
1	A	64	PRO	2.6
1	A	212	GLU	2.6
1	B	285	VAL	2.6
1	B	310	VAL	2.6
1	C	65	GLN	2.6
1	C	175	SER	2.6
1	F	65	GLN	2.6
1	E	118	LEU	2.6
1	F	150	LEU	2.6
1	F	245	GLU	2.6
1	C	260	ARG	2.6
1	E	181	THR	2.6
1	E	346	LYS	2.6
1	A	303	PHE	2.6
1	C	176	GLY	2.6
1	C	185	PRO	2.6
1	C	187	LEU	2.6
1	F	161	ASP	2.6
1	E	168	THR	2.6
1	E	251	THR	2.6
1	F	350	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	47	ALA	2.6
1	A	20	PRO	2.6
1	A	331	PRO	2.6
1	C	118	LEU	2.6
1	E	33	PRO	2.6
1	E	125	THR	2.6
1	F	49	GLU	2.6
1	E	141	ALA	2.6
1	A	269	LEU	2.5
1	C	171	TYR	2.5
1	E	34	PRO	2.5
1	E	339	GLU	2.5
1	C	103	ILE	2.5
1	D	22	ARG	2.5
1	E	246	ILE	2.5
1	F	321	GLN	2.5
1	E	144	ASN	2.5
1	F	53	VAL	2.5
1	C	330	LEU	2.5
1	A	356	ILE	2.5
1	B	169	ILE	2.5
1	D	44	ASP	2.5
1	E	132	TRP	2.5
1	E	256	ALA	2.5
1	C	21	PRO	2.5
1	B	171	TYR	2.5
1	C	190	ILE	2.5
1	E	177	MET	2.5
1	B	151	ASN	2.5
1	F	47	ALA	2.5
1	C	76	PHE	2.5
1	F	79	GLN	2.5
1	B	121	VAL	2.5
1	E	58	VAL	2.5
1	E	160	VAL	2.5
1	B	71	PRO	2.5
1	B	213	HIS	2.5
1	F	249	ASP	2.5
1	E	113	THR	2.5
1	F	246	ILE	2.5
1	C	111	TYR	2.5
1	C	63	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	65	GLN	2.5
1	E	290	GLY	2.5
1	A	71	PRO	2.5
1	A	152	LYS	2.5
1	C	322	LYS	2.5
1	F	178	ASP	2.5
1	B	334	ILE	2.5
1	C	23	GLU	2.5
1	B	362	LYS	2.4
1	E	70	ASP	2.4
1	E	75	GLY	2.4
1	E	188	GLY	2.4
1	E	306	GLY	2.4
1	C	193	SER	2.4
1	F	335	ARG	2.4
1	A	322	LYS	2.4
1	B	167	LYS	2.4
1	F	315	GLY	2.4
1	C	134	ILE	2.4
1	F	90	ILE	2.4
1	E	170	GLN	2.4
1	B	361	VAL	2.4
1	A	68	LEU	2.4
1	A	98	LEU	2.4
1	E	52	LEU	2.4
1	C	141	ALA	2.4
1	D	323	ALA	2.4
1	D	213	HIS	2.4
1	E	213	HIS	2.4
1	F	151	ASN	2.4
1	E	253	LEU	2.4
1	F	187	LEU	2.4
1	C	178	ASP	2.4
1	D	334	ILE	2.4
1	F	356	ILE	2.4
1	F	219	ALA	2.4
1	C	188	GLY	2.4
1	A	149	LEU	2.4
1	B	252	VAL	2.4
1	C	172	LEU	2.4
1	D	26	VAL	2.4
1	F	22	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	157	SER	2.4
1	E	169	ILE	2.4
1	A	267	ALA	2.4
1	E	26	VAL	2.4
1	A	263	ILE	2.4
1	A	214	GLY	2.3
1	F	297	TYR	2.3
1	C	96	VAL	2.3
1	A	175	SER	2.3
1	B	312	LYS	2.3
1	A	34	PRO	2.3
1	D	306	GLY	2.3
1	E	328	CYS	2.3
1	B	260	ARG	2.3
1	A	65	GLN	2.3
1	E	326	TYR	2.3
1	C	163	ARG	2.3
1	C	180	ARG	2.3
1	C	147	GLY	2.3
1	C	194	PHE	2.3
1	A	115	LEU	2.3
1	A	157	SER	2.3
1	B	163	ARG	2.3
1	C	218	LEU	2.3
1	A	251	THR	2.3
1	B	26	VAL	2.3
1	F	147	GLY	2.3
1	B	221	ILE	2.3
1	F	62	TRP	2.3
1	F	349	PRO	2.3
1	F	157	SER	2.3
1	C	243	LEU	2.3
1	E	158	GLY	2.3
1	F	33	PRO	2.3
1	C	334	ILE	2.2
1	F	103	ILE	2.2
1	C	261	LYS	2.2
1	B	92	ASP	2.2
1	B	215	ASP	2.2
1	E	150	LEU	2.2
1	E	176	GLY	2.2
1	E	320	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	171	TYR	2.2
1	D	34	PRO	2.2
1	A	259	MET	2.2
1	B	162	MET	2.2
1	D	312	LYS	2.2
1	B	357	PHE	2.2
1	C	161	ASP	2.2
1	C	255	PHE	2.2
1	B	243	LEU	2.2
1	B	339	GLU	2.2
1	E	109	PRO	2.2
1	F	305	VAL	2.2
1	E	63	GLN	2.2
1	E	73	SER	2.2
1	E	151	ASN	2.2
1	C	324	GLN	2.2
1	B	335	ARG	2.2
1	E	22	ARG	2.2
1	E	31	SER	2.2
1	F	30	HIS	2.2
1	F	134	ILE	2.2
1	C	315	GLY	2.2
1	B	18	PHE	2.2
1	E	27	GLN	2.2
1	E	112	GLN	2.2
1	C	240	VAL	2.2
1	D	310	VAL	2.2
1	E	174	GLY	2.2
1	F	300	ILE	2.2
1	A	46	TRP	2.2
1	E	62	TRP	2.2
1	E	303	PHE	2.2
1	B	125	THR	2.2
1	E	192	THR	2.2
1	B	240	VAL	2.2
1	C	99	VAL	2.2
1	A	75	GLY	2.2
1	F	177	MET	2.2
1	F	67	PHE	2.2
1	E	156	LEU	2.2
1	A	208	ARG	2.2
1	B	22	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	152	LYS	2.2
1	B	72	ALA	2.1
1	B	94	TYR	2.1
1	B	131	SER	2.1
1	C	254	ALA	2.1
1	F	264	SER	2.1
1	C	309	LYS	2.1
1	D	329	ARG	2.1
1	F	66	ASP	2.1
1	F	327	VAL	2.1
1	C	98	LEU	2.1
1	D	18	PHE	2.1
1	E	185	PRO	2.1
1	C	135	TRP	2.1
1	E	114	MET	2.1
1	F	102	MET	2.1
1	A	95	PHE	2.1
1	E	95	PHE	2.1
1	A	306	GLY	2.1
1	D	46	TRP	2.1
1	A	148	ASP	2.1
1	C	220	GLN	2.1
1	A	156	LEU	2.1
1	C	357	PHE	2.1
1	C	307	ARG	2.1
1	C	53	VAL	2.1
1	E	324	GLN	2.1
1	A	304	LEU	2.1
1	E	243	LEU	2.1
1	F	166	GLU	2.1
1	A	317	SER	2.1
1	B	227	ALA	2.1
1	A	97	VAL	2.1
1	C	151	ASN	2.1
1	C	333	ARG	2.1
1	A	153	TYR	2.1
1	A	174	GLY	2.1
1	A	255	PHE	2.1
1	B	353	PHE	2.1
1	A	31	SER	2.1
1	D	317	SER	2.1
1	F	101	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	141	ALA	2.0
1	F	159	ARG	2.0
1	A	239	ILE	2.0
1	D	246	ILE	2.0
1	F	56	LYS	2.0
1	A	189	PHE	2.0
1	C	83	LEU	2.0
1	F	164	GLN	2.0
1	F	207	ALA	2.0
1	E	167	LYS	2.0
1	E	103	ILE	2.0
1	C	332	PRO	2.0
1	E	139	TRP	2.0
1	B	271	TYR	2.0
1	C	236	TYR	2.0
1	E	255	PHE	2.0
1	C	145	ARG	2.0
1	D	260	ARG	2.0
1	D	56	LYS	2.0
1	D	242	LYS	2.0
1	B	32	MET	2.0
1	E	305	VAL	2.0
1	F	158	GLY	2.0
1	A	167	LYS	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, 95^{th} 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
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.