



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:56 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 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>

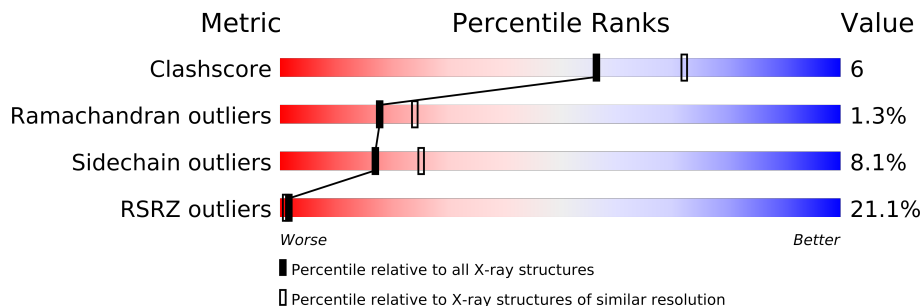
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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. 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	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	AZI	B	1366	X	X
3	AZI	C	2366	-	X
3	AZI	D	3366	X	X
3	AZI	E	4366	-	X

2 Entry composition

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

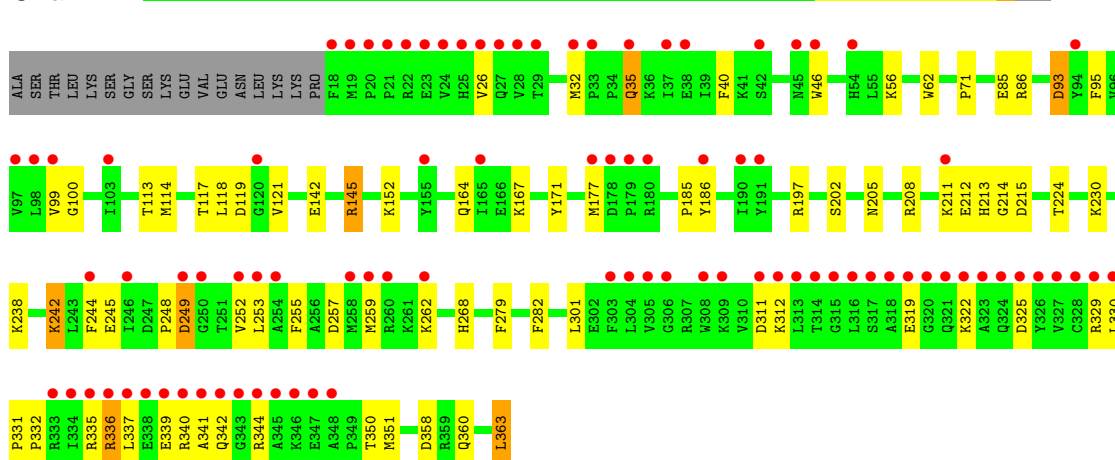
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	60	Total O 60 60	0	0
4	B	64	Total O 64 64	0	0
4	C	60	Total O 60 60	0	0
4	D	65	Total O 65 65	0	0
4	E	66	Total O 66 66	0	0
4	F	53	Total O 53 53	0	0

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 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.

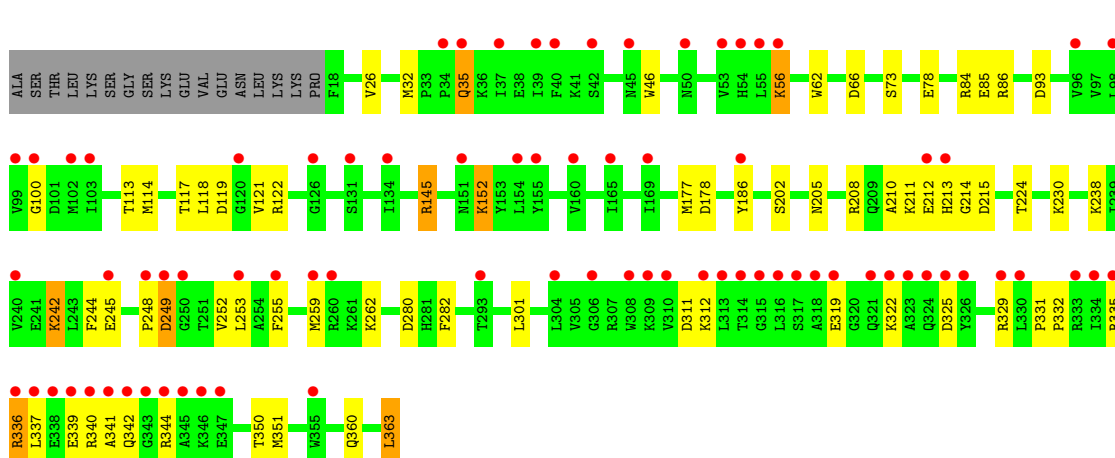
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain A:



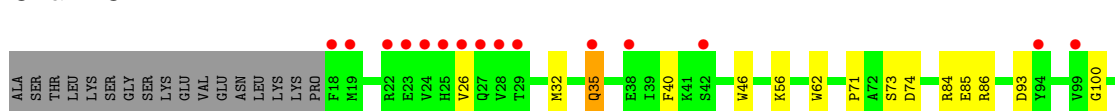
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

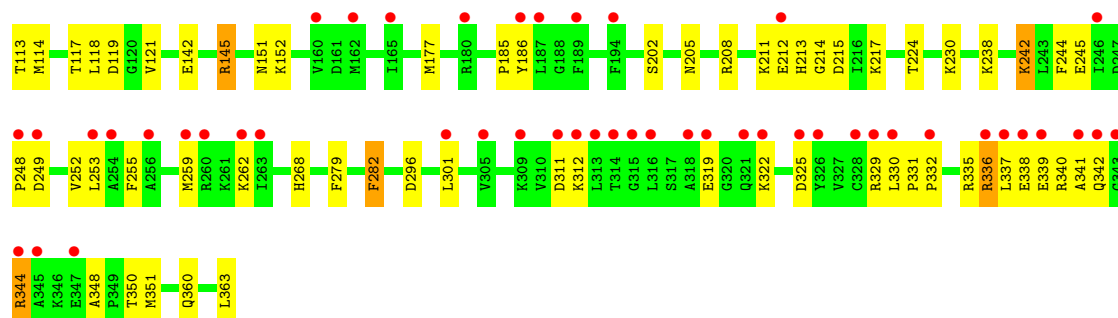
Chain B:



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

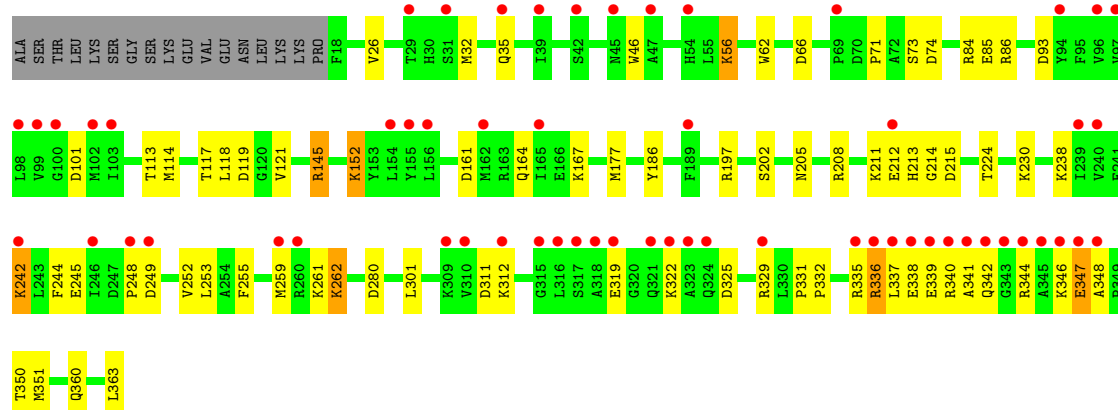
Chain C:





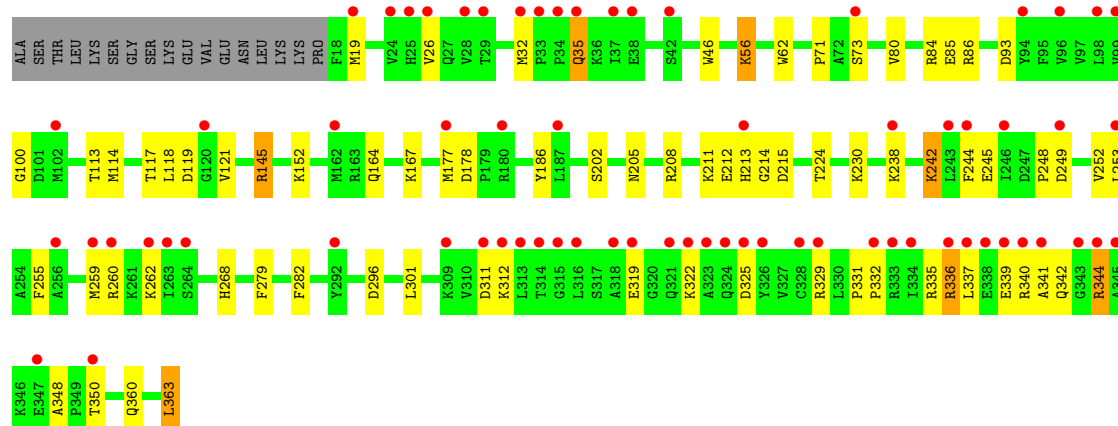
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain D:



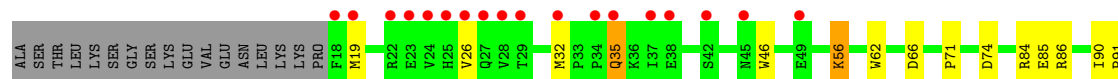
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

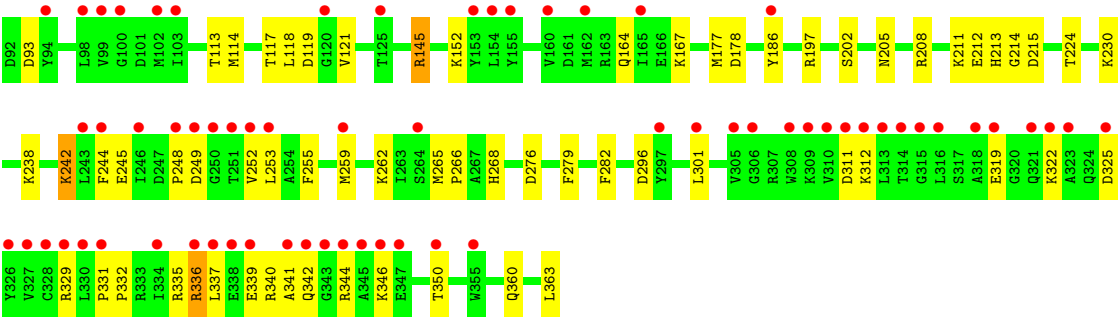
Chain E:



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

Chain F:





4 Data and refinement statistics

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)	0.31 , -4.3	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 90115 reflections	Xtriage
F_o, F_c correlation	0.86	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.

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 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	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

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 6.

All (214) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:A:46:TRP:CZ2	1:A:242:LYS:HG3	2.39	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	Distance(Å)	Clash(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%)	19	26
1	B	344/363 (95%)	328 (95%)	12 (4%)	4 (1%)	19	26
1	C	345/363 (95%)	329 (95%)	12 (4%)	4 (1%)	19	26
1	D	344/363 (95%)	327 (95%)	11 (3%)	6 (2%)	14	17
1	E	344/363 (95%)	325 (94%)	15 (4%)	4 (1%)	19	26
1	F	344/363 (95%)	328 (95%)	11 (3%)	5 (2%)	15	20
All	All	2065/2178 (95%)	1965 (95%)	73 (4%)	27 (1%)	18	24

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ARG
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

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Mol	Chain	Res	Type
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%)	17	26
1	B	300/315 (95%)	276 (92%)	24 (8%)	17	26
1	C	301/315 (96%)	277 (92%)	24 (8%)	17	26
1	D	300/315 (95%)	276 (92%)	24 (8%)	17	26
1	E	300/315 (95%)	276 (92%)	24 (8%)	17	26
1	F	300/315 (95%)	275 (92%)	25 (8%)	16	24
All	All	1801/1890 (95%)	1656 (92%)	145 (8%)	17	25

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

Mol	Chain	Res	Type
1	A	26	VAL

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 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 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	2,2,2	1.64	0	0,1,1	0.00	-
3	AZI	B	1366	2	2,2,2	2.21	2 (100%)	0,1,1	0.00	-
3	AZI	C	2366	2	2,2,2	1.92	1 (50%)	0,1,1	0.00	-
3	AZI	D	3366	2	2,2,2	2.22	2 (100%)	0,1,1	0.00	-
3	AZI	E	4366	2	2,2,2	1.91	0	0,1,1	0.00	-
3	AZI	F	5366	2	2,2,2	1.81	0	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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1366	AZI	N3-N2	-2.29	1.13	1.21
3	D	3366	AZI	N1-N2	-2.24	1.13	1.21
3	D	3366	AZI	N3-N2	-2.21	1.13	1.21
3	C	2366	AZI	N3-N2	-2.12	1.13	1.21
3	B	1366	AZI	N1-N2	-2.12	1.13	1.21

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%)	1.44	90 (26%) 1 1	5, 12, 21, 25	6 (1%)
1	B	346/363 (95%)	1.35	78 (22%) 1 1	4, 11, 21, 25	6 (1%)
1	C	346/363 (95%)	1.16	63 (18%) 2 1	4, 11, 20, 25	6 (1%)
1	D	346/363 (95%)	1.18	59 (17%) 2 1	5, 12, 21, 25	6 (1%)
1	E	346/363 (95%)	1.21	69 (19%) 2 1	5, 12, 21, 25	6 (1%)
1	F	346/363 (95%)	1.35	83 (23%) 1 1	4, 11, 21, 25	6 (1%)
All	All	2076/2178 (95%)	1.28	442 (21%) 1 1	4, 12, 21, 25	36 (1%)

All (442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	ALA	13.0
1	D	343	GLY	12.6
1	D	341	ALA	11.5
1	A	341	ALA	11.1
1	A	343	GLY	11.1
1	B	345	ALA	10.7
1	D	342	GLN	10.6
1	F	343	GLY	10.3
1	A	344	ARG	10.2
1	D	345	ALA	9.4
1	F	344	ARG	8.2
1	F	345	ALA	8.2
1	B	344	ARG	8.1
1	D	344	ARG	7.2
1	A	329	ARG	7.0
1	B	316	LEU	6.9
1	A	314	THR	6.2
1	F	341	ALA	6.2
1	C	344	ARG	6.1

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Mol	Chain	Res	Type	RSRZ
1	F	346	LYS	6.1
1	C	347	GLU	6.1
1	B	341	ALA	6.0
1	B	322	LYS	6.0
1	A	342	GLN	5.9
1	A	24	VAL	5.8
1	A	311	ASP	5.8
1	F	330	LEU	5.8
1	E	35	GLN	5.8
1	D	338	GLU	5.7
1	E	344	ARG	5.7
1	A	338	GLU	5.6
1	F	329	ARG	5.4
1	F	322	LYS	5.4
1	B	338	GLU	5.3
1	C	338	GLU	5.3
1	A	326	TYR	5.3
1	B	343	GLY	5.3
1	C	249	ASP	5.2
1	B	309	LYS	5.2
1	B	249	ASP	5.2
1	B	313	LEU	5.2
1	D	340	ARG	5.2
1	F	326	TYR	5.1
1	F	29	THR	5.1
1	A	318	ALA	5.1
1	C	343	GLY	5.1
1	B	35	GLN	5.1
1	E	340	ARG	5.1
1	E	315	GLY	5.0
1	F	253	LEU	5.0
1	F	334	ILE	5.0
1	A	346	LYS	4.9
1	D	337	LEU	4.9
1	F	338	GLU	4.8
1	B	253	LEU	4.8
1	B	42	SER	4.7
1	D	347	GLU	4.7
1	C	329	ARG	4.7
1	A	35	GLN	4.7
1	B	53	VAL	4.6
1	A	246	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	345	ALA	4.6
1	A	28	VAL	4.6
1	E	338	GLU	4.6
1	F	347	GLU	4.6
1	E	318	ALA	4.6
1	E	42	SER	4.5
1	E	323	ALA	4.5
1	F	316	LEU	4.5
1	C	337	LEU	4.5
1	B	319	GLU	4.5
1	E	322	LYS	4.5
1	B	333	ARG	4.5
1	C	94	TYR	4.4
1	E	336	ARG	4.4
1	B	315	GLY	4.4
1	C	25	HIS	4.4
1	C	18	PHE	4.3
1	A	27	GLN	4.3
1	F	314	THR	4.3
1	B	310	VAL	4.3
1	B	336	ARG	4.3
1	C	28	VAL	4.2
1	A	316	LEU	4.2
1	A	320	GLY	4.2
1	D	42	SER	4.2
1	B	330	LEU	4.2
1	E	263	ILE	4.2
1	E	337	LEU	4.2
1	B	346	LYS	4.2
1	C	314	THR	4.2
1	C	35	GLN	4.2
1	C	262	LYS	4.1
1	B	337	LEU	4.1
1	C	336	ARG	4.1
1	D	339	GLU	4.1
1	F	313	LEU	4.1
1	C	26	VAL	4.1
1	E	260	ARG	4.1
1	F	337	LEU	4.1
1	A	29	THR	4.0
1	B	312	LYS	4.0
1	D	249	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	342	GLN	4.0
1	C	325	ASP	4.0
1	F	342	GLN	4.0
1	A	18	PHE	4.0
1	E	316	LEU	3.9
1	F	94	TYR	3.9
1	D	346	LYS	3.9
1	B	318	ALA	3.9
1	D	99	VAL	3.9
1	D	35	GLN	3.9
1	B	347	GLU	3.9
1	A	260	ARG	3.9
1	B	326	TYR	3.9
1	B	323	ALA	3.8
1	F	315	GLY	3.8
1	F	28	VAL	3.8
1	A	334	ILE	3.8
1	A	322	LYS	3.8
1	E	38	GLU	3.8
1	B	321	GLN	3.7
1	A	325	ASP	3.7
1	B	329	ARG	3.7
1	A	26	VAL	3.7
1	B	165	ILE	3.7
1	C	321	GLN	3.7
1	C	24	VAL	3.6
1	A	180	ARG	3.6
1	A	37	ILE	3.6
1	A	321	GLN	3.6
1	E	333	ARG	3.6
1	D	165	ILE	3.6
1	C	342	GLN	3.6
1	D	312	LYS	3.6
1	D	309	LYS	3.6
1	E	343	GLY	3.5
1	E	259	MET	3.5
1	E	94	TYR	3.5
1	A	253	LEU	3.5
1	A	327	VAL	3.5
1	E	309	LYS	3.5
1	B	334	ILE	3.5
1	F	325	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	262	LYS	3.5
1	A	249	ASP	3.5
1	D	322	LYS	3.5
1	F	259	MET	3.5
1	F	249	ASP	3.5
1	F	319	GLU	3.4
1	A	319	GLU	3.4
1	E	329	ARG	3.4
1	A	339	GLU	3.4
1	D	246	ILE	3.4
1	F	45	ASN	3.4
1	F	35	GLN	3.4
1	A	313	LEU	3.4
1	F	321	GLN	3.4
1	C	312	LYS	3.4
1	C	19	MET	3.4
1	F	318	ALA	3.4
1	B	314	THR	3.4
1	F	42	SER	3.4
1	F	336	ARG	3.3
1	E	238	LYS	3.3
1	C	253	LEU	3.3
1	E	325	ASP	3.3
1	D	335	ARG	3.3
1	A	25	HIS	3.3
1	D	336	ARG	3.3
1	F	25	HIS	3.3
1	A	94	TYR	3.3
1	E	256	ALA	3.2
1	C	248	PRO	3.2
1	F	34	PRO	3.2
1	F	19	MET	3.2
1	D	319	GLU	3.2
1	F	246	ILE	3.2
1	E	249	ASP	3.2
1	E	341	ALA	3.2
1	E	37	ILE	3.2
1	E	326	TYR	3.2
1	D	45	ASN	3.2
1	A	315	GLY	3.2
1	F	331	PRO	3.2
1	F	165	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	3.2
1	E	345	ALA	3.2
1	E	99	VAL	3.2
1	F	99	VAL	3.2
1	B	34	PRO	3.1
1	B	54	HIS	3.1
1	C	326	TYR	3.1
1	E	24	VAL	3.1
1	F	264	SER	3.1
1	D	98	LEU	3.1
1	A	22	ARG	3.1
1	E	32	MET	3.1
1	F	32	MET	3.1
1	B	99	VAL	3.1
1	E	321	GLN	3.1
1	A	312	LYS	3.1
1	D	103	ILE	3.1
1	D	316	LEU	3.0
1	E	314	THR	3.0
1	C	315	GLY	3.0
1	C	309	LYS	3.0
1	C	322	LYS	3.0
1	A	262	LYS	3.0
1	C	318	ALA	3.0
1	A	328	CYS	3.0
1	F	328	CYS	3.0
1	C	42	SER	3.0
1	B	50	ASN	3.0
1	C	212	GLU	3.0
1	C	256	ALA	3.0
1	F	339	GLU	3.0
1	A	333	ARG	3.0
1	F	301	LEU	3.0
1	D	102	MET	3.0
1	F	186	TYR	3.0
1	B	56	LYS	2.9
1	F	26	VAL	2.9
1	A	304	LEU	2.9
1	E	19	MET	2.9
1	A	211	LYS	2.9
1	C	263	ILE	2.9
1	D	248	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	332	PRO	2.9
1	A	252	VAL	2.9
1	E	244	PHE	2.9
1	C	311	ASP	2.9
1	A	19	MET	2.9
1	B	96	VAL	2.9
1	B	154	LEU	2.9
1	E	253	LEU	2.9
1	D	259	MET	2.9
1	F	312	LYS	2.9
1	D	39	ILE	2.9
1	B	250	GLY	2.9
1	E	319	GLU	2.9
1	D	154	LEU	2.9
1	B	324	GLN	2.9
1	A	165	ILE	2.9
1	D	96	VAL	2.8
1	F	154	LEU	2.8
1	A	250	GLY	2.8
1	B	335	ARG	2.8
1	D	212	GLU	2.8
1	F	248	PRO	2.8
1	E	180	ARG	2.8
1	E	25	HIS	2.8
1	A	21	PRO	2.8
1	C	27	GLN	2.8
1	A	54	HIS	2.8
1	B	37	ILE	2.8
1	A	336	ARG	2.8
1	D	54	HIS	2.8
1	E	28	VAL	2.8
1	A	317	SER	2.7
1	B	240	VAL	2.7
1	C	313	LEU	2.7
1	A	23	GLU	2.7
1	A	103	ILE	2.7
1	B	102	MET	2.7
1	B	245	GLU	2.7
1	F	38	GLU	2.7
1	A	308	TRP	2.7
1	C	259	MET	2.7
1	A	323	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	103	ILE	2.7
1	B	325	ASP	2.7
1	C	328	CYS	2.6
1	B	126	GLY	2.6
1	C	316	LEU	2.6
1	C	341	ALA	2.6
1	C	160	VAL	2.6
1	D	97	VAL	2.6
1	A	178	ASP	2.6
1	C	330	LEU	2.6
1	D	329	ARG	2.6
1	C	194	PHE	2.6
1	D	348	ALA	2.6
1	A	259	MET	2.6
1	F	160	VAL	2.6
1	A	45	ASN	2.6
1	F	24	VAL	2.6
1	F	305	VAL	2.6
1	D	100	GLY	2.6
1	B	248	PRO	2.6
1	D	315	GLY	2.5
1	A	347	GLU	2.5
1	F	244	PHE	2.5
1	E	120	GLY	2.5
1	B	98	LEU	2.5
1	A	258	MET	2.5
1	C	23	GLU	2.5
1	A	99	VAL	2.5
1	C	165	ILE	2.5
1	D	323	ALA	2.5
1	E	312	LYS	2.5
1	A	340	ARG	2.5
1	B	306	GLY	2.5
1	A	306	GLY	2.5
1	F	120	GLY	2.5
1	E	264	SER	2.5
1	F	252	VAL	2.5
1	C	246	ILE	2.5
1	F	27	GLN	2.5
1	A	305	VAL	2.5
1	C	254	ALA	2.5
1	F	308	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	254	ALA	2.4
1	B	100	GLY	2.4
1	B	304	LEU	2.4
1	E	29	THR	2.4
1	A	309	LYS	2.4
1	D	310	VAL	2.4
1	D	318	ALA	2.4
1	E	328	CYS	2.4
1	D	242	LYS	2.4
1	E	334	ILE	2.4
1	C	22	ARG	2.4
1	C	186	TYR	2.4
1	D	31	SER	2.4
1	A	186	TYR	2.4
1	F	162	MET	2.4
1	B	308	TRP	2.4
1	B	45	ASN	2.3
1	A	335	ARG	2.3
1	C	339	GLU	2.3
1	E	339	GLU	2.3
1	D	162	MET	2.3
1	B	40	PHE	2.3
1	B	255	PHE	2.3
1	D	189	PHE	2.3
1	F	49	GLU	2.3
1	E	246	ILE	2.3
1	E	34	PRO	2.3
1	A	32	MET	2.3
1	F	125	THR	2.3
1	F	350	THR	2.3
1	B	340	ARG	2.3
1	C	260	ARG	2.3
1	B	131	SER	2.3
1	A	98	LEU	2.3
1	C	180	ARG	2.3
1	A	120	GLY	2.3
1	E	98	LEU	2.3
1	F	153	TYR	2.3
1	F	155	TYR	2.3
1	E	162	MET	2.3
1	F	100	GLY	2.3
1	B	160	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	311	ASP	2.3
1	F	98	LEU	2.3
1	F	323	ALA	2.3
1	E	96	VAL	2.3
1	E	347	GLU	2.3
1	E	324	GLN	2.2
1	E	102	MET	2.2
1	D	317	SER	2.2
1	B	151	ASN	2.2
1	A	337	LEU	2.2
1	E	311	ASP	2.2
1	A	244	PHE	2.2
1	D	155	TYR	2.2
1	F	37	ILE	2.2
1	D	69	PRO	2.2
1	A	303	PHE	2.2
1	B	259	MET	2.2
1	D	324	GLN	2.2
1	A	190	ILE	2.2
1	C	29	THR	2.2
1	E	33	PRO	2.2
1	D	321	GLN	2.2
1	F	102	MET	2.2
1	F	310	VAL	2.2
1	F	250	GLY	2.2
1	B	55	LEU	2.2
1	F	251	THR	2.2
1	F	355	TRP	2.2
1	E	292	TYR	2.2
1	D	47	ALA	2.2
1	B	260	ARG	2.2
1	F	18	PHE	2.2
1	F	23	GLU	2.2
1	A	191	TYR	2.2
1	B	186	TYR	2.2
1	A	97	VAL	2.1
1	A	20	PRO	2.1
1	B	169	ILE	2.1
1	C	301	LEU	2.1
1	E	213	HIS	2.1
1	B	39	ILE	2.1
1	E	313	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	155	TYR	2.1
1	D	94	TYR	2.1
1	A	38	GLU	2.1
1	C	319	GLU	2.1
1	A	177	MET	2.1
1	C	187	LEU	2.1
1	D	156	LEU	2.1
1	E	243	LEU	2.1
1	F	243	LEU	2.1
1	F	306	GLY	2.1
1	A	155	TYR	2.1
1	A	324	GLN	2.1
1	F	22	ARG	2.1
1	B	212	GLU	2.1
1	B	293	THR	2.1
1	F	103	ILE	2.1
1	B	355	TRP	2.1
1	D	29	THR	2.1
1	E	26	VAL	2.1
1	B	213	HIS	2.1
1	B	120	GLY	2.1
1	E	177	MET	2.1
1	A	46	TRP	2.1
1	C	305	VAL	2.1
1	E	350	THR	2.1
1	B	339	GLU	2.1
1	A	42	SER	2.1
1	F	309	LYS	2.1
1	C	332	PRO	2.0
1	F	327	VAL	2.0
1	F	297	TYR	2.0
1	C	189	PHE	2.0
1	C	162	MET	2.0
1	D	260	ARG	2.0
1	A	179	PRO	2.0
1	C	38	GLU	2.0
1	A	348	ALA	2.0
1	B	317	SER	2.0
1	B	134	ILE	2.0
1	C	99	VAL	2.0
1	D	240	VAL	2.0
1	E	73	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	187	LEU	2.0
1	D	239	ILE	2.0
1	A	33	PRO	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
3	AZI	E	4366	3/3	0.33	6.35	2,2,4,5	0
3	AZI	D	3366	3/3	0.29	4.76	2,2,4,6	0
3	AZI	B	1366	3/3	0.30	3.69	2,2,4,5	0
3	AZI	C	2366	3/3	0.22	3.68	2,2,4,6	0
3	AZI	A	366	3/3	0.19	0.60	2,2,4,6	0
3	AZI	F	5366	3/3	0.15	-1.00	2,2,4,5	0
2	FE	B	365	1/1	0.10	-2.51	22,22,22,22	0
2	FE	A	364	1/1	0.10	-2.74	32,32,32,32	0
2	FE	F	364	1/1	0.10	-3.08	32,32,32,32	0
2	FE	C	364	1/1	0.10	-3.13	31,31,31,31	0
2	FE	A	365	1/1	0.06	-3.43	22,22,22,22	0
2	FE	B	364	1/1	0.10	-3.48	31,31,31,31	0
2	FE	E	365	1/1	0.08	-3.95	22,22,22,22	0
2	FE	D	365	1/1	0.08	-4.05	23,23,23,23	0
2	FE	E	364	1/1	0.07	-4.54	32,32,32,32	0
2	FE	D	364	1/1	0.07	-4.93	32,32,32,32	0
2	FE	F	365	1/1	0.04	-6.22	23,23,23,23	0
2	FE	C	365	1/1	0.05	-7.05	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.