Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 05:09 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

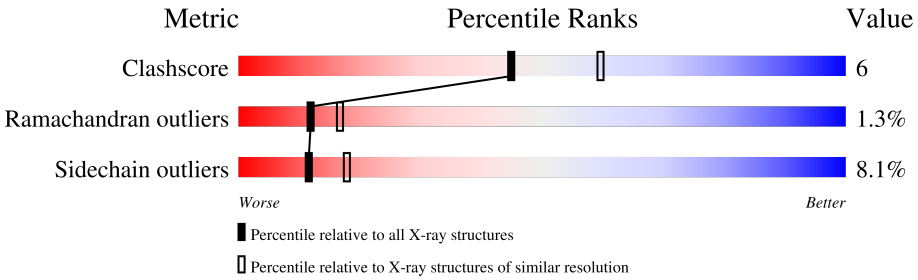
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	363	74% 20% • 5%
1	B	363	76% 17% • 5%
1	C	363	74% 20% • 5%
1	D	363	74% 19% • 5%
1	E	363	75% 19% • 5%
1	F	363	74% 20% • 5%

2 Entry composition (i)

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.

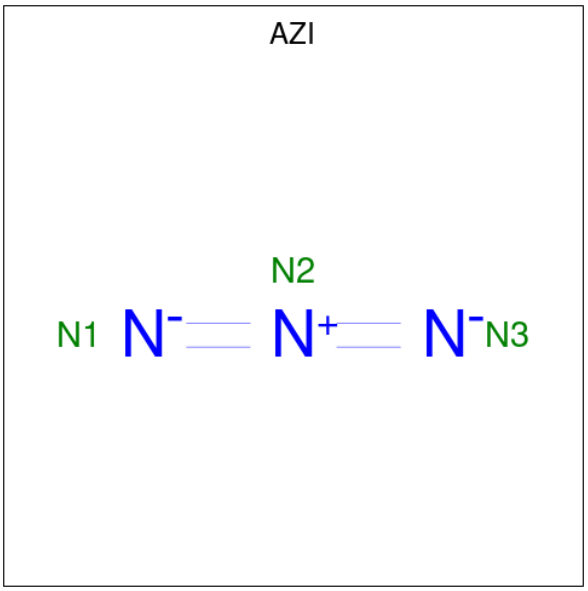
- Molecule 1 is a protein called Acyl-[acyl-carrier protein] desaturase.

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	A	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	D	2	Total	Fe	0	0
			2	2		
2	E	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.

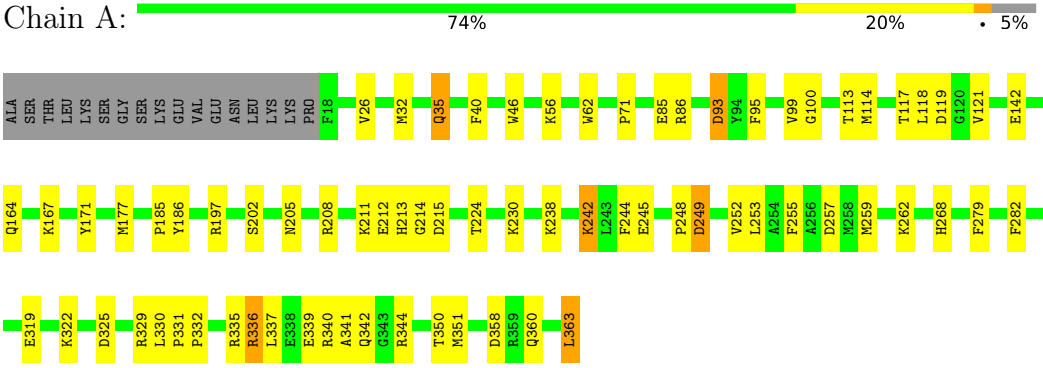
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	60	Total O 60 60	0	0
4	B	64	Total O 64 64	0	0
4	C	60	Total O 60 60	0	0
4	D	65	Total O 65 65	0	0
4	E	66	Total O 66 66	0	0
4	F	53	Total O 53 53	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

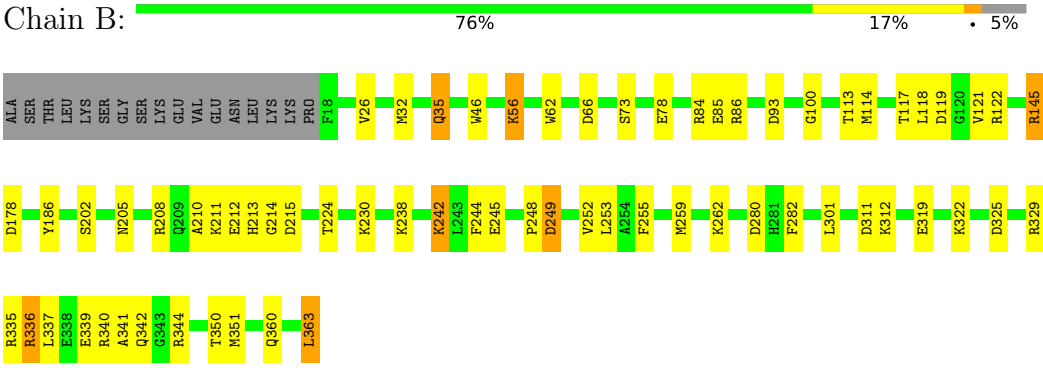
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain A:



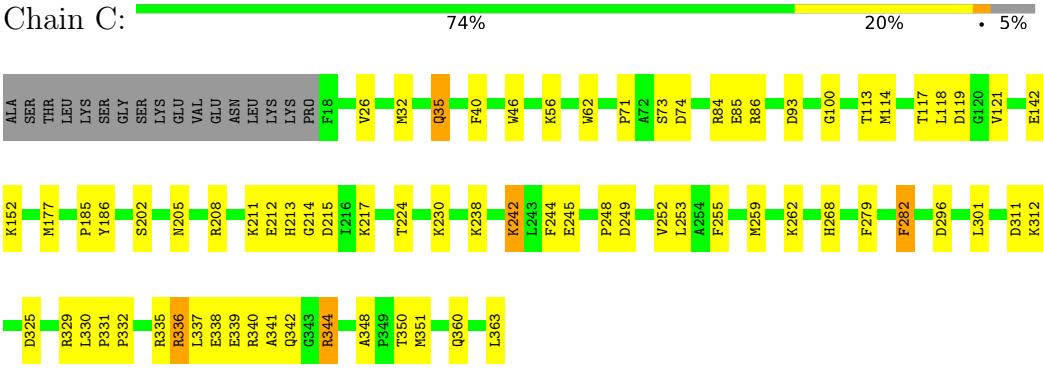
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain B:



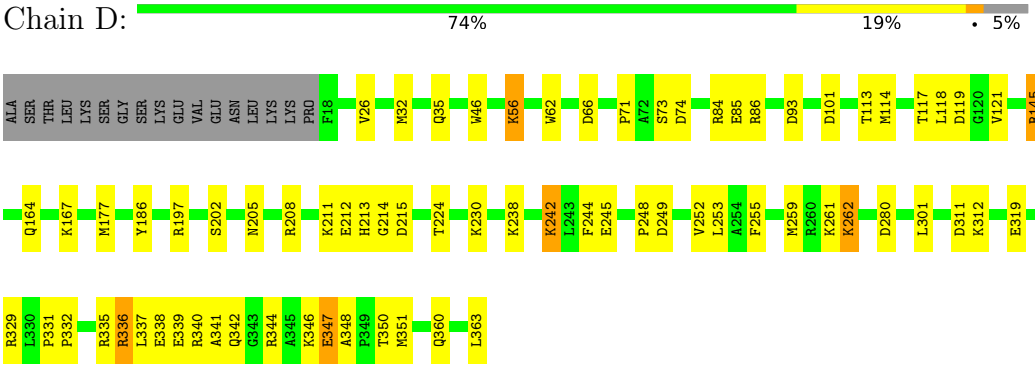
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain C:



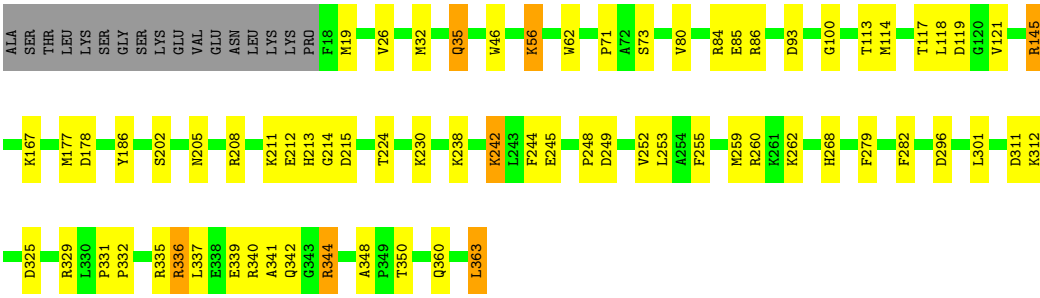
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain D:



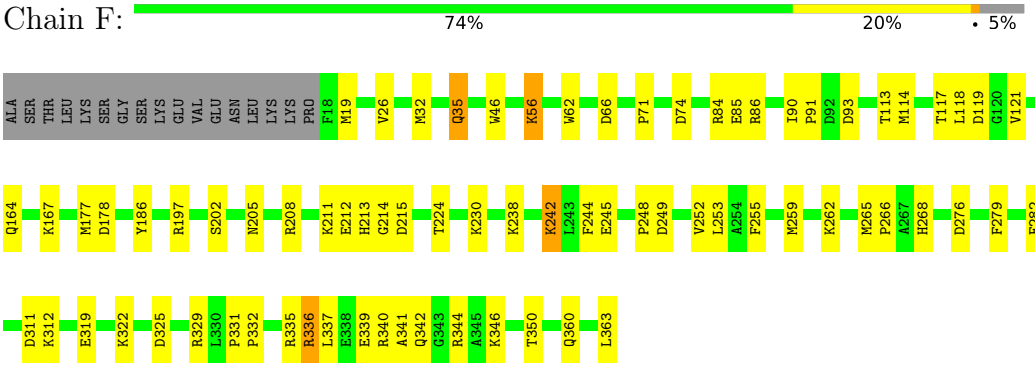
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

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	2236 reflections (2.48%)	wwPDB-VP
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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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:HG3	1:B:145:ARG:HH11	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:HH11	1:C:145:ARG:HG3	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:HE	1:F:336:ARG:HA	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:HA	1:C:336:ARG:HE	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:E:248:PRO:O	1:E:252:VAL:HG23	2.05	0.56
1:F:46:TRP:CZ2	1:F:242:LYS:HG3	2.40	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:HG3	1:D:145:ARG:NH1	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:HA	1:F:336:ARG:NE	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:HA	1:D:336:ARG:NE	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:HA	1:A:336:ARG:NE	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:HA	1:C:336:ARG:NE	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:HG3	1:A:145:ARG:NH1	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:H	1:A:35:GLN:HG3	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:HG3	1:E:145:ARG:NH1	2.27	0.46
1:A:93:ASP:OD1	1:A:93:ASP:N	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:H	1:E:35:GLN:HG3	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:46:TRP:CE2	1:C:242:LYS:HG3	2.52	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:HD2	1:D:56:LYS:HA	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:HD12	1:E:363:LEU:HA	1.89	0.43
1:F:46:TRP:CE2	1:F:242:LYS:HG3	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:H	1:F:35:GLN:HG3	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:HG3	1:C:145:ARG:NH1	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:HD12	1:A:363:LEU:HA	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: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: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:D:164:GLN:OE1	1:D:167:LYS:HE2	2.21	0.41
1:F:90:ILE:HA	1:F:91:PRO:HD3	1.93	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:HD12	1:B:363:LEU:HA	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 (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%)	13	19
1	B	344/363 (95%)	328 (95%)	12 (4%)	4 (1%)	13	19
1	C	345/363 (95%)	329 (95%)	12 (4%)	4 (1%)	13	19
1	D	344/363 (95%)	327 (95%)	11 (3%)	6 (2%)	9	11
1	E	344/363 (95%)	325 (94%)	15 (4%)	4 (1%)	13	19
1	F	344/363 (95%)	328 (95%)	11 (3%)	5 (2%)	10	14
All	All	2065/2178 (95%)	1965 (95%)	73 (4%)	27 (1%)	12	17

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%)	12 18
1	B	300/315 (95%)	276 (92%)	24 (8%)	12 18
1	C	301/315 (96%)	277 (92%)	24 (8%)	12 18
1	D	300/315 (95%)	276 (92%)	24 (8%)	12 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	300/315 (95%)	276 (92%)	24 (8%)	12 18
1	F	300/315 (95%)	275 (92%)	25 (8%)	11 17
All	All	1801/1890 (95%)	1656 (92%)	145 (8%)	11 18

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

Sometimes 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 monosaccharides 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	B	1366	2	0,2,2	-	-	0,1,1	-	-
3	AZI	A	366	2	0,2,2	-	-	0,1,1	-	-
3	AZI	C	2366	2	0,2,2	-	-	0,1,1	-	-
3	AZI	E	4366	2	0,2,2	-	-	0,1,1	-	-
3	AZI	F	5366	2	0,2,2	-	-	0,1,1	-	-
3	AZI	D	3366	2	0,2,2	-	-	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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