



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:57 AM UTC

PDB ID : 6I97 / pdb_00006i97
Title : Structure of the ferrioxamine B transporter FoxA from *Pseudomonas aeruginosa* in complex with ferrioxamine B and a C-terminal TonB fragment
Authors : Josts, I.; Tidow, H.
Deposited on : 2018-11-22
Resolution : 3.35 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:

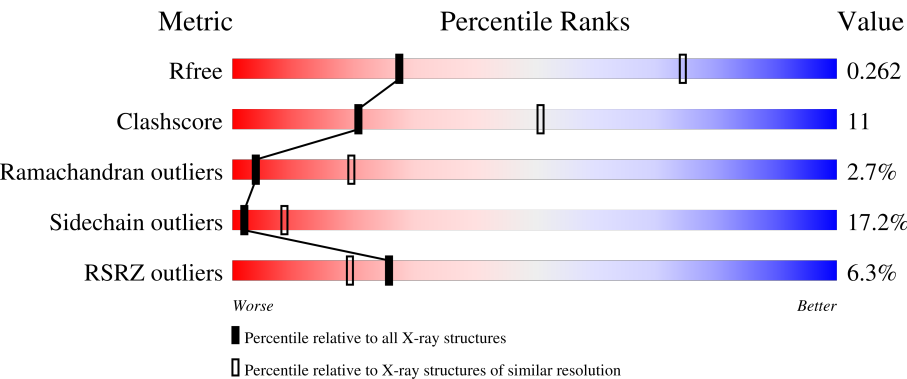
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.35 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))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	768	6% 61% 30% 7% ..
1	B	768	6% 62% 29% 7% ..
2	D	90	8% 60% 24% 13% .
2	E	90	8% 54% 39% 7%

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
3	0UE	A	901	X	-	-	-
3	0UE	B	901	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13442 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.

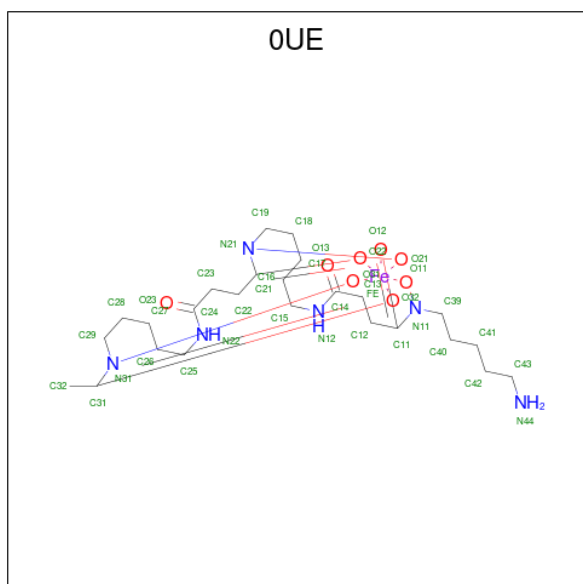
- Molecule 1 is a protein called Metal-pseudopaline receptor CntO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	763	Total	C	N	O	S	0	0	0
			5962	3738	1024	1188	12			
1	B	759	Total	C	N	O	S	0	0	0
			5936	3723	1019	1182	12			

- Molecule 2 is a protein called Protein TonB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	90	Total	C	N	O	S	0	0	0
			732	465	135	127	5			
2	E	90	Total	C	N	O	S	0	0	0
			732	465	135	127	5			

- Molecule 3 is Ferrioxamine B (CCD ID: 0UE) (formula: $C_{25}H_{45}FeN_6O_8$).

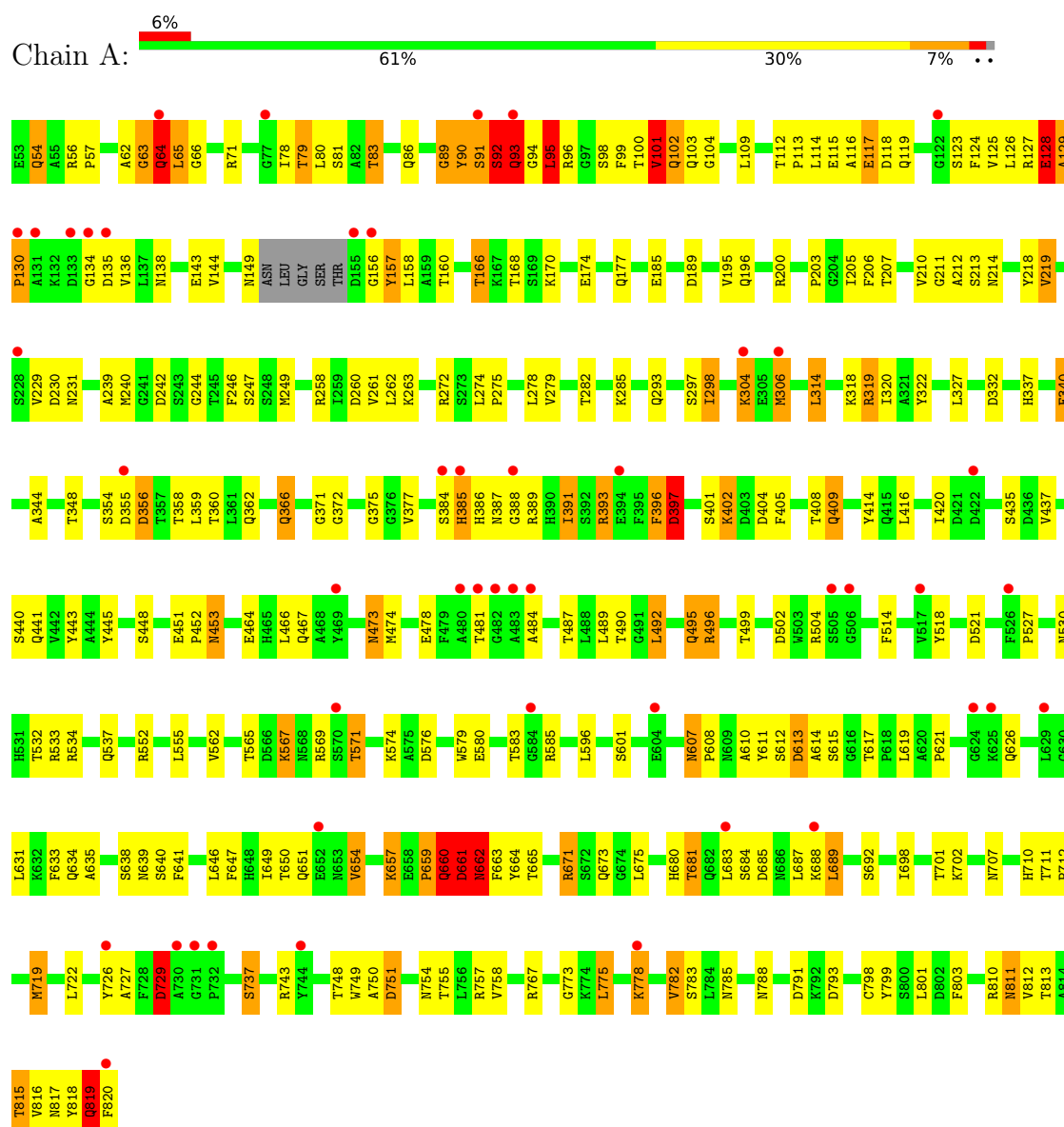


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			40	25	1	6	8		
3	B	1	Total	C	Fe	N	O	0	0
			40	25	1	6	8		

3 Residue-property plots

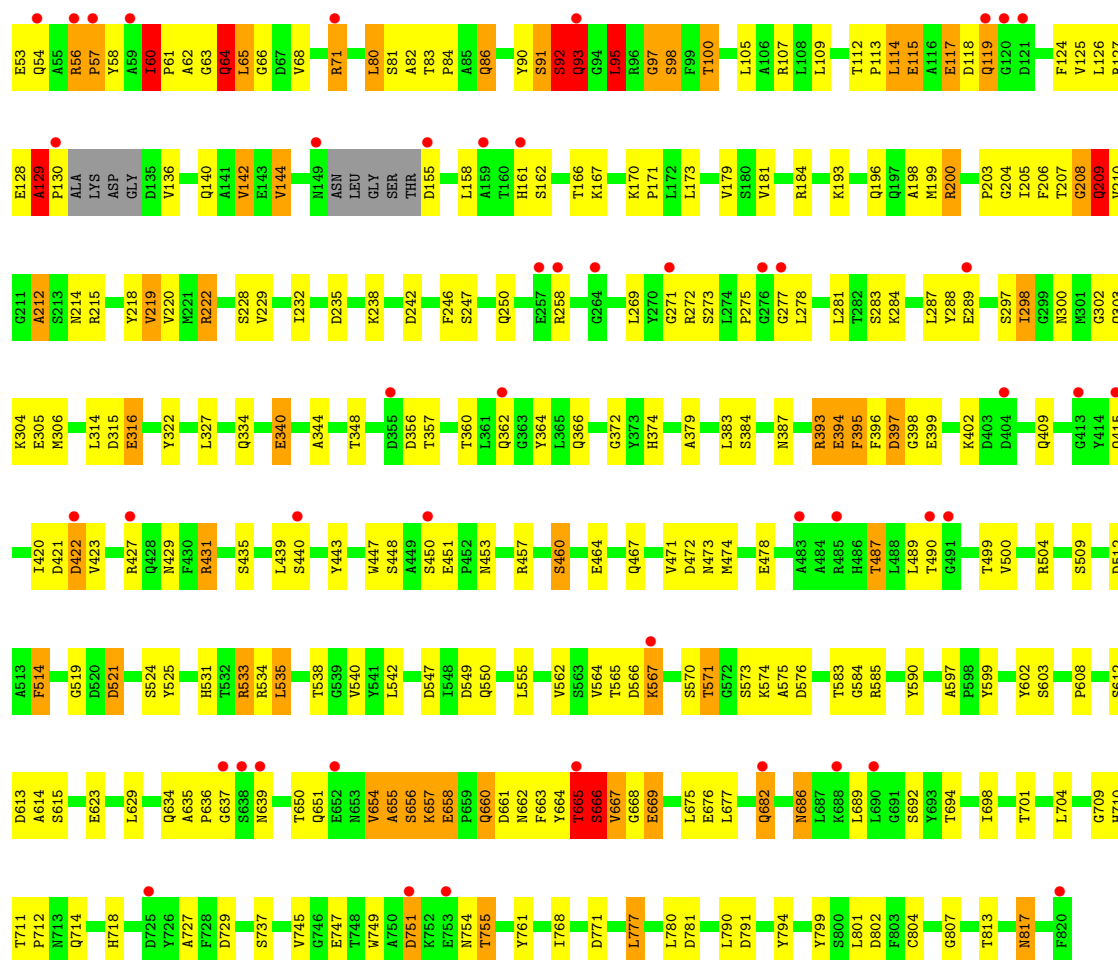
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Metal-pseudopaline receptor CntO



• Molecule 1: Metal-pseudopaline receptor CntO

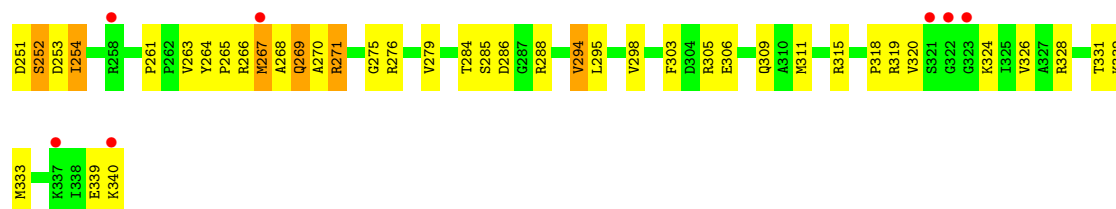




• Molecule 2: Protein TonB



• Molecule 2: Protein TonB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	163.64Å 174.40Å 214.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 – 3.35 48.84 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.84-3.35) 99.9 (48.84-3.35)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.229 , 0.264 (Not available) , 0.262	Depositor DCC
R_{free} test set	4363 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13442	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0UE

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	1.33	28/6097 (0.5%)	1.43	54/8272 (0.7%)
1	B	1.41	39/6070 (0.6%)	1.48	69/8235 (0.8%)
2	D	1.46	4/746 (0.5%)	1.60	14/999 (1.4%)
2	E	1.33	5/746 (0.7%)	1.46	9/999 (0.9%)
All	All	1.37	76/13659 (0.6%)	1.46	146/18505 (0.8%)

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	A	0	2
1	B	0	1
2	E	0	1
All	All	0	4

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	657	LYS	CA-C	-12.50	1.44	1.52
1	B	657	LYS	N-CA	-11.77	1.33	1.46
1	B	751	ASP	CB-CG	10.06	1.77	1.52
1	B	181	VAL	C-O	-9.34	1.14	1.24
2	D	271	ARG	CA-C	-8.74	1.45	1.53
1	A	96	ARG	C-O	-7.95	1.16	1.23
1	A	617	THR	C-O	-7.64	1.14	1.24
1	A	94	GLY	C-O	-7.49	1.16	1.23
2	E	252	SER	N-CA	7.17	1.54	1.46
1	B	547	ASP	CA-C	6.95	1.60	1.53
1	A	94	GLY	N-CA	6.82	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	729	ASP	N-CA	6.70	1.55	1.45
2	D	251	ASP	N-CA	6.61	1.58	1.46
1	A	385	HIS	CA-CB	6.57	1.63	1.53
1	B	208	GLY	C-O	-6.57	1.15	1.23
1	A	386	HIS	N-CA	6.55	1.54	1.46
1	B	198	ALA	C-O	6.41	1.32	1.24
1	B	60	ILE	N-CA	6.31	1.50	1.45
1	B	549	ASP	CA-C	6.20	1.58	1.52
1	A	496	ARG	CD-NE	6.12	1.54	1.46
1	B	447	TRP	N-CA	6.10	1.53	1.45
1	B	271	GLY	C-O	6.10	1.31	1.23
1	B	755	THR	CB-OG1	6.01	1.53	1.43
1	B	421	ASP	CA-C	-5.98	1.47	1.53
1	B	158	LEU	CA-C	-5.96	1.45	1.52
1	B	669	GLU	N-CA	5.93	1.53	1.46
1	B	200	ARG	CD-NE	5.92	1.54	1.46
1	A	71	ARG	NE-CZ	5.92	1.39	1.33
2	E	251	ASP	CA-CB	5.91	1.65	1.53
1	B	669	GLU	CA-C	5.88	1.60	1.52
1	B	534	ARG	CA-C	5.87	1.59	1.52
1	A	78	ILE	CA-C	-5.83	1.47	1.52
1	B	91	SER	CA-CB	5.78	1.63	1.53
1	B	281	LEU	C-O	5.69	1.30	1.23
1	A	567	LYS	N-CA	5.66	1.53	1.46
2	E	251	ASP	CB-CG	5.65	1.66	1.52
1	A	298	ILE	CB-CG1	5.65	1.64	1.53
2	E	294	VAL	C-O	-5.64	1.17	1.24
1	B	277	GLY	C-O	5.62	1.30	1.23
1	B	362	GLN	CA-C	5.61	1.59	1.52
1	A	261	VAL	C-O	-5.58	1.18	1.24
1	B	525	TYR	CA-CB	5.55	1.62	1.53
1	A	239	ALA	N-CA	5.54	1.52	1.46
1	B	215	ARG	CZ-NH1	5.46	1.40	1.32
1	A	635	ALA	C-N	5.43	1.39	1.33
2	D	251	ASP	CB-CG	5.43	1.65	1.52
1	A	231	ASN	CA-C	5.37	1.60	1.52
1	B	567	LYS	CA-CB	5.36	1.61	1.53
1	B	525	TYR	CA-C	5.36	1.59	1.52
1	B	129	ALA	C-N	5.35	1.43	1.34
1	B	200	ARG	NE-CZ	5.34	1.39	1.33
1	B	71	ARG	CD-NE	5.33	1.53	1.46
1	B	184	ARG	CA-C	-5.33	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	310	ALA	CA-C	-5.33	1.46	1.52
1	B	71	ARG	NE-CZ	5.32	1.39	1.33
1	B	397	ASP	CA-CB	5.30	1.61	1.53
1	A	619	LEU	C-O	5.28	1.30	1.23
1	A	63	GLY	N-CA	5.27	1.50	1.45
1	A	567	LYS	CA-C	-5.27	1.46	1.52
1	B	666	SER	N-CA	5.24	1.52	1.46
1	A	218	TYR	C-O	-5.24	1.17	1.24
1	B	567	LYS	CA-C	-5.19	1.46	1.52
1	A	496	ARG	CA-C	5.18	1.58	1.52
1	A	409	GLN	CA-C	-5.15	1.46	1.52
1	A	71	ARG	CD-NE	5.14	1.53	1.46
1	A	262	LEU	CA-C	-5.12	1.46	1.52
1	B	714	GLN	CA-C	5.12	1.59	1.53
1	B	567	LYS	N-CA	5.12	1.52	1.46
1	A	356	ASP	CA-C	5.11	1.59	1.52
1	B	136	VAL	N-CA	5.10	1.52	1.46
1	A	397	ASP	N-CA	5.10	1.52	1.46
1	B	599	TYR	N-CA	5.10	1.52	1.46
1	A	496	ARG	NE-CZ	5.09	1.38	1.33
1	A	757	ARG	CD-NE	5.08	1.53	1.46
1	B	550	GLN	CA-C	5.04	1.59	1.52
2	E	288	ARG	CA-C	5.03	1.59	1.52

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	668	GLY	N-CA-C	-17.25	88.15	111.09
1	A	117	GLU	N-CA-C	14.36	126.62	110.97
1	A	129	ALA	CA-C-N	11.01	133.61	119.84
1	A	129	ALA	C-N-CA	11.01	133.61	119.84
2	D	269	GLN	N-CA-C	-11.00	98.82	111.03
1	B	271	GLY	N-CA-C	10.94	126.77	112.77
1	B	669	GLU	N-CA-C	9.82	123.01	110.24
1	A	662	ASN	N-CA-C	-8.38	100.48	111.71
1	B	129	ALA	N-CA-C	8.31	128.18	109.81
1	B	612	SER	N-CA-C	8.27	122.92	109.85
1	B	136	VAL	N-CA-C	8.12	119.61	107.75
1	B	571	THR	CB-CA-C	-8.00	96.06	110.70
1	B	519	GLY	N-CA-C	-7.94	102.72	112.33
1	A	567	LYS	N-CA-CB	7.59	121.72	109.95
1	B	654	VAL	N-CA-C	7.37	117.97	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	PHE	CA-C-O	-7.35	113.17	120.89
1	A	83	THR	CA-C-N	7.32	128.98	119.84
1	A	83	THR	C-N-CA	7.32	128.98	119.84
1	B	92	SER	N-CA-C	7.29	126.33	110.80
2	E	252	SER	N-CA-C	7.24	119.14	108.14
1	A	388	GLY	N-CA-C	7.21	126.45	114.48
1	A	92	SER	CB-CA-C	-7.15	96.20	110.42
1	A	567	LYS	N-CA-C	-7.11	98.46	109.76
1	A	385	HIS	N-CA-C	-6.98	97.04	108.41
1	B	71	ARG	N-CA-C	-6.92	102.80	111.11
1	B	799	TYR	N-CA-C	-6.90	104.99	113.41
1	B	656	SER	O-C-N	6.88	130.82	122.84
1	A	571	THR	CB-CA-C	-6.87	97.92	110.63
1	A	391	ILE	N-CA-C	-6.85	98.46	108.87
1	B	817	ASN	N-CA-C	6.85	120.57	109.40
1	A	95	LEU	N-CA-C	6.85	119.67	110.35
1	B	514	PHE	N-CA-C	-6.83	97.83	109.24
1	B	422	ASP	N-CA-C	-6.66	103.84	112.23
1	A	285	LYS	CA-C-N	-6.66	113.79	120.31
1	A	285	LYS	C-N-CA	-6.66	113.79	120.31
1	B	60	ILE	CA-C-N	6.65	128.15	119.84
1	B	60	ILE	C-N-CA	6.65	128.15	119.84
1	B	567	LYS	N-CA-CB	6.57	121.00	110.16
1	B	657	LYS	CA-C-O	-6.53	112.08	119.98
2	D	286	ASP	N-CA-CB	-6.49	101.06	110.47
1	B	114	LEU	CA-C-N	6.48	133.93	121.54
1	B	114	LEU	C-N-CA	6.48	133.93	121.54
2	D	270	ALA	N-CA-C	-6.48	100.23	109.96
1	B	95	LEU	N-CA-C	6.46	119.68	108.76
1	B	709	GLY	N-CA-C	-6.43	107.04	114.69
1	B	571	THR	N-CA-C	6.41	119.57	111.69
2	D	319	ARG	CA-C-N	-6.40	115.25	123.19
2	D	319	ARG	C-N-CA	-6.40	115.25	123.19
1	A	89	GLY	N-CA-C	-6.40	98.02	113.18
1	B	93	GLN	N-CA-C	6.33	124.28	110.80
1	A	396	PHE	N-CA-CB	6.24	118.96	110.10
1	A	306	MET	CG-SD-CE	6.24	114.62	100.90
1	B	599	TYR	N-CA-C	6.21	118.29	108.79
1	A	654	VAL	N-CA-C	-6.21	101.57	109.58
1	B	464	GLU	N-CA-C	6.17	118.51	108.26
1	A	298	ILE	N-CA-C	-6.11	99.40	108.45
1	B	662	ASN	N-CA-C	-6.10	102.41	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	755	THR	OG1-CB-CG2	6.10	121.50	109.30
1	B	60	ILE	CA-C-O	-6.08	116.78	119.94
1	A	71	ARG	N-CA-C	-6.07	103.83	111.11
2	D	286	ASP	CB-CA-C	6.05	121.15	110.37
1	B	100	THR	N-CA-C	-6.01	103.01	110.41
1	A	661	ASP	N-CA-CB	6.01	120.64	110.49
1	B	162	SER	N-CA-C	5.99	119.25	109.24
1	A	496	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	B	668	GLY	CA-C-O	-5.98	115.86	121.96
1	B	212	ALA	N-CA-C	5.97	123.51	110.80
1	B	298	ILE	N-CA-C	-5.97	99.57	108.46
1	A	304	LYS	CB-CG-CD	5.86	124.78	111.30
1	B	682	GLN	N-CA-C	-5.86	100.79	109.11
1	A	298	ILE	CB-CG1-CD1	5.85	126.09	113.80
1	A	90	TYR	N-CA-C	-5.83	99.10	108.55
1	B	397	ASP	N-CA-C	5.83	119.69	112.47
1	A	95	LEU	CB-CA-C	-5.81	99.22	109.62
2	D	252	SER	N-CA-C	5.80	116.21	108.38
1	A	64	GLN	CA-C-N	5.78	132.59	121.54
1	A	64	GLN	C-N-CA	5.78	132.59	121.54
1	A	157	TYR	N-CA-C	5.77	123.09	110.80
1	B	86	GLN	CB-CA-C	5.76	118.36	109.03
1	B	298	ILE	CB-CG1-CD1	5.76	125.89	113.80
2	E	270	ALA	N-CA-C	-5.75	105.09	111.36
2	E	295	LEU	N-CA-C	5.74	118.41	111.40
1	A	119	GLN	N-CA-C	5.73	119.33	111.54
2	D	271	ARG	N-CA-C	-5.73	104.21	110.91
1	B	179	VAL	N-CA-C	5.70	116.49	108.17
1	A	504	ARG	N-CA-C	-5.65	99.93	108.46
2	E	284	THR	CA-C-N	5.62	128.59	120.79
2	E	284	THR	C-N-CA	5.62	128.59	120.79
1	B	575	ALA	N-CA-C	-5.57	101.51	110.14
1	B	567	LYS	N-CA-C	-5.56	100.22	109.46
1	B	200	ARG	CB-CG-CD	5.55	124.08	111.30
2	E	315	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	A	63	GLY	N-CA-C	5.52	118.43	111.09
1	A	385	HIS	CB-CA-C	5.51	119.31	110.16
1	B	460	SER	CA-C-N	5.49	125.84	121.61
1	B	460	SER	C-N-CA	5.49	125.84	121.61
1	A	78	ILE	CB-CA-C	-5.49	103.53	112.03
1	A	585	ARG	N-CA-C	5.49	117.52	109.24
2	E	315	ARG	NE-CZ-NH2	5.48	124.14	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	SER	CA-C-N	5.48	132.01	121.54
1	B	92	SER	C-N-CA	5.48	132.01	121.54
1	B	64	GLN	CB-CG-CD	5.47	121.89	112.60
1	A	94	GLY	N-CA-C	5.46	120.99	112.31
1	B	667	VAL	CB-CA-C	5.46	120.25	111.29
1	B	91	SER	N-CA-C	-5.45	99.19	110.80
1	B	215	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	A	337	HIS	N-CA-C	5.41	119.18	112.47
1	B	443	TYR	N-CA-C	5.40	117.47	108.99
1	A	116	ALA	N-CA-C	5.39	117.20	108.41
1	A	751	ASP	N-CA-CB	-5.39	101.76	110.71
2	D	314	TRP	N-CA-C	5.37	117.22	110.24
1	B	228	SER	N-CA-C	5.35	119.56	113.19
1	B	209	GLN	N-CA-C	-5.33	107.43	114.04
1	B	340	GLU	N-CA-C	-5.31	101.03	109.59
1	A	117	GLU	CB-CA-C	-5.30	102.80	110.96
1	B	710	HIS	N-CA-C	5.30	116.93	110.41
1	B	657	LYS	O-C-N	5.30	127.85	121.76
1	B	200	ARG	CG-CD-NE	5.26	123.58	112.00
1	A	819	GLN	CA-C-N	5.24	131.14	121.70
1	A	819	GLN	C-N-CA	5.24	131.14	121.70
2	D	292	ILE	CB-CA-C	-5.24	103.30	111.26
1	A	340	GLU	N-CA-C	-5.21	99.61	108.26
2	E	311	MET	N-CA-C	-5.21	105.78	111.82
1	A	206	PHE	CA-C-O	5.17	125.90	120.36
2	D	326	VAL	N-CA-CB	-5.17	103.75	112.44
1	A	812	VAL	N-CA-C	5.16	116.02	108.58
1	B	635	ALA	CA-C-N	5.16	126.28	119.84
1	B	635	ALA	C-N-CA	5.16	126.28	119.84
1	B	665	THR	N-CA-CB	5.15	118.38	110.61
1	A	496	ARG	CB-CG-CD	5.14	123.11	111.30
1	B	431	ARG	CG-CD-NE	5.14	123.30	112.00
1	B	656	SER	CA-C-N	-5.13	116.33	122.44
1	B	656	SER	C-N-CA	-5.13	116.33	122.44
2	D	310	ALA	O-C-N	5.13	128.38	122.17
1	A	366	GLN	N-CA-C	5.12	117.76	108.69
1	A	246	PHE	N-CA-C	-5.12	107.20	113.50
1	A	684	SER	N-CA-C	5.12	114.38	108.49
1	B	718	HIS	N-CA-C	5.12	117.83	109.59
1	B	768	ILE	N-CA-C	-5.10	100.55	108.86
2	D	306	GLU	N-CA-C	-5.08	105.44	111.69
1	A	621	PRO	CA-C-N	5.07	128.06	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	PRO	C-N-CA	5.07	128.06	120.87
1	B	547	ASP	N-CA-C	5.06	117.20	107.44
2	D	293	GLN	N-CA-C	-5.06	99.74	108.69
1	B	584	GLY	N-CA-C	5.03	118.79	110.55
2	E	253	ASP	N-CA-C	5.02	116.91	109.69

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	GLU	Mainchain
1	A	93	GLN	Peptide
1	B	95	LEU	Peptide
2	E	298	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5962	0	5656	138	0
1	B	5936	0	5630	124	0
2	D	732	0	756	9	0
2	E	732	0	756	19	0
3	A	40	0	45	7	0
3	B	40	0	45	9	0
All	All	13442	0	12888	291	0

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 11.

All (291) 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:B:751:ASP:CG	1:B:751:ASP:CB	1.77	1.57
1:B:115:GLU:OE1	1:B:128:GLU:O	1.73	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:LEU:H	1:B:777:LEU:HD12	1.46	0.80
1:A:393:ARG:HG2	1:A:393:ARG:HH11	1.47	0.79
2:E:266:ARG:O	2:E:266:ARG:HD3	1.82	0.79
1:B:82:ALA:HB1	1:B:126:LEU:HD12	1.64	0.78
1:B:117:GLU:O	1:B:124:PHE:HD1	1.64	0.78
1:A:158:LEU:HD12	1:A:680:HIS:HB2	1.66	0.78
1:B:119:GLN:HE21	1:B:119:GLN:HA	1.48	0.77
1:A:396:PHE:O	1:A:397:ASP:CB	2.34	0.76
1:B:315:ASP:OD1	1:B:315:ASP:N	2.18	0.76
1:A:596:LEU:HD12	1:A:633:PHE:HB2	1.69	0.75
1:B:654:VAL:O	1:B:655:ALA:HB3	1.85	0.74
3:A:901:0UE:H9	3:A:901:0UE:O13	1.89	0.72
3:A:901:0UE:O13	3:A:901:0UE:H37	1.88	0.72
1:B:112:THR:OG1	1:B:113:PRO:HD2	1.87	0.72
1:A:396:PHE:HB3	1:A:518:TYR:OH	1.89	0.71
1:A:83:THR:HG22	1:B:144:VAL:HA	1.74	0.70
1:A:115:GLU:HB2	1:A:129:ALA:HB2	1.72	0.70
1:A:92:SER:OG	1:A:93:GLN:N	2.20	0.67
1:A:297:SER:HB2	1:A:815:THR:HG23	1.75	0.67
1:A:95:LEU:HD13	1:A:99:PHE:CD2	2.30	0.66
1:A:401:SER:OG	1:A:401:SER:O	2.11	0.66
1:B:118:ASP:O	1:B:124:PHE:CE1	2.49	0.66
1:B:199:MET:HE1	1:B:219:VAL:HG11	1.76	0.66
1:A:205:ILE:O	1:A:719:MET:HE1	1.97	0.65
1:A:565:THR:HG22	1:A:576:ASP:HA	1.77	0.65
1:B:62:ALA:HB2	1:B:93:GLN:O	1.97	0.65
3:B:901:0UE:O23	3:B:901:0UE:H25	1.96	0.65
1:B:614:ALA:HB2	1:B:663:PHE:CE1	2.32	0.64
2:D:259:MET:HE3	2:D:314:TRP:CH2	2.32	0.64
1:B:64:GLN:O	1:B:66:GLY:N	2.31	0.64
1:B:745:VAL:HG21	1:B:761:TYR:CE2	2.33	0.63
1:B:60:ILE:HG23	1:B:71:ARG:HD2	1.79	0.63
1:B:119:GLN:HE21	1:B:119:GLN:CA	2.10	0.63
1:B:82:ALA:CB	1:B:126:LEU:HD12	2.29	0.62
1:B:654:VAL:O	1:B:655:ALA:CB	2.47	0.62
1:B:535:LEU:HD12	1:B:564:VAL:HG22	1.82	0.61
1:A:200:ARG:HG2	1:A:207:THR:HG21	1.83	0.61
1:A:466:LEU:HD23	1:A:467:GLN:N	2.14	0.61
1:B:521:ASP:OD1	1:B:521:ASP:N	2.34	0.61
1:A:210:VAL:HG12	1:A:210:VAL:O	2.02	0.60
1:B:210:VAL:HG12	1:B:210:VAL:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:THR:HB	1:A:484:ALA:HB3	1.83	0.59
1:B:657:LYS:HD2	3:B:901:0UE:H11	1.83	0.59
1:B:170:LYS:HG3	1:B:171:PRO:HD2	1.85	0.59
1:A:340:GLU:HG3	1:A:372:GLY:CA	2.32	0.59
1:A:662:ASN:OD1	1:A:662:ASN:N	2.32	0.59
1:A:258:ARG:NH2	1:A:260:ASP:OD2	2.36	0.58
1:B:478:GLU:HG2	1:B:487:THR:HG23	1.85	0.58
1:A:478:GLU:HG2	1:A:487:THR:HG23	1.85	0.58
1:A:639:ASN:HD22	1:A:639:ASN:N	2.01	0.58
1:A:396:PHE:O	1:A:397:ASP:HB3	2.03	0.57
1:A:79:THR:O	1:A:123:SER:O	2.22	0.57
1:A:112:THR:HB	1:A:113:PRO:HD2	1.87	0.57
1:B:246:PHE:CE2	1:B:439:LEU:HD22	2.40	0.57
1:B:669:GLU:HG3	1:B:701:THR:OG1	2.05	0.57
1:B:63:GLY:O	1:B:65:LEU:N	2.38	0.57
1:B:119:GLN:HA	1:B:119:GLN:NE2	2.20	0.57
1:B:399:GLU:OE1	1:B:457:ARG:NH2	2.35	0.57
1:B:711:THR:H	1:B:754:ASN:HD21	1.53	0.56
1:A:100:THR:HG22	1:A:103:GLN:NE2	2.21	0.56
1:B:64:GLN:HA	1:B:91:SER:HA	1.87	0.56
1:B:222:ARG:HD3	1:B:676:GLU:OE1	2.06	0.56
1:B:415:GLN:HG2	1:B:429:ASN:OD1	2.06	0.56
1:A:86:GLN:OE1	2:E:261:PRO:HG3	2.05	0.56
1:A:64:GLN:O	1:A:66:GLY:N	2.40	0.55
1:A:95:LEU:HD13	1:A:99:PHE:CE2	2.41	0.55
1:B:117:GLU:HG2	1:B:127:ARG:HD2	1.88	0.55
1:B:686:ASN:ND2	1:B:729:ASP:OD1	2.39	0.55
1:A:63:GLY:O	1:A:65:LEU:N	2.40	0.55
1:A:348:THR:HG23	1:A:362:GLN:HG2	1.88	0.55
1:B:448:SER:HB3	1:B:451:GLU:O	2.06	0.55
1:A:62:ALA:CB	1:A:93:GLN:HA	2.37	0.55
1:A:443:TYR:CD2	3:A:901:0UE:H28	2.42	0.55
1:A:91:SER:O	1:A:92:SER:CB	2.55	0.54
1:A:219:VAL:HG21	1:A:279:VAL:HG21	1.89	0.54
1:A:100:THR:HG23	1:A:100:THR:O	2.07	0.54
1:B:203:PRO:HB3	1:B:692:SER:HB2	1.89	0.54
1:A:607:ASN:C	1:A:607:ASN:HD22	2.17	0.53
1:A:318:LYS:HG3	2:D:299:PRO:HB3	1.89	0.53
1:A:448:SER:HB3	1:A:451:GLU:O	2.08	0.53
2:E:266:ARG:HD3	2:E:266:ARG:C	2.30	0.53
2:E:266:ARG:CD	2:E:266:ARG:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:SER:CB	1:A:815:THR:HG23	2.38	0.53
1:B:698:ILE:HG23	1:B:712:PRO:HD2	1.89	0.53
1:B:302:GLY:O	1:B:304:LYS:HE3	2.08	0.53
1:B:283:SER:O	1:B:284:LYS:HB3	2.09	0.53
1:A:249:MET:SD	1:A:409:GLN:HG2	2.49	0.53
1:B:613:ASP:HB3	1:B:615:SER:H	1.73	0.52
1:A:393:ARG:HH12	1:A:793:ASP:HA	1.74	0.52
2:E:266:ARG:CD	2:E:266:ARG:N	2.72	0.52
1:B:196:GLN:HG2	1:B:207:THR:HG23	1.92	0.52
1:B:379:ALA:HB1	1:B:383:LEU:HD12	1.92	0.52
1:B:58:TYR:H	1:B:97:GLY:HA2	1.75	0.52
1:B:790:LEU:O	1:B:791:ASP:C	2.53	0.52
1:B:665:THR:C	1:B:666:SER:O	2.48	0.51
1:A:158:LEU:HD11	1:A:641:PHE:HB2	1.93	0.51
1:A:647:PHE:O	1:A:673:GLN:HA	2.10	0.51
1:A:240:MET:CE	1:A:272:ARG:HH21	2.24	0.51
1:B:218:TYR:CE2	3:B:901:OUE:H8	2.46	0.51
1:B:246:PHE:CD2	1:B:439:LEU:HD22	2.46	0.51
1:B:364:TYR:OH	1:B:366:GLN:NE2	2.44	0.51
1:A:773:GLY:HA2	1:A:778:LYS:HA	1.92	0.51
1:B:83:THR:HB	1:B:84:PRO:HD2	1.93	0.51
2:E:266:ARG:HD3	2:E:266:ARG:N	2.26	0.51
2:E:276:ARG:HD2	2:E:333:MET:CE	2.41	0.51
1:A:128:GLU:O	1:A:128:GLU:HG2	2.09	0.51
1:B:167:LYS:HG3	1:B:269:LEU:HD13	1.92	0.51
1:B:669:GLU:CG	1:B:701:THR:OG1	2.59	0.51
1:A:275:PRO:HB2	1:A:651:GLN:HE21	1.76	0.51
1:A:818:TYR:CD1	1:A:818:TYR:C	2.89	0.51
1:B:91:SER:C	1:B:92:SER:OG	2.52	0.51
2:D:267:MET:SD	2:D:271:ARG:NH1	2.84	0.51
1:A:101:VAL:O	1:A:104:GLY:N	2.44	0.50
1:B:686:ASN:HB3	1:B:727:ALA:O	2.11	0.50
1:A:240:MET:HE1	1:A:495:GLN:OE1	2.11	0.50
1:A:749:TRP:O	1:A:750:ALA:HB3	2.12	0.50
2:D:252:SER:OG	2:D:253:ASP:N	2.44	0.50
1:A:396:PHE:O	1:A:397:ASP:HB2	2.10	0.50
1:B:780:LEU:HA	1:B:817:ASN:O	2.12	0.50
2:E:264:TYR:CD1	2:E:269:GLN:HB3	2.46	0.50
1:B:57:PRO:HA	1:B:98:SER:H	1.76	0.49
2:E:275:GLY:HA3	2:E:303:PHE:CE2	2.47	0.49
1:A:62:ALA:HB1	1:A:93:GLN:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:ASN:C	1:A:811:ASN:HD22	2.20	0.49
1:A:393:ARG:NH1	1:A:793:ASP:HA	2.27	0.49
1:B:218:TYR:HE2	3:B:901:0UE:H8	1.78	0.49
1:B:246:PHE:HE1	3:B:901:0UE:H46	1.77	0.49
1:A:671:ARG:O	1:A:698:ILE:HA	2.13	0.49
1:B:396:PHE:CE2	1:B:398:GLY:O	2.66	0.49
1:A:340:GLU:HG3	1:A:372:GLY:HA2	1.95	0.49
1:A:727:ALA:HB2	1:A:737:SER:HB3	1.94	0.49
1:B:91:SER:O	1:B:92:SER:CB	2.61	0.48
1:A:562:VAL:HG12	1:A:579:TRP:HB2	1.94	0.48
1:A:240:MET:HE2	1:A:240:MET:HA	1.95	0.48
1:A:156:GLY:O	1:A:158:LEU:N	2.46	0.48
1:A:640:SER:OG	1:A:681:THR:HA	2.12	0.48
1:A:687:LEU:HA	1:A:726:TYR:HB3	1.95	0.48
1:B:314:LEU:HD21	1:B:322:TYR:CD1	2.49	0.48
1:B:562:VAL:HG11	1:B:608:PRO:HB3	1.96	0.48
1:B:393:ARG:NH2	1:B:791:ASP:OD1	2.46	0.48
1:B:771:ASP:HA	1:B:781:ASP:HB3	1.96	0.48
1:A:360:THR:O	1:A:414:TYR:HA	2.14	0.47
1:A:750:ALA:HA	1:A:798:CYS:HB2	1.96	0.47
1:B:374:HIS:NE2	3:B:901:0UE:H21	2.29	0.47
1:B:288:TYR:CD1	2:E:271:ARG:HG2	2.49	0.47
1:A:502:ASP:HA	1:A:530:ASN:OD1	2.14	0.47
1:A:203:PRO:HB3	1:A:692:SER:HB2	1.96	0.47
3:A:901:0UE:H8	3:A:901:0UE:H12	1.39	0.47
1:A:174:GLU:OE1	1:A:552:ARG:HD2	2.15	0.47
1:A:158:LEU:CD2	1:A:160:THR:HG23	2.45	0.47
1:B:112:THR:HG23	1:B:114:LEU:H	1.79	0.47
1:A:532:THR:OG1	1:A:569:ARG:HD2	2.15	0.46
1:A:371:GLY:HA3	1:A:405:PHE:HB3	1.96	0.46
1:B:112:THR:OG1	1:B:113:PRO:CD	2.62	0.46
1:A:278:LEU:HD12	1:A:278:LEU:C	2.41	0.46
1:B:199:MET:HE1	1:B:219:VAL:CG1	2.42	0.46
1:B:661:ASP:HB3	1:B:663:PHE:CD2	2.51	0.46
1:A:319:ARG:HG2	1:A:319:ARG:HH11	1.80	0.46
1:B:751:ASP:HB2	1:B:801:LEU:HG	1.98	0.46
1:A:89:GLY:O	1:A:90:TYR:CG	2.69	0.46
1:A:611:TYR:HB3	1:A:664:TYR:CD1	2.49	0.46
1:B:204:GLY:HA2	1:B:694:THR:HG21	1.97	0.46
1:A:129:ALA:HA	1:A:130:PRO:HD3	1.55	0.46
1:A:354:SER:HB3	1:A:356:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ASP:OD1	1:A:521:ASP:N	2.48	0.46
1:B:777:LEU:HD12	1:B:777:LEU:N	2.23	0.46
2:E:266:ARG:H	2:E:266:ARG:HD2	1.80	0.46
1:A:90:TYR:CD1	1:A:112:THR:HG22	2.51	0.45
1:A:240:MET:HE1	1:A:272:ARG:HH21	1.81	0.45
2:D:304:ASP:OD1	2:D:304:ASP:N	2.40	0.45
2:E:269:GLN:C	2:E:269:GLN:CD	2.84	0.45
1:B:80:LEU:HD23	1:B:80:LEU:HA	1.65	0.45
1:B:214:ASN:HB2	1:B:340:GLU:OE1	2.16	0.45
1:B:613:ASP:HB3	1:B:615:SER:N	2.31	0.45
1:A:359:LEU:HD13	1:A:416:LEU:HD13	1.98	0.45
1:A:661:ASP:HB3	1:A:663:PHE:H	1.81	0.45
1:A:819:GLN:O	1:A:820:PHE:CD2	2.70	0.45
1:B:112:THR:HG23	1:B:114:LEU:N	2.32	0.45
1:B:272:ARG:HG2	1:B:608:PRO:HD2	1.98	0.45
1:B:316:GLU:OE2	1:B:316:GLU:HA	2.17	0.45
2:D:254:ILE:HG13	2:D:283:ILE:HD12	1.97	0.45
2:E:275:GLY:HA3	2:E:303:PHE:HE2	1.80	0.45
1:A:247:SER:N	1:A:464:GLU:OE1	2.48	0.45
1:A:445:TYR:CE1	1:A:660:GLN:HG2	2.51	0.45
1:A:596:LEU:HD11	1:A:631:LEU:HD11	1.99	0.45
1:B:209:GLN:HG3	1:B:220:VAL:HG21	1.99	0.45
1:B:314:LEU:HD21	1:B:322:TYR:HD1	1.82	0.45
1:B:344:ALA:HB2	1:B:366:GLN:HG3	1.99	0.45
1:B:374:HIS:CD2	1:B:374:HIS:O	2.70	0.45
1:A:272:ARG:HG3	1:A:608:PRO:HD2	1.99	0.45
1:A:200:ARG:HD2	1:A:743:ARG:NE	2.32	0.45
1:A:533:ARG:NH2	1:A:610:ALA:O	2.46	0.44
1:B:246:PHE:CE1	3:B:901:OUE:H41	2.52	0.44
1:B:173:LEU:HD22	1:B:634:GLN:HB3	1.99	0.44
1:B:471:VAL:HG22	1:B:472:ASP:N	2.33	0.44
1:A:214:ASN:HB2	1:A:340:GLU:OE2	2.17	0.44
1:B:284:LYS:O	1:B:284:LYS:HG2	2.17	0.44
1:B:387:ASN:ND2	1:B:453:ASN:OD1	2.51	0.44
1:A:729:ASP:OD1	1:A:729:ASP:N	2.51	0.44
1:B:275:PRO:HB2	1:B:651:GLN:HG2	1.99	0.44
1:A:613:ASP:HB3	1:A:615:SER:H	1.82	0.44
1:B:278:LEU:C	1:B:278:LEU:HD12	2.43	0.44
1:B:535:LEU:HD12	1:B:564:VAL:CG2	2.47	0.44
1:A:314:LEU:HB2	1:A:320:ILE:HG22	2.00	0.43
1:B:118:ASP:O	1:B:124:PHE:HE1	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:901:0UE:H24	3:B:901:0UE:H30	1.63	0.43
2:D:276:ARG:HE	2:D:298:VAL:CG2	2.31	0.43
1:A:707:ASN:O	1:A:710:HIS:HB2	2.18	0.43
1:A:62:ALA:HB2	1:A:93:GLN:HA	2.00	0.43
1:A:466:LEU:HD23	1:A:466:LEU:C	2.43	0.43
1:A:683:LEU:HD23	1:A:687:LEU:HD23	2.01	0.43
1:A:453:ASN:HD22	1:A:453:ASN:HA	1.57	0.43
1:B:602:TYR:CD2	1:B:602:TYR:C	2.96	0.43
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.84	0.43
1:A:788:ASN:O	1:A:810:ARG:HG3	2.19	0.43
1:A:818:TYR:C	1:A:818:TYR:HD1	2.25	0.43
1:B:531:HIS:ND1	1:B:566:ASP:OD1	2.44	0.43
2:E:263:VAL:O	2:E:263:VAL:HG13	2.19	0.43
1:A:659:PRO:HG2	1:A:803:PHE:CD2	2.54	0.43
1:A:473:ASN:HD22	1:A:492:LEU:HD23	1.83	0.43
1:A:247:SER:HA	1:A:437:VAL:HG21	2.00	0.42
1:B:394:GLU:O	1:B:395:PHE:HB3	2.19	0.42
1:A:782:VAL:HG13	1:A:783:SER:N	2.35	0.42
1:B:200:ARG:HD2	1:B:207:THR:HG21	2.00	0.42
1:B:590:TYR:O	1:B:597:ALA:HA	2.19	0.42
1:A:189:ASP:O	1:A:767:ARG:HD2	2.20	0.42
1:A:393:ARG:NH2	1:A:791:ASP:OD1	2.52	0.42
1:A:614:ALA:HB2	1:A:663:PHE:CE2	2.54	0.42
1:A:711:THR:HA	1:A:712:PRO:HD3	1.92	0.42
1:B:287:LEU:CD1	1:B:287:LEU:N	2.82	0.42
1:B:379:ALA:HB2	1:B:804:CYS:SG	2.59	0.42
1:B:334:GLN:O	1:B:394:GLU:OE1	2.36	0.42
1:B:450:SER:OG	1:B:451:GLU:N	2.52	0.42
2:D:264:TYR:CD1	2:D:265:PRO:HD2	2.55	0.42
1:B:660:GLN:HE21	1:B:660:GLN:HB2	1.71	0.42
1:A:86:GLN:NE2	1:A:126:LEU:O	2.50	0.42
1:B:90:TYR:CE2	1:B:140:GLN:HG2	2.54	0.42
1:B:196:GLN:HG3	1:B:218:TYR:O	2.20	0.42
1:B:749:TRP:CZ2	1:B:754:ASN:HB3	2.55	0.42
1:A:57:PRO:HA	1:A:98:SER:HA	2.01	0.42
1:B:420:ILE:HD13	1:B:420:ILE:HG21	1.82	0.42
1:A:91:SER:OG	1:A:92:SER:N	2.49	0.42
1:A:166:THR:O	1:A:168:THR:HG22	2.20	0.42
1:A:211:GLY:O	1:A:213:SER:N	2.53	0.42
1:A:657:LYS:HG2	3:A:901:0UE:H13	2.01	0.42
1:B:63:GLY:O	1:B:68:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:PHE:HB3	1:B:220:VAL:HB	2.02	0.42
1:B:664:TYR:CD1	1:B:664:TYR:N	2.88	0.42
1:A:375:GLY:HA2	3:A:901:0UE:C25	2.50	0.41
1:A:100:THR:HG22	1:A:103:GLN:CD	2.45	0.41
1:B:142:VAL:CG2	2:E:332:LYS:HE3	2.50	0.41
2:E:267:MET:HB2	2:E:267:MET:HE2	1.46	0.41
1:A:115:GLU:CB	1:A:129:ALA:HB2	2.47	0.41
1:A:344:ALA:HB2	1:A:366:GLN:HG3	2.03	0.41
1:A:626:GLN:HG3	1:A:649:ILE:CG1	2.49	0.41
1:A:689:LEU:HD22	1:A:722:LEU:HD11	2.02	0.41
1:B:129:ALA:HB3	1:B:130:PRO:HD3	2.02	0.41
2:E:305:ARG:O	2:E:309:GLN:HG3	2.20	0.41
2:E:306:GLU:H	2:E:306:GLU:HG2	1.60	0.41
1:B:246:PHE:CE2	1:B:439:LEU:CD2	3.03	0.41
1:B:300:ASN:O	1:B:303:GLN:HG3	2.20	0.41
1:A:100:THR:O	1:A:101:VAL:C	2.64	0.41
1:A:195:VAL:O	1:A:196:GLN:C	2.62	0.41
1:A:634:GLN:HG3	1:A:640:SER:O	2.21	0.41
1:B:65:LEU:HD23	1:B:90:TYR:HB2	2.01	0.41
1:B:161:HIS:O	1:B:258:ARG:NH2	2.54	0.41
1:A:242:ASP:C	1:A:242:ASP:OD1	2.63	0.41
1:A:210:VAL:O	1:A:210:VAL:CG1	2.69	0.41
1:A:244:GLY:O	3:A:901:0UE:H43	2.21	0.41
1:A:322:TYR:CD1	1:A:322:TYR:C	2.99	0.41
1:A:751:ASP:HB3	1:A:754:ASN:H	1.86	0.41
1:B:794:TYR:CZ	1:B:807:GLY:HA3	2.56	0.41
1:A:54:GLN:OE1	1:A:54:GLN:N	2.54	0.41
1:A:130:PRO:O	1:A:130:PRO:CD	2.69	0.41
1:B:196:GLN:NE2	1:B:218:TYR:H	2.18	0.41
2:E:264:TYR:CD1	2:E:265:PRO:HD2	2.56	0.41
1:A:646:LEU:HD13	1:A:675:LEU:HD13	2.01	0.40
1:B:242:ASP:OD1	1:B:533:ARG:NH1	2.54	0.40
1:B:56:ARG:HB3	1:B:57:PRO:CD	2.51	0.40
1:A:319:ARG:HG2	1:A:319:ARG:NH1	2.37	0.40
1:A:626:GLN:HB2	1:A:649:ILE:HG12	2.03	0.40
1:B:396:PHE:O	1:B:396:PHE:CG	2.74	0.40
1:B:427:ARG:HB3	1:B:474:MET:HE3	2.03	0.40
1:A:401:SER:O	1:A:402:LYS:HB2	2.22	0.40
1:A:496:ARG:HH12	1:A:534:ARG:NH1	2.20	0.40
1:A:537:GLN:HB2	1:A:562:VAL:HG23	2.03	0.40
1:B:565:THR:HG22	1:B:576:ASP:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:901:0UE:H31	3:B:901:0UE:H34	1.93	0.40
2:D:271:ARG:O	2:D:272:GLY:C	2.64	0.40

There are no symmetry-related clashes.

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	759/768 (99%)	667 (88%)	71 (9%)	21 (3%)	4	19
1	B	753/768 (98%)	655 (87%)	79 (10%)	19 (2%)	4	20
2	D	88/90 (98%)	74 (84%)	11 (12%)	3 (3%)	3	16
2	E	88/90 (98%)	81 (92%)	4 (4%)	3 (3%)	3	16
All	All	1688/1716 (98%)	1477 (88%)	165 (10%)	46 (3%)	4	20

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	65	LEU
1	A	92	SER
1	A	118	ASP
1	A	157	TYR
1	A	212	ALA
1	A	397	ASP
1	A	402	LYS
1	A	775	LEU
1	B	61	PRO
1	B	64	GLN
1	B	65	LEU
1	B	98	SER

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Mol	Chain	Res	Type
1	B	129	ALA
1	B	212	ALA
2	D	254	ILE
2	E	286	ASP
1	A	130	PRO
1	A	134	GLY
1	A	387	ASN
1	A	661	ASP
1	B	208	GLY
1	B	372	GLY
1	B	655	ALA
2	E	268	ALA
1	A	101	VAL
1	A	102	GLN
1	A	124	PHE
1	A	135	ASP
1	A	659	PRO
1	B	666	SER
1	B	667	VAL
2	D	268	ALA
1	A	660	GLN
1	B	97	GLY
1	B	658	GLU
1	A	638	SER
1	B	394	GLU
1	B	395	PHE
1	B	423	VAL
2	D	272	GLY
1	A	452	PRO
1	B	57	PRO
1	B	636	PRO
1	B	637	GLY
2	E	254	ILE

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	629/633 (99%)	526 (84%)	103 (16%)	2	10
1	B	627/633 (99%)	525 (84%)	102 (16%)	2	10
2	D	79/79 (100%)	58 (73%)	21 (27%)	0	1
2	E	79/79 (100%)	62 (78%)	17 (22%)	1	3
All	All	1414/1424 (99%)	1171 (83%)	243 (17%)	2	8

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	56	ARG
1	A	79	THR
1	A	80	LEU
1	A	81	SER
1	A	91	SER
1	A	93	GLN
1	A	95	LEU
1	A	101	VAL
1	A	102	GLN
1	A	109	LEU
1	A	117	GLU
1	A	125	VAL
1	A	127	ARG
1	A	128	GLU
1	A	136	VAL
1	A	138	ASN
1	A	143	GLU
1	A	144	VAL
1	A	149	ASN
1	A	166	THR
1	A	170	LYS
1	A	177	GLN
1	A	185	GLU
1	A	219	VAL
1	A	229	VAL
1	A	230	ASP
1	A	263	LYS
1	A	274	LEU
1	A	282	THR
1	A	293	GLN
1	A	298	ILE
1	A	304	LYS

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Mol	Chain	Res	Type
1	A	306	MET
1	A	314	LEU
1	A	319	ARG
1	A	327	LEU
1	A	332	ASP
1	A	355	ASP
1	A	358	THR
1	A	377	VAL
1	A	384	SER
1	A	385	HIS
1	A	389	ARG
1	A	391	ILE
1	A	393	ARG
1	A	404	ASP
1	A	408	THR
1	A	420	ILE
1	A	435	SER
1	A	440	SER
1	A	441	GLN
1	A	453	ASN
1	A	473	ASN
1	A	474	MET
1	A	489	LEU
1	A	490	THR
1	A	492	LEU
1	A	495	GLN
1	A	499	THR
1	A	514	PHE
1	A	527	PRO
1	A	555	LEU
1	A	567	LYS
1	A	571	THR
1	A	574	LYS
1	A	580	GLU
1	A	583	THR
1	A	601	SER
1	A	607	ASN
1	A	612	SER
1	A	613	ASP
1	A	650	THR
1	A	654	VAL
1	A	657	LYS

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Mol	Chain	Res	Type
1	A	660	GLN
1	A	662	ASN
1	A	665	THR
1	A	671	ARG
1	A	681	THR
1	A	685	ASP
1	A	688	LYS
1	A	689	LEU
1	A	701	THR
1	A	702	LYS
1	A	719	MET
1	A	729	ASP
1	A	737	SER
1	A	748	THR
1	A	755	THR
1	A	758	VAL
1	A	775	LEU
1	A	778	LYS
1	A	782	VAL
1	A	785	ASN
1	A	799	TYR
1	A	801	LEU
1	A	811	ASN
1	A	813	THR
1	A	815	THR
1	A	816	VAL
1	A	817	ASN
1	A	819	GLN
1	B	53	GLU
1	B	54	GLN
1	B	56	ARG
1	B	60	ILE
1	B	80	LEU
1	B	81	SER
1	B	86	GLN
1	B	92	SER
1	B	93	GLN
1	B	95	LEU
1	B	100	THR
1	B	105	LEU
1	B	107	ARG
1	B	109	LEU

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Mol	Chain	Res	Type
1	B	115	GLU
1	B	117	GLU
1	B	119	GLN
1	B	125	VAL
1	B	142	VAL
1	B	144	VAL
1	B	155	ASP
1	B	166	THR
1	B	193	LYS
1	B	205	ILE
1	B	209	GLN
1	B	219	VAL
1	B	222	ARG
1	B	229	VAL
1	B	232	ILE
1	B	235	ASP
1	B	238	LYS
1	B	247	SER
1	B	250	GLN
1	B	273	SER
1	B	289	GLU
1	B	297	SER
1	B	298	ILE
1	B	305	GLU
1	B	306	MET
1	B	316	GLU
1	B	327	LEU
1	B	348	THR
1	B	356	ASP
1	B	357	THR
1	B	360	THR
1	B	384	SER
1	B	393	ARG
1	B	397	ASP
1	B	402	LYS
1	B	409	GLN
1	B	422	ASP
1	B	431	ARG
1	B	435	SER
1	B	440	SER
1	B	460	SER
1	B	467	GLN

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Mol	Chain	Res	Type
1	B	473	ASN
1	B	487	THR
1	B	489	LEU
1	B	490	THR
1	B	499	THR
1	B	500	VAL
1	B	504	ARG
1	B	509	SER
1	B	512	ASP
1	B	514	PHE
1	B	521	ASP
1	B	524	SER
1	B	533	ARG
1	B	535	LEU
1	B	538	THR
1	B	540	VAL
1	B	542	LEU
1	B	555	LEU
1	B	567	LYS
1	B	570	SER
1	B	571	THR
1	B	573	SER
1	B	574	LYS
1	B	583	THR
1	B	585	ARG
1	B	603	SER
1	B	623	GLU
1	B	629	LEU
1	B	639	ASN
1	B	650	THR
1	B	656	SER
1	B	658	GLU
1	B	660	GLN
1	B	665	THR
1	B	675	LEU
1	B	677	LEU
1	B	682	GLN
1	B	686	ASN
1	B	689	LEU
1	B	704	LEU
1	B	737	SER
1	B	747	GLU

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Mol	Chain	Res	Type
1	B	755	THR
1	B	777	LEU
1	B	802	ASP
1	B	813	THR
2	D	251	ASP
2	D	252	SER
2	D	258	ARG
2	D	263	VAL
2	D	267	MET
2	D	269	GLN
2	D	271	ARG
2	D	276	ARG
2	D	286	ASP
2	D	293	GLN
2	D	294	VAL
2	D	297	SER
2	D	304	ASP
2	D	306	GLU
2	D	309	GLN
2	D	311	MET
2	D	317	GLU
2	D	326	VAL
2	D	328	ARG
2	D	331	THR
2	D	340	LYS
2	E	252	SER
2	E	254	ILE
2	E	267	MET
2	E	269	GLN
2	E	271	ARG
2	E	279	VAL
2	E	285	SER
2	E	294	VAL
2	E	318	PRO
2	E	319	ARG
2	E	320	VAL
2	E	324	LYS
2	E	326	VAL
2	E	328	ARG
2	E	331	THR
2	E	339	GLU
2	E	340	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	103	GLN
1	A	293	GLN
1	A	387	ASN
1	A	409	GLN
1	A	515	ASN
1	A	607	ASN
1	A	639	ASN
1	A	651	GLN
1	A	686	ASN
1	A	785	ASN
1	A	811	ASN
1	A	817	ASN
1	A	819	GLN
1	B	64	GLN
1	B	86	GLN
1	B	119	GLN
1	B	161	HIS
1	B	196	GLN
1	B	366	GLN
1	B	385	HIS
1	B	550	GLN
1	B	559	GLN
1	B	626	GLN
1	B	660	GLN
1	B	718	HIS
1	B	754	ASN
2	D	269	GLN
2	E	269	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	0UE	A	901	-	44,44,44	2.92	11 (25%)	44,66,66	4.90	12 (27%)
3	0UE	B	901	-	44,44,44	2.78	10 (22%)	44,66,66	4.41	11 (25%)

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	0UE	A	901	-	2/2/9/11	15/34/88/88	0/3/5/5
3	0UE	B	901	-	2/2/9/11	13/34/88/88	0/3/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	0UE	O11-N11	-10.23	1.20	1.38
3	B	901	0UE	O11-N11	-9.64	1.21	1.38
3	A	901	0UE	O21-N21	-9.53	1.21	1.38
3	A	901	0UE	O31-N31	-8.85	1.23	1.38
3	B	901	0UE	O31-N31	-8.67	1.23	1.38
3	B	901	0UE	O21-N21	-8.37	1.23	1.38
3	B	901	0UE	O32-FE	-4.27	1.92	2.04
3	A	901	0UE	O32-FE	-4.17	1.93	2.04
3	B	901	0UE	O21-FE	-3.95	1.90	1.99
3	A	901	0UE	O31-FE	-3.92	1.90	1.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	0UE	O22-FE	-3.88	1.94	2.04
3	A	901	0UE	O22-FE	-3.70	1.94	2.04
3	A	901	0UE	O21-FE	-3.63	1.91	1.99
3	B	901	0UE	O31-FE	-3.48	1.91	1.99
3	B	901	0UE	O12-FE	-3.09	1.96	2.04
3	A	901	0UE	C21-N21	3.08	1.36	1.31
3	B	901	0UE	C21-N21	2.91	1.36	1.31
3	B	901	0UE	O12-C11	-2.46	1.23	1.28
3	A	901	0UE	O12-FE	-2.29	1.98	2.04
3	A	901	0UE	C31-N31	2.14	1.37	1.31
3	A	901	0UE	O12-C11	-2.13	1.24	1.28

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	0UE	O11-N11-C11	-24.95	100.12	116.42
3	B	901	0UE	O11-N11-C11	-19.29	103.82	116.42
3	B	901	0UE	O12-C11-N11	-12.97	108.48	118.38
3	A	901	0UE	O12-C11-N11	-12.84	108.58	118.38
3	B	901	0UE	O21-N21-C21	9.91	122.89	116.42
3	A	901	0UE	O21-N21-C21	8.72	122.11	116.42
3	B	901	0UE	C19-N21-C21	-7.64	119.85	128.89
3	A	901	0UE	O11-N11-C39	7.57	126.78	114.13
3	B	901	0UE	O11-N11-C39	6.92	125.69	114.13
3	B	901	0UE	C12-C11-N11	6.40	129.07	121.07
3	A	901	0UE	C12-C11-N11	6.06	128.64	121.07
3	A	901	0UE	O22-C21-N21	-4.73	114.77	118.38
3	A	901	0UE	C19-N21-C21	-4.62	123.42	128.89
3	B	901	0UE	O22-C21-N21	-4.56	114.90	118.38
3	B	901	0UE	O31-N31-C31	4.36	123.69	116.68
3	A	901	0UE	O31-N31-C31	3.87	122.91	116.68
3	A	901	0UE	C39-N11-C11	3.54	133.08	128.89
3	B	901	0UE	C22-C21-N21	2.72	124.48	121.07
3	A	901	0UE	O32-C31-N31	-2.50	114.26	118.42
3	A	901	0UE	O12-C11-C12	2.48	122.74	120.13
3	A	901	0UE	C22-C21-N21	2.32	123.97	121.07
3	B	901	0UE	O32-C31-N31	-2.21	114.74	118.42
3	B	901	0UE	O12-C11-C12	2.17	122.42	120.13

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	901	0UE	N31
3	A	901	0UE	N21
3	B	901	0UE	N31
3	B	901	0UE	N21

All (28) torsion outliers are listed below:

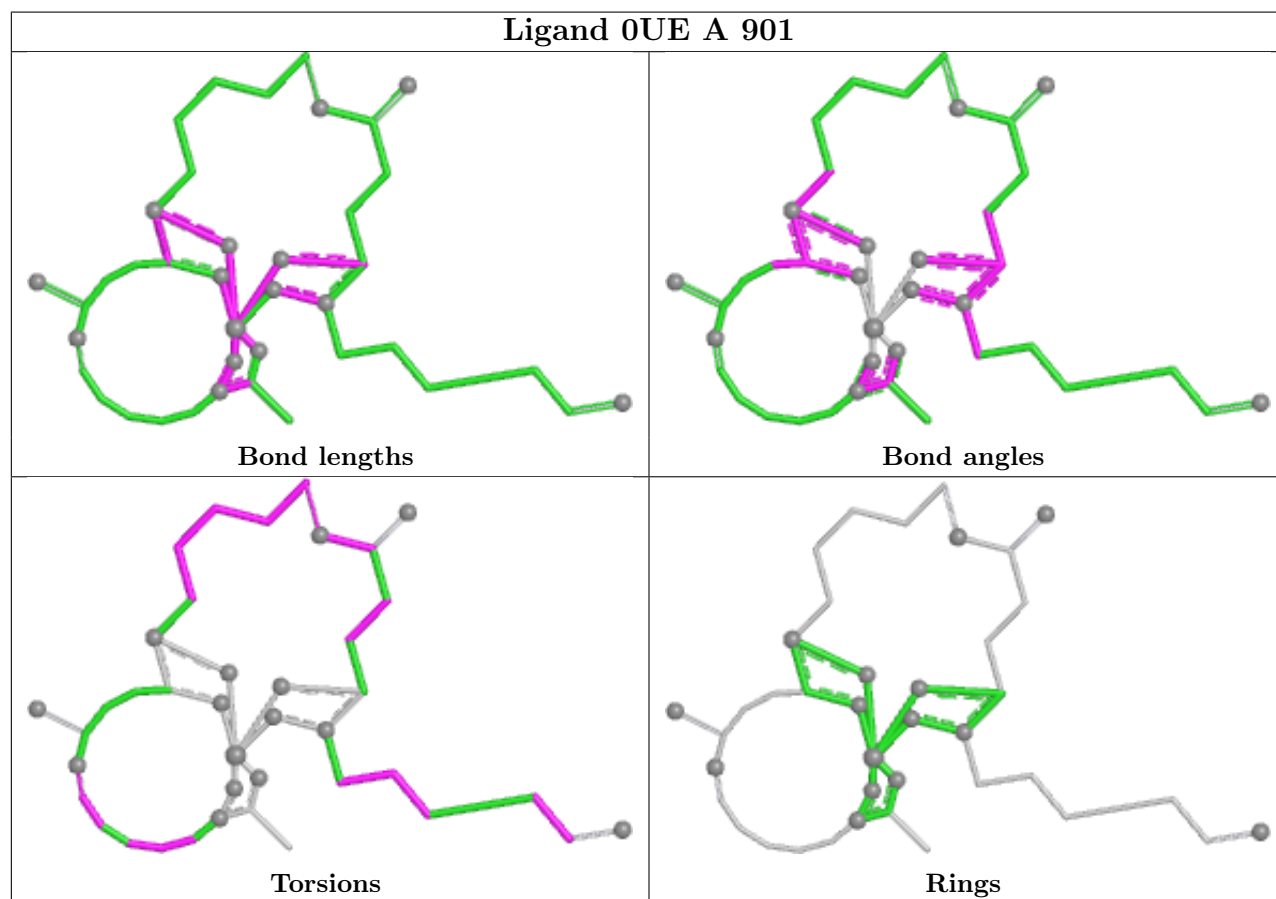
Mol	Chain	Res	Type	Atoms
3	A	901	0UE	C11-C12-C13-C14
3	A	901	0UE	C17-C18-C19-N21
3	A	901	0UE	C27-C28-C29-N31
3	A	901	0UE	N11-C39-C40-C41
3	B	901	0UE	N11-C39-C40-C41
3	B	901	0UE	C26-C25-N22-C24
3	A	901	0UE	C16-C15-N12-C14
3	A	901	0UE	C26-C25-N22-C24
3	A	901	0UE	C15-C16-C17-C18
3	A	901	0UE	O13-C14-N12-C15
3	A	901	0UE	N12-C15-C16-C17
3	A	901	0UE	C13-C14-N12-C15
3	A	901	0UE	N22-C25-C26-C27
3	B	901	0UE	C25-C26-C27-C28
3	A	901	0UE	C26-C27-C28-C29
3	A	901	0UE	C41-C42-C43-N44
3	B	901	0UE	C12-C13-C14-N12
3	A	901	0UE	C39-C40-C41-C42
3	B	901	0UE	C12-C13-C14-O13
3	B	901	0UE	N12-C15-C16-C17
3	A	901	0UE	C16-C17-C18-C19
3	B	901	0UE	C27-C28-C29-N31
3	B	901	0UE	O23-C24-N22-C25
3	B	901	0UE	N22-C25-C26-C27
3	B	901	0UE	C23-C24-N22-C25
3	B	901	0UE	C11-C12-C13-C14
3	B	901	0UE	C16-C17-C18-C19
3	B	901	0UE	C40-C39-N11-O11

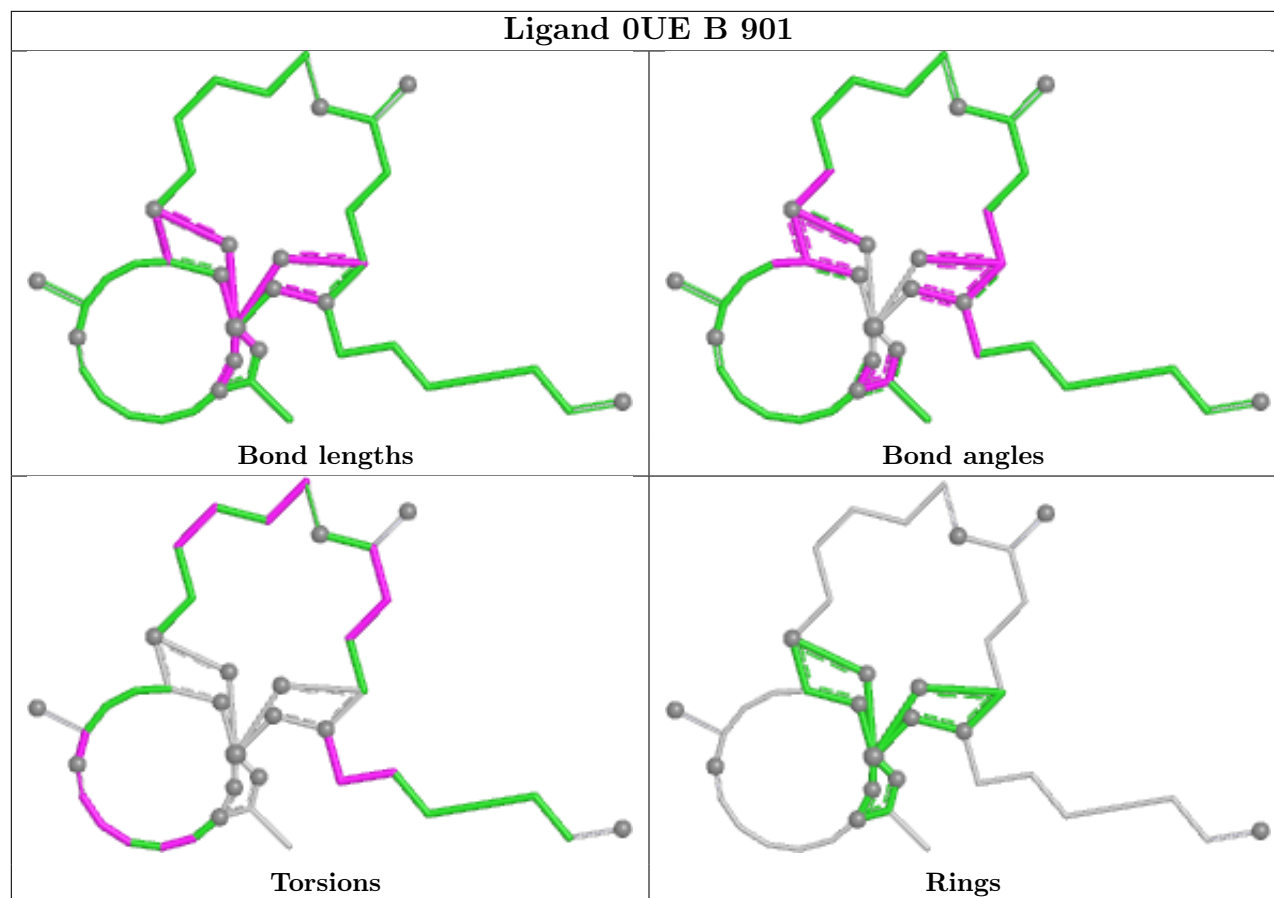
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	0UE	7	0
3	B	901	0UE	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

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	763/768 (99%)	0.22	47 (6%) 26 20	62, 89, 119, 145	0
1	B	759/768 (98%)	0.33	47 (6%) 26 20	63, 85, 117, 150	0
2	D	90/90 (100%)	0.25	7 (7%) 19 15	62, 83, 116, 135	0
2	E	90/90 (100%)	0.25	7 (7%) 19 15	65, 82, 106, 122	0
All	All	1702/1716 (99%)	0.27	108 (6%) 26 19	62, 86, 118, 150	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	ASP	7.6
1	B	155	ASP	6.3
1	B	130	PRO	5.3
1	A	134	GLY	5.1
1	A	730	ALA	4.5
1	B	639	ASN	4.5
1	B	637	GLY	4.4
1	B	54	GLN	4.4
1	A	484	ALA	4.3
1	A	130	PRO	4.3
1	B	149	ASN	4.3
1	A	133	ASP	4.3
1	B	427	ARG	4.2
1	B	355	ASP	4.1
1	B	665	THR	4.1
1	A	422	ASP	4.0
2	E	321	SER	4.0
1	A	155	ASP	4.0
1	B	120	GLY	3.7
1	B	682	GLN	3.6
1	A	480	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	820	PHE	3.6
1	A	304	LYS	3.6
1	A	482	GLY	3.5
1	B	688	LYS	3.5
1	B	450	SER	3.5
1	A	481	THR	3.5
1	A	726	TYR	3.4
1	A	64	GLN	3.4
1	B	440	SER	3.3
1	A	384	SER	3.3
1	B	257	GLU	3.3
1	B	277	GLY	3.3
2	E	323	GLY	3.2
1	B	121	ASP	3.2
1	A	228	SER	3.1
2	E	340	LYS	3.1
1	A	683	LEU	3.0
1	A	570	SER	3.0
1	A	625	LYS	2.9
1	B	362	GLN	2.9
2	D	322	GLY	2.9
2	D	251	ASP	2.8
1	B	93	GLN	2.8
1	A	652	GLU	2.8
1	B	57	PRO	2.8
1	A	156	GLY	2.8
1	A	629	LEU	2.8
1	B	820	PHE	2.7
2	D	305	ARG	2.7
1	B	483	ALA	2.7
1	A	688	LYS	2.7
1	B	404	ASP	2.7
1	B	725	ASP	2.7
1	B	289	GLU	2.7
2	D	306	GLU	2.7
1	A	91	SER	2.6
1	B	491	GLY	2.6
2	E	322	GLY	2.6
1	A	483	ALA	2.6
1	A	732	PRO	2.5
1	B	638	SER	2.5
1	A	604	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	276	GLY	2.5
1	B	119	GLN	2.5
2	E	267	MET	2.5
1	A	778	LYS	2.5
1	B	753	GLU	2.4
1	B	56	ARG	2.4
1	A	77	GLY	2.4
1	A	624	GLY	2.4
1	B	159	ALA	2.4
1	B	751	ASP	2.4
1	B	161	HIS	2.4
1	A	131	ALA	2.4
1	A	731	GLY	2.3
1	B	71	ARG	2.3
1	B	690	LEU	2.3
2	D	304	ASP	2.3
1	B	422	ASP	2.3
1	B	567	LYS	2.3
1	B	271	GLY	2.2
1	A	517	VAL	2.2
1	A	505	SER	2.2
1	B	652	GLU	2.2
1	A	744	TYR	2.2
2	E	258	ARG	2.2
1	A	122	GLY	2.1
1	B	258	ARG	2.1
1	A	135	ASP	2.1
2	D	340	LYS	2.1
1	A	388	GLY	2.1
1	B	490	THR	2.1
1	A	306	MET	2.1
1	A	93	GLN	2.1
1	B	415	GLN	2.1
1	A	394	GLU	2.1
1	B	485	ARG	2.1
2	D	267	MET	2.1
1	A	469	TYR	2.1
1	A	506	GLY	2.1
2	E	337	LYS	2.0
1	A	385	HIS	2.0
1	B	59	ALA	2.0
1	A	526	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	413	GLY	2.0
1	A	584	GLY	2.0
1	B	264	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

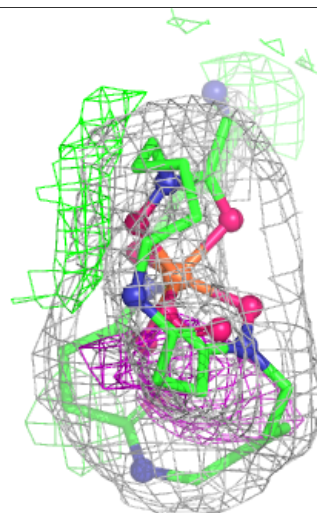
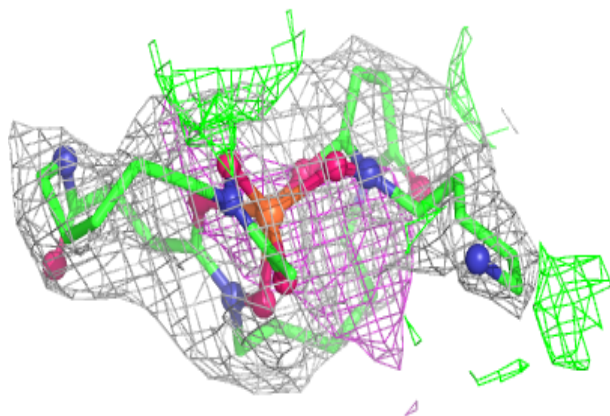
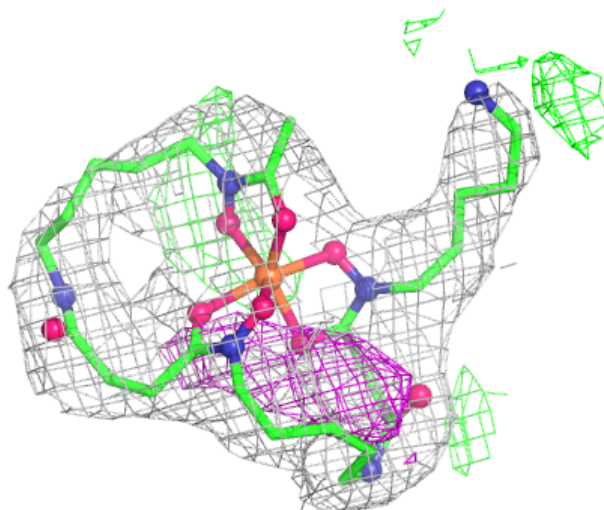
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	0UE	A	901	40/40	0.96	0.14	59,81,103,140	0
3	0UE	B	901	40/40	0.96	0.13	46,71,94,109	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

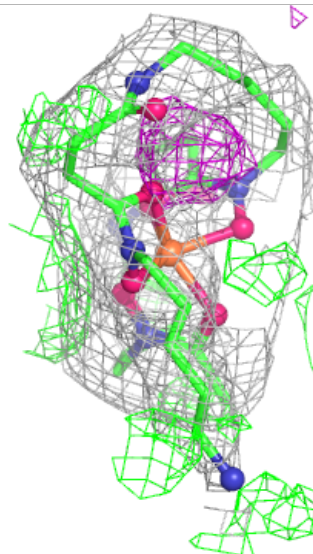
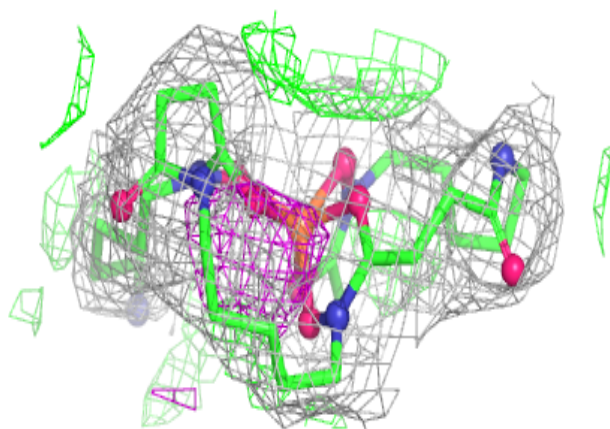
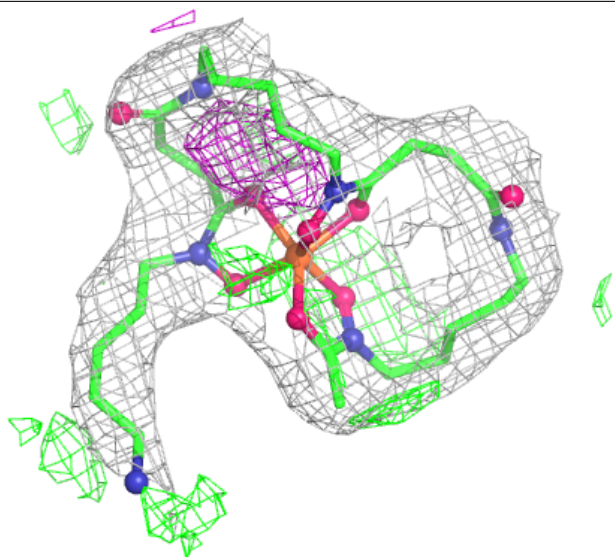
Electron density around 0UE A 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 0UE B 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.