Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:53 am BST

PDB ID	:	6I97
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 following versions of software and data (see references ⓘ) were used in the production of this report:

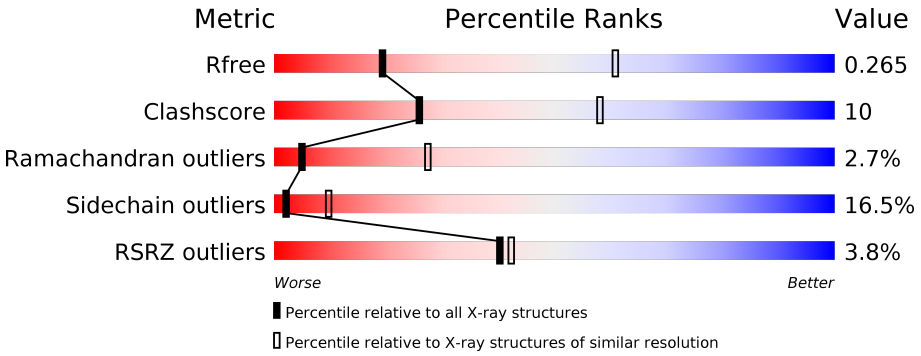
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 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% 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	5% 64% 28% 6%
1	B	768	3% 65% 27% 6%
2	D	90	4% 62% 29% 9%
2	E	90	% 61% 32% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	0UE	A	901	X	-	-	-
3	0UE	B	901	X	-	-	-

2 Entry composition

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.

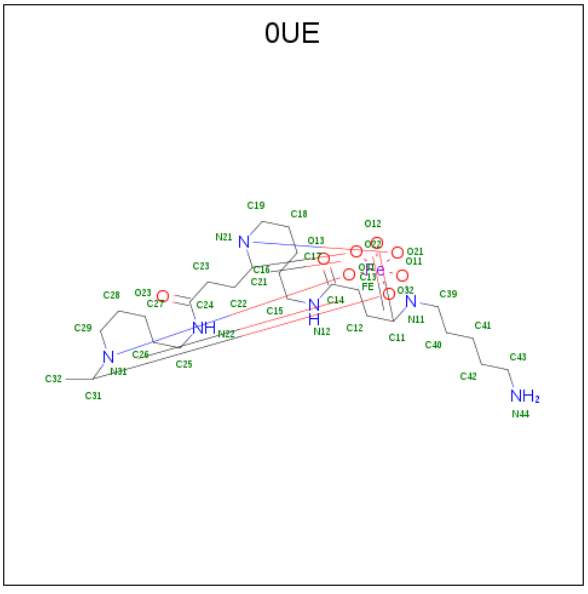
- Molecule 1 is a protein called TonB-dependent receptor.

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 (three-letter code: 0UE) (formula: $C_{25}H_{45}FeN_6O_8$).



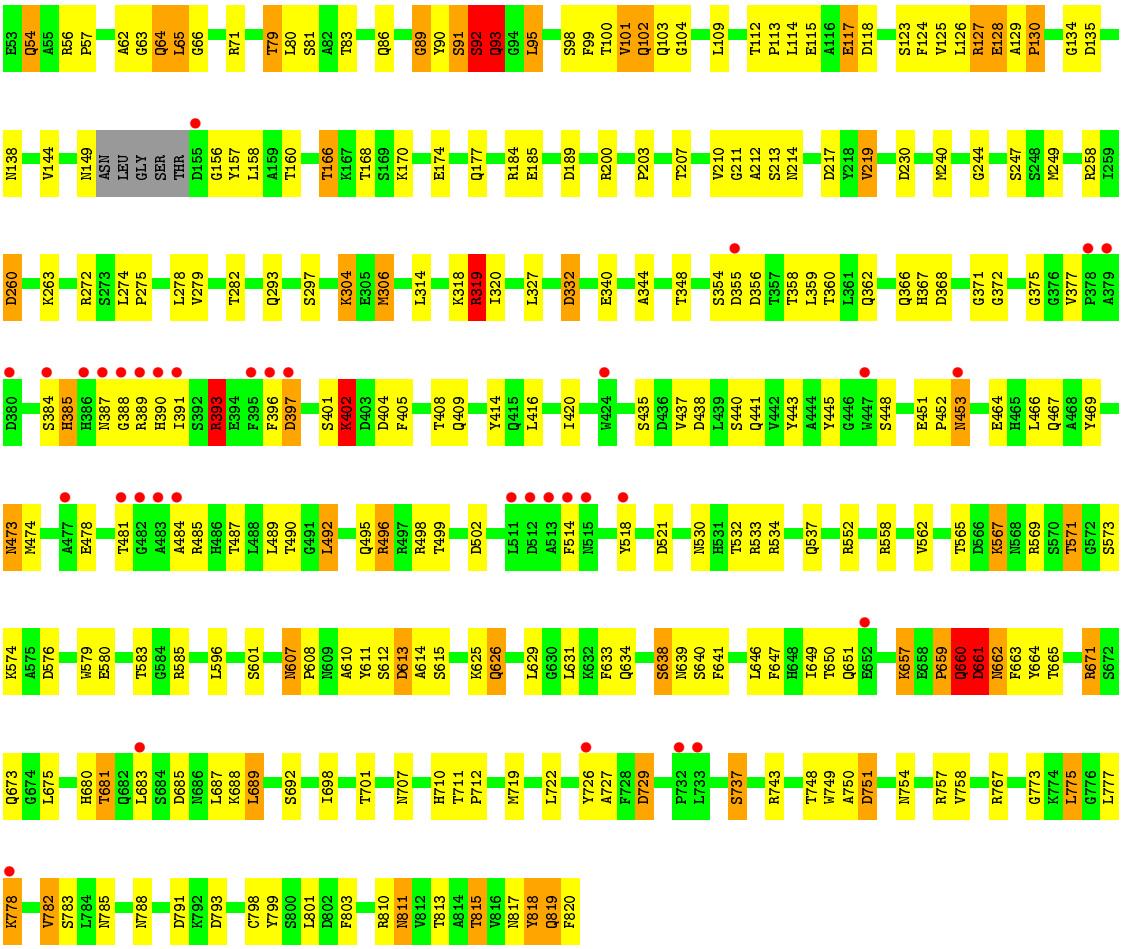
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			40	25	1	6	8		
3	B	1	Total	C	Fe	N	O	0	0
			40	25	1	6	8		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

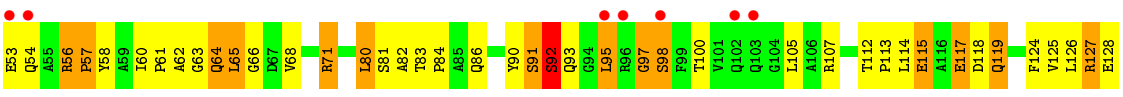
- Molecule 1: TonB-dependent receptor

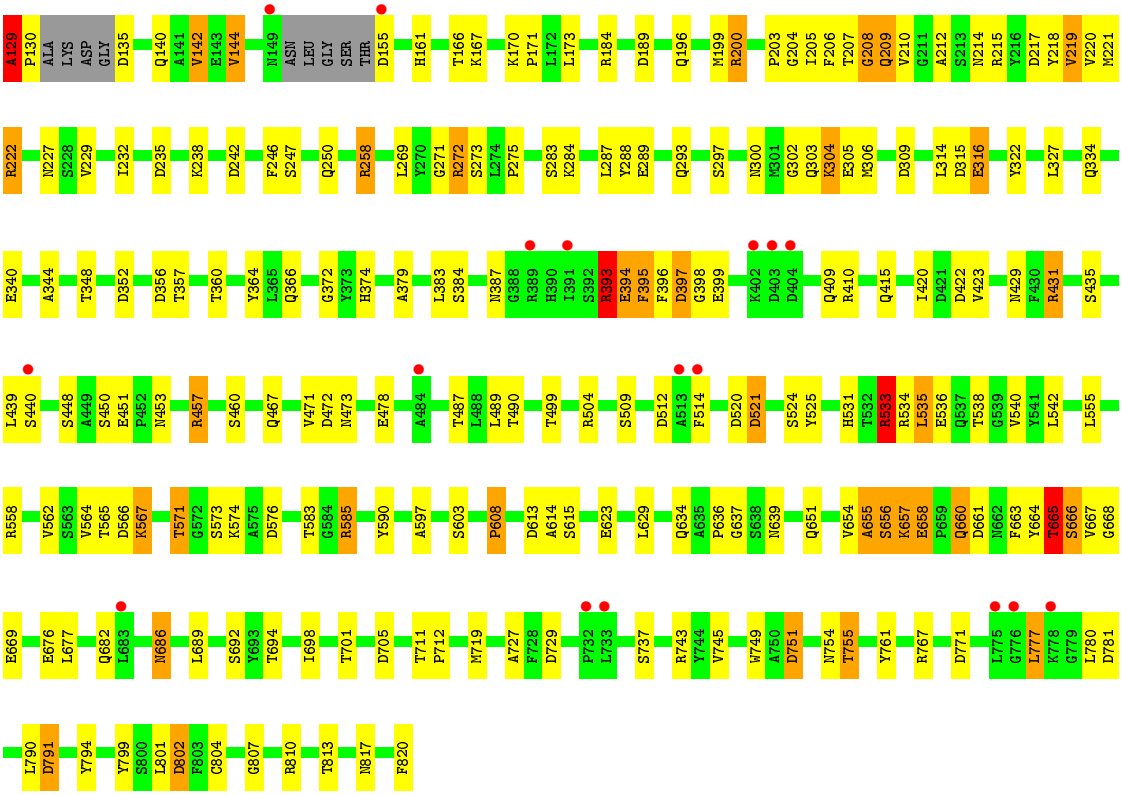
Chain A:



- Molecule 1: TonB-dependent receptor

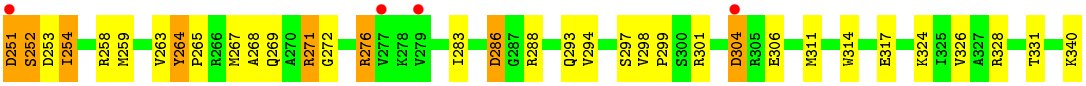
Chain B:





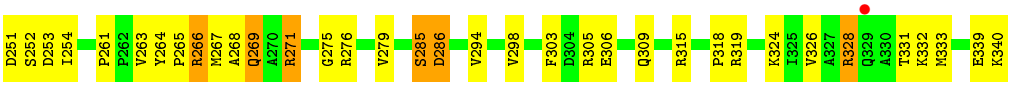
- Molecule 2: Protein TonB

Chain D:



- Molecule 2: Protein TonB

Chain E:



4 Data and refinement statistics (i)

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)	135.22 – 3.35 48.84 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (135.22-3.35) 99.9 (48.84-3.35)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.229 , 0.264 0.236 , 0.265	Depositor DCC
R_{free} test set	4361 reflections (4.93%)	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)	0.30 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	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.*

[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

5.1 Standard geometry

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	0.99	2/6097 (0.0%)	1.19	29/8272 (0.4%)
1	B	1.08	12/6070 (0.2%)	1.26	43/8235 (0.5%)
2	D	1.07	2/746 (0.3%)	1.24	3/999 (0.3%)
2	E	1.02	3/746 (0.4%)	1.18	3/999 (0.3%)
All	All	1.04	19/13659 (0.1%)	1.23	78/18505 (0.4%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	751	ASP	CB-CG	12.12	1.77	1.51
2	E	251	ASP	CB-CG	6.87	1.66	1.51
1	B	91	SER	CA-CB	6.86	1.63	1.52
2	D	251	ASP	CB-CG	6.60	1.65	1.51
1	B	657	LYS	N-CA	-6.23	1.33	1.46
2	D	251	ASP	N-CA	6.23	1.58	1.46
1	B	289	GLU	CG-CD	6.07	1.61	1.51
1	B	536	GLU	CD-OE1	5.71	1.31	1.25
1	B	215	ARG	CZ-NH1	5.64	1.40	1.33
1	A	469	TYR	CG-CD2	5.64	1.46	1.39
1	B	525	TYR	CB-CG	5.57	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	SER	CB-OG	5.49	1.49	1.42
1	B	397	ASP	CB-CG	5.42	1.63	1.51
1	B	208	GLY	C-O	-5.38	1.15	1.23
2	E	285	SER	CB-OG	5.35	1.49	1.42
2	E	251	ASP	CA-CB	5.15	1.65	1.53
1	B	755	THR	CB-OG1	5.05	1.53	1.43
1	B	665	THR	CB-CG2	5.02	1.69	1.52
1	A	71	ARG	NE-CZ	5.01	1.39	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	A	393	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	B	668	GLY	N-CA-C	-9.98	88.15	113.10
1	B	200	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	B	71	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	A	306	MET	CG-SD-CE	9.01	114.62	100.20
1	A	332	ASP	CB-CG-OD2	-8.89	110.30	118.30
2	E	315	ARG	NE-CZ-NH1	-8.69	115.95	120.30
1	A	496	ARG	NE-CZ-NH2	8.57	124.59	120.30
1	B	215	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	332	ASP	CB-CG-OD1	8.37	125.83	118.30
1	B	309	ASP	CB-CG-OD1	7.83	125.35	118.30
2	E	315	ARG	NE-CZ-NH2	7.67	124.14	120.30
1	A	71	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	485	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	B	272	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	B	810	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	92	SER	CB-CA-C	-7.32	96.20	110.10
1	B	705	ASP	CB-CG-OD2	7.26	124.84	118.30
1	A	319	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	410	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	B	457	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	368	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	802	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	B	751	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	534	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	A	757	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	B	585	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	B	217	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	393	ARG	NE-CZ-NH1	6.49	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	777	LEU	CA-CB-CG	6.39	130.01	115.30
1	B	129	ALA	N-CA-C	6.36	128.18	111.00
2	E	328	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	B	92	SER	CA-C-N	-6.21	103.55	117.20
1	A	567	LYS	N-CA-CB	6.18	121.72	110.60
1	A	89	GLY	N-CA-C	-6.03	98.02	113.10
1	A	393	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	498	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	184	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	B	127	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	304	LYS	CD-CE-NZ	5.82	125.09	111.70
1	B	791	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	558	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	117	GLU	N-CA-C	5.79	126.62	111.00
1	A	95	LEU	CB-CA-C	-5.78	99.22	110.20
1	B	567	LYS	N-CA-CB	5.78	121.00	110.60
1	B	571	THR	CB-CA-C	-5.76	96.06	111.60
1	A	585	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	558	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	221	MET	CG-SD-CE	-5.71	91.07	100.20
1	B	743	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	92	SER	N-CA-C	5.68	126.33	111.00
1	B	184	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	B	200	ARG	CG-CD-NE	5.61	123.58	111.80
1	A	558	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	661	ASP	N-CA-CB	5.58	120.64	110.60
1	B	189	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	431	ARG	CG-CD-NE	5.48	123.30	111.80
1	B	271	GLY	N-CA-C	5.47	126.77	113.10
2	D	286	ASP	CB-CA-C	5.37	121.15	110.40
1	A	388	GLY	N-CA-C	5.34	126.45	113.10
1	B	135	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	352	ASP	CB-CG-OD1	5.33	123.09	118.30
2	D	286	ASP	N-CA-CB	-5.30	101.06	110.60
1	A	217	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	705	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	B	71	ARG	CD-NE-CZ	5.25	130.95	123.60
1	B	309	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	127	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	D	288	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	71	ARG	CD-NE-CZ	5.20	130.88	123.60
1	A	385	HIS	N-CA-C	-5.17	97.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	767	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	258	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	533	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	656	SER	O-C-N	5.08	130.82	122.70
1	A	304	LYS	CB-CG-CD	5.07	124.78	111.60
1	A	571	THR	CB-CA-C	-5.07	97.92	111.60

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 (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	5962	0	5656	129	0
1	B	5936	0	5630	121	0
2	D	732	0	756	8	0
2	E	732	0	756	17	0
3	A	40	0	45	7	0
3	B	40	0	45	9	0
All	All	13442	0	12888	276	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 10.

All (276) 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:CB	1:B:751:ASP:CG	1.77	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLU:OE1	1:B:128:GLU:O	1.73	1.02
1:B:777:LEU:HD12	1:B:777:LEU:H	1.46	0.80
1:A:393:ARG:HH11	1:A:393:ARG:HG2	1.47	0.79
2:E:266:ARG:HD3	2:E:266:ARG:O	1.82	0.79
1:B:117:GLU:O	1:B:124:PHE:HD1	1.64	0.78
1:B:82:ALA:HB1	1:B:126:LEU:HD12	1.64	0.78
1:A:158:LEU:HD12	1:A:680:HIS:HB2	1.66	0.78
1:B:119:GLN:HA	1:B:119:GLN:HE21	1.48	0.77
1:A:396:PHE:O	1:A:397:ASP:CB	2.34	0.76
1:B:315:ASP:N	1:B:315:ASP:OD1	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	0.75
1:A:92:SER:OG	1:A:93:GLN:N	2.20	0.73
3:A:901:0UE:O13	3:A:901:0UE:H9	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:240:MET:HE1	1:A:272:ARG:HH21	1.57	0.69
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:O	1:A:401:SER:OG	2.11	0.66
1:B:118:ASP:O	1:B:124:PHE:CE1	2.49	0.66
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:H25	3:B:901:0UE:O23	1.96	0.65
1:B:614:ALA:HB2	1:B:663:PHE:CE1	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:CA	1:B:119:GLN:HE21	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:N	1:B:521:ASP:OD1	2.34	0.61
1:A:210:VAL:HG12	1:A:210:VAL:O	2.02	0.60
1:B:210:VAL:O	1:B:210:VAL:HG12	2.02	0.59
1:A:481:THR:HB	1:A:484:ALA:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:639:ASN:HD22	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: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:63:GLY:O	1:B:65:LEU:N	2.38	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:348:THR:HG23	1:A:362:GLN:HG2	1.88	0.55
1:A:63:GLY:O	1:A:65:LEU:N	2.40	0.55
1:B:448:SER:HB3	1:B:451:GLU:O	2.06	0.55
1:A:443:TYR:CD2	3:A:901:0UE:H28	2.42	0.55
1:A:62:ALA:CB	1:A:93:GLN:HA	2.37	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:448:SER:HB3	1:A:451:GLU:O	2.08	0.53
1:A:318:LYS:HG3	2:D:299:PRO:HB3	1.89	0.53
2:E:266:ARG:H	2:E:266:ARG:CD	2.22	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:364:TYR:OH	1:B:366:GLN:NE2	2.44	0.51
1:B:246:PHE:CD2	1:B:439:LEU:HD22	2.46	0.51
1:B:218:TYR:CE2	3:B:901:0UE:H8	2.46	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:240:MET:CE	1:A:272:ARG:HH21	2.24	0.51
1:A:275:PRO:HB2	1:A:651:GLN:HE21	1.76	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: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
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:A:607:ASN:HD22	1:A:607:ASN:C	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:E:266:ARG:HD3	2:E:266:ARG:C	2.30	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
1:B:790:LEU:O	1:B:791:ASP:C	2.53	0.47
3:A:901:0UE:H12	3:A:901:0UE:H8	1.39	0.47
1:B:665:THR:C	1:B:666:SER:O	2.48	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:B:205:ILE:O	1:B:719:MET:HE1	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:B:661:ASP:HB3	1:B:663:PHE:CD2	2.51	0.46
1:A:319:ARG:HH11	1:A:319:ARG:HG2	1.80	0.46
1:B:751:ASP:HB2	1:B:801:LEU:HG	1.98	0.46
1:A:818:TYR:CD1	1:A:818:TYR:C	2.89	0.46
1:A:89:GLY:O	1:A:90:TYR:CG	2.69	0.46
1:B:91:SER:C	1:B:92:SER:OG	2.52	0.46
2:D:304:ASP:N	2:D:304:ASP:OD1	2.40	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
1:A:521:ASP:N	1:A:521:ASP:OD1	2.48	0.46
1:B:777:LEU:HD12	1:B:777:LEU:N	2.23	0.46
2:E:266:ARG:HD2	2:E:266:ARG:H	1.80	0.46
1:A:90:TYR:CD1	1:A:112:THR:HG22	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:80:LEU:HA	1:B:80:LEU:HD23	1.65	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:316:GLU:OE2	1:B:316:GLU:HA	2.17	0.45
1:B:272:ARG:HG2	1:B:608:PRO:HD2	1.98	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:596:LEU:HD11	1:A:631:LEU:HD11	1.99	0.45
1:A:445:TYR:CE1	1:A:660:GLN:HG2	2.51	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:811:ASN:HD22	1:A:811:ASN:C	2.20	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:901:0UE:H41	2.52	0.44
1:B:471:VAL:HG22	1:B:472:ASP:N	2.33	0.44
1:B:173:LEU:HD22	1:B:634:GLN:HB3	1.99	0.44
1:A:214:ASN:HB2	1:A:340:GLU:OE2	2.17	0.44
1:B:284:LYS:HG2	1:B:284:LYS:O	2.17	0.44
1:B:387:ASN:ND2	1:B:453:ASN:OD1	2.51	0.44
1:A:729:ASP:N	1:A:729:ASP:OD1	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
2:D:259:MET:HE3	2:D:314:TRP:CH2	2.53	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
3:B:901:0UE:H30	3:B:901:0UE:H24	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:683:LEU:HD23	1:A:687:LEU:HD23	2.01	0.43
1:A:453:ASN:HA	1:A:453:ASN:HD22	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HB2	1:B:660:GLN:HE21	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:HG21	1:B:420:ILE:HD13	1.82	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:A:91:SER:OG	1:A:92:SER:N	2.49	0.42
1:B:206:PHE:HB3	1:B:220:VAL:HB	2.02	0.42
1:B:63:GLY:O	1:B:68:VAL:HG23	2.19	0.42
1:B:664:TYR:N	1:B:664:TYR:CD1	2.88	0.42
1:A:375:GLY:HA2	3:A:901:0UE:C25	2.50	0.41
1:A:278:LEU:C	1:A:278:LEU:HD12	2.41	0.41
1:B:142:VAL:CG2	2:E:332:LYS:HE3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:634:GLN:HG3	1:A:640:SER:O	2.21	0.41
1:B:161:HIS:O	1:B:258:ARG:NH2	2.54	0.41
1:B:65:LEU:HD23	1:B:90:TYR:HB2	2.01	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: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:130:PRO:O	1:A:130:PRO:CD	2.69	0.41
1:A:240:MET:HE1	1:A:272:ARG:NH2	2.32	0.41
1:A:54:GLN:OE1	1:A:54:GLN:N	2.54	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:NH1	1:A:319:ARG:HG2	2.37	0.40
1:A:626:GLN:HB2	1:A:649:ILE:HG12	2.03	0.40
1:B:199:MET:HE1	1:B:219:VAL:HG11	2.03	0.40
1:B:396:PHE:CG	1:B:396:PHE:O	2.74	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
3:B:901:0UE:H34	3:B:901:0UE:H31	1.93	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%)	5 26
1	B	753/768 (98%)	655 (87%)	79 (10%)	19 (2%)	5 29
2	D	88/90 (98%)	74 (84%)	11 (12%)	3 (3%)	3 23
2	E	88/90 (98%)	81 (92%)	4 (4%)	3 (3%)	3 23
All	All	1688/1716 (98%)	1477 (88%)	165 (10%)	46 (3%)	5 27

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
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

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Mol	Chain	Res	Type
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 (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	629/633 (99%)	528 (84%)	101 (16%)	2 10
1	B	627/633 (99%)	534 (85%)	93 (15%)	3 13
2	D	79/79 (100%)	57 (72%)	22 (28%)	0 1
2	E	79/79 (100%)	61 (77%)	18 (23%)	1 3
All	All	1414/1424 (99%)	1180 (84%)	234 (16%)	2 10

All (234) 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	102	GLN

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Mol	Chain	Res	Type
1	A	109	LEU
1	A	117	GLU
1	A	125	VAL
1	A	127	ARG
1	A	138	ASN
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	230	ASP
1	A	260	ASP
1	A	263	LYS
1	A	274	LEU
1	A	282	THR
1	A	293	GLN
1	A	304	LYS
1	A	306	MET
1	A	319	ARG
1	A	327	LEU
1	A	332	ASP
1	A	355	ASP
1	A	358	THR
1	A	367	HIS
1	A	377	VAL
1	A	384	SER
1	A	385	HIS
1	A	389	ARG
1	A	390	HIS
1	A	391	ILE
1	A	393	ARG
1	A	402	LYS
1	A	404	ASP
1	A	408	THR
1	A	420	ILE
1	A	435	SER
1	A	438	ASP
1	A	440	SER
1	A	441	GLN
1	A	453	ASN

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Mol	Chain	Res	Type
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	567	LYS
1	A	571	THR
1	A	573	SER
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	625	LYS
1	A	626	GLN
1	A	629	LEU
1	A	638	SER
1	A	650	THR
1	A	657	LYS
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	719	MET
1	A	729	ASP
1	A	737	SER
1	A	748	THR
1	A	751	ASP
1	A	758	VAL
1	A	775	LEU
1	A	778	LYS
1	A	782	VAL

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Mol	Chain	Res	Type
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	817	ASN
1	A	818	TYR
1	A	819	GLN
1	B	53	GLU
1	B	54	GLN
1	B	56	ARG
1	B	80	LEU
1	B	81	SER
1	B	86	GLN
1	B	92	SER
1	B	95	LEU
1	B	100	THR
1	B	105	LEU
1	B	107	ARG
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	209	GLN
1	B	219	VAL
1	B	222	ARG
1	B	227	ASN
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	293	GLN
1	B	297	SER
1	B	305	GLU

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Mol	Chain	Res	Type
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	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
1	B	473	ASN
1	B	489	LEU
1	B	490	THR
1	B	499	THR
1	B	504	ARG
1	B	509	SER
1	B	512	ASP
1	B	514	PHE
1	B	520	ASP
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	571	THR
1	B	573	SER
1	B	574	LYS
1	B	583	THR
1	B	585	ARG
1	B	603	SER
1	B	608	PRO

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Mol	Chain	Res	Type
1	B	623	GLU
1	B	629	LEU
1	B	639	ASN
1	B	656	SER
1	B	658	GLU
1	B	660	GLN
1	B	665	THR
1	B	677	LEU
1	B	682	GLN
1	B	686	ASN
1	B	689	LEU
1	B	737	SER
1	B	755	THR
1	B	777	LEU
1	B	799	TYR
1	B	802	ASP
1	B	813	THR
1	B	820	PHE
2	D	251	ASP
2	D	252	SER
2	D	258	ARG
2	D	263	VAL
2	D	264	TYR
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	301	ARG
2	D	304	ASP
2	D	306	GLU
2	D	311	MET
2	D	317	GLU
2	D	324	LYS
2	D	326	VAL
2	D	328	ARG
2	D	331	THR
2	D	340	LYS
2	E	252	SER
2	E	253	ASP

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Mol	Chain	Res	Type
2	E	266	ARG
2	E	267	MET
2	E	269	GLN
2	E	271	ARG
2	E	279	VAL
2	E	285	SER
2	E	286	ASP
2	E	294	VAL
2	E	318	PRO
2	E	319	ARG
2	E	324	LYS
2	E	326	VAL
2	E	328	ARG
2	E	331	THR
2	E	339	GLU
2	E	340	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	149	ASN
1	A	293	GLN
1	A	387	ASN
1	A	409	GLN
1	A	453	ASN
1	A	515	ASN
1	A	639	ASN
1	A	651	GLN
1	A	682	GLN
1	A	686	ASN
1	A	785	ASN
1	A	811	ASN
1	A	817	ASN
1	B	64	GLN
1	B	86	GLN
1	B	119	GLN
1	B	196	GLN
1	B	366	GLN
1	B	660	GLN
2	D	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	B	901	-	44,44,44	2.77	10 (22%)	44,66,66	4.41	11 (25%)
3	0UE	A	901	-	44,44,44	2.90	11 (25%)	44,66,66	4.90	12 (27%)

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	-4.11	1.92	2.04
3	A	901	0UE	O32-FE	-4.00	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
3	B	901	0UE	O22-FE	-3.73	1.94	2.04
3	A	901	0UE	O21-FE	-3.63	1.91	1.99
3	A	901	0UE	O22-FE	-3.56	1.94	2.04
3	B	901	0UE	O31-FE	-3.48	1.91	1.99
3	A	901	0UE	C21-N21	3.08	1.36	1.31
3	B	901	0UE	O12-FE	-2.96	1.96	2.04
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	-2.20	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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	B	901	0UE	N31
3	B	901	0UE	N21
3	A	901	0UE	N31
3	A	901	0UE	N21

All (28) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	B	901	0UE	C23-C24-N22-C25
3	B	901	0UE	C16-C17-C18-C19
3	B	901	0UE	C40-C39-N11-O11

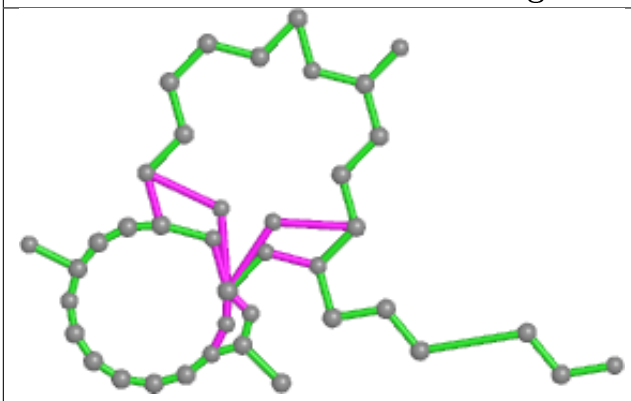
There are no ring outliers.

2 monomers are involved in 16 short contacts:

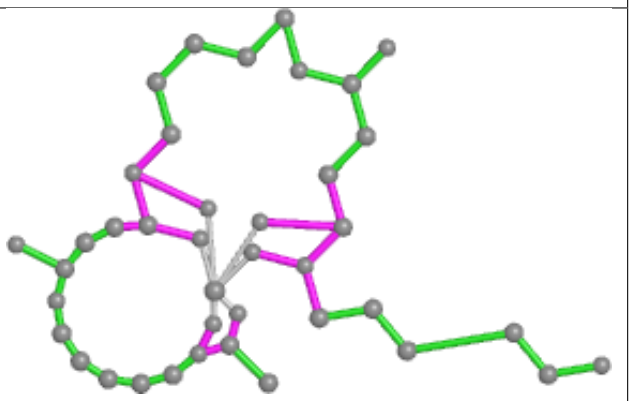
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	0UE	9	0
3	A	901	0UE	7	0

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 then 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.

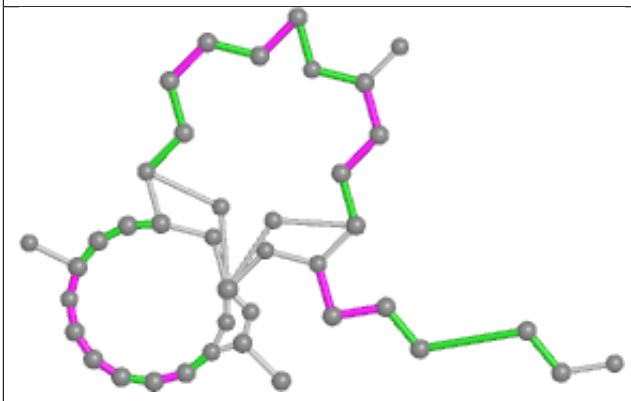
Ligand 0UE B 901



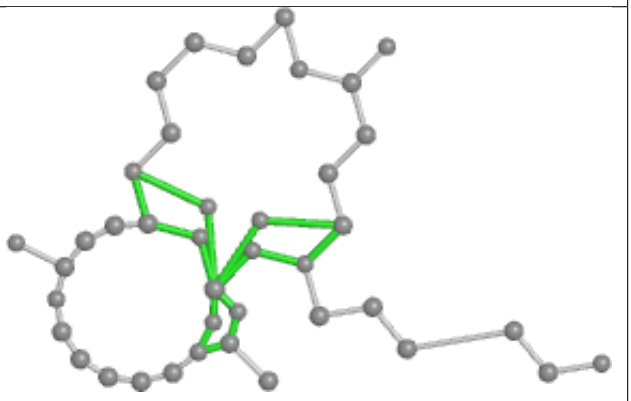
Bond lengths



Bond angles

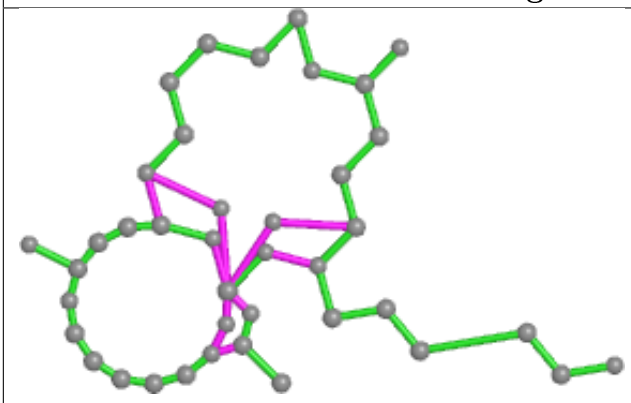


Torsions

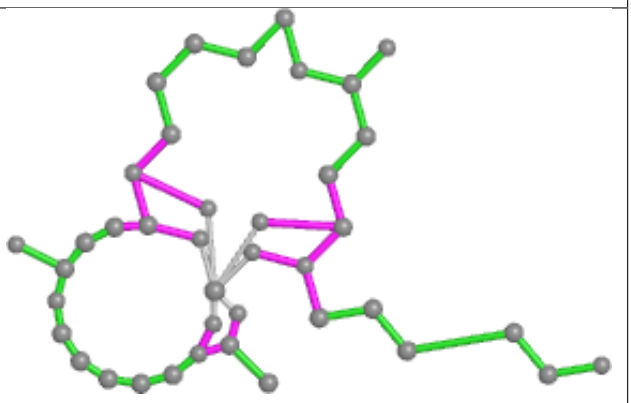


Rings

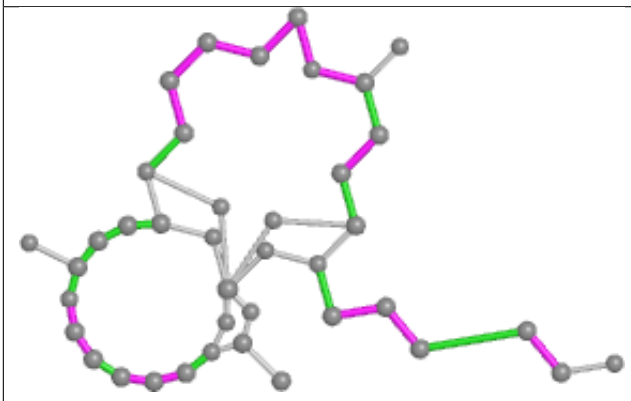
Ligand 0UE A 901



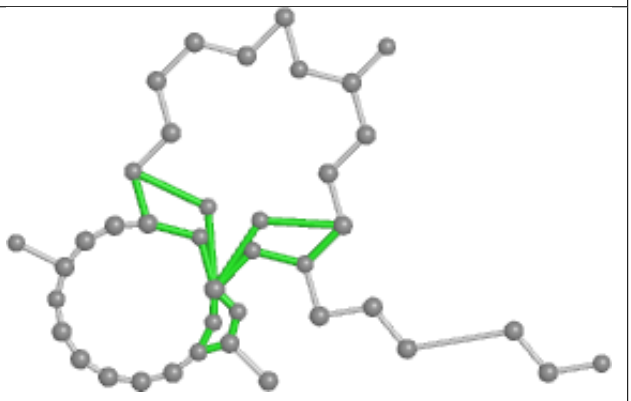
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	763/768 (99%)	0.13	35 (4%) 32 35	62, 89, 119, 145	0
1	B	759/768 (98%)	0.09	24 (3%) 47 50	63, 85, 117, 150	0
2	D	90/90 (100%)	0.30	4 (4%) 34 37	62, 83, 116, 135	0
2	E	90/90 (100%)	0.15	1 (1%) 80 84	65, 82, 106, 122	0
All	All	1702/1716 (99%)	0.12	64 (3%) 40 42	62, 86, 118, 150	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	ALA	4.0
1	B	775	LEU	3.8
1	A	683	LEU	3.8
1	A	514	PHE	3.7
1	A	155	ASP	3.6
1	A	484	ALA	3.6
1	A	453	ASN	3.5
1	A	386	HIS	3.5
1	A	395	PHE	3.4
1	A	732	PRO	3.2
1	A	384	SER	3.2
1	B	732	PRO	3.2
1	B	155	ASP	3.2
1	A	379	ALA	3.1
1	B	733	LEU	3.1
1	A	447	TRP	3.0
1	B	102	GLN	3.0
1	A	726	TYR	3.0
1	B	404	ASP	2.8
1	A	355	ASP	2.8
1	A	482	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	483	ALA	2.7
1	A	380	ASP	2.7
2	D	251	ASP	2.6
1	B	484	ALA	2.6
1	B	402	LYS	2.5
1	B	149	ASN	2.5
1	A	389	ARG	2.5
1	A	733	LEU	2.5
1	A	390	HIS	2.5
1	A	481	THR	2.4
1	A	387	ASN	2.4
1	B	776	GLY	2.4
1	A	378	PRO	2.4
2	D	279	VAL	2.3
1	A	424	TRP	2.3
1	B	778	LYS	2.3
2	E	329	GLN	2.3
1	B	54	GLN	2.3
1	A	391	ILE	2.2
1	A	477	ALA	2.2
1	B	389	ARG	2.2
1	A	511	LEU	2.2
1	B	96	ARG	2.2
2	D	277	VAL	2.2
1	B	403	ASP	2.2
1	B	440	SER	2.2
1	B	683	LEU	2.2
1	A	396	PHE	2.2
1	B	95	LEU	2.1
1	A	512	ASP	2.1
1	A	388	GLY	2.1
1	B	103	GLN	2.1
1	B	513	ALA	2.1
1	A	515	ASN	2.1
1	B	53	GLU	2.1
1	B	98	SER	2.1
1	A	778	LYS	2.0
2	D	304	ASP	2.0
1	B	391	ILE	2.0
1	A	397	ASP	2.0
1	A	652	GLU	2.0
1	A	518	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	514	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

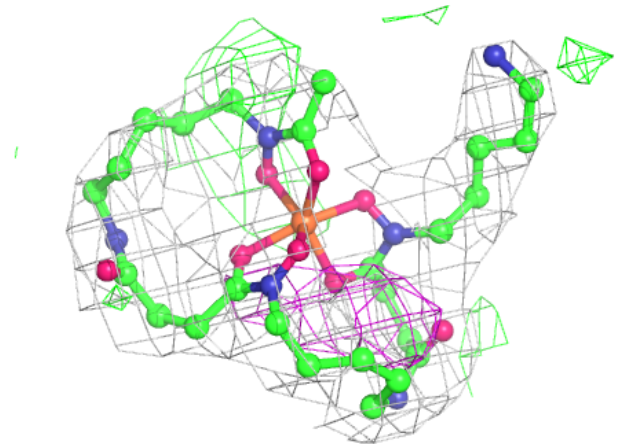
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

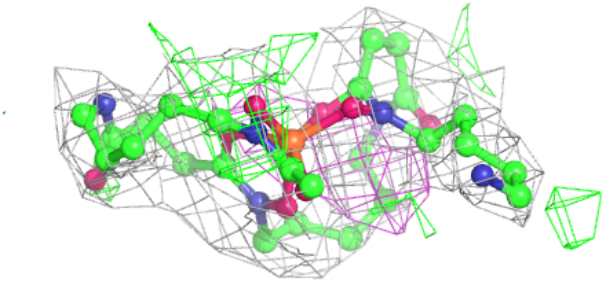
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	0UE	A	901	40/40	0.96	0.24	59,81,103,140	0
3	0UE	B	901	40/40	0.97	0.21	46,71,94,109	0

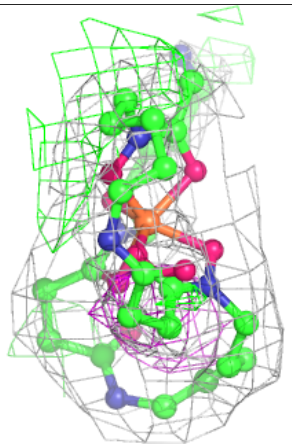
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

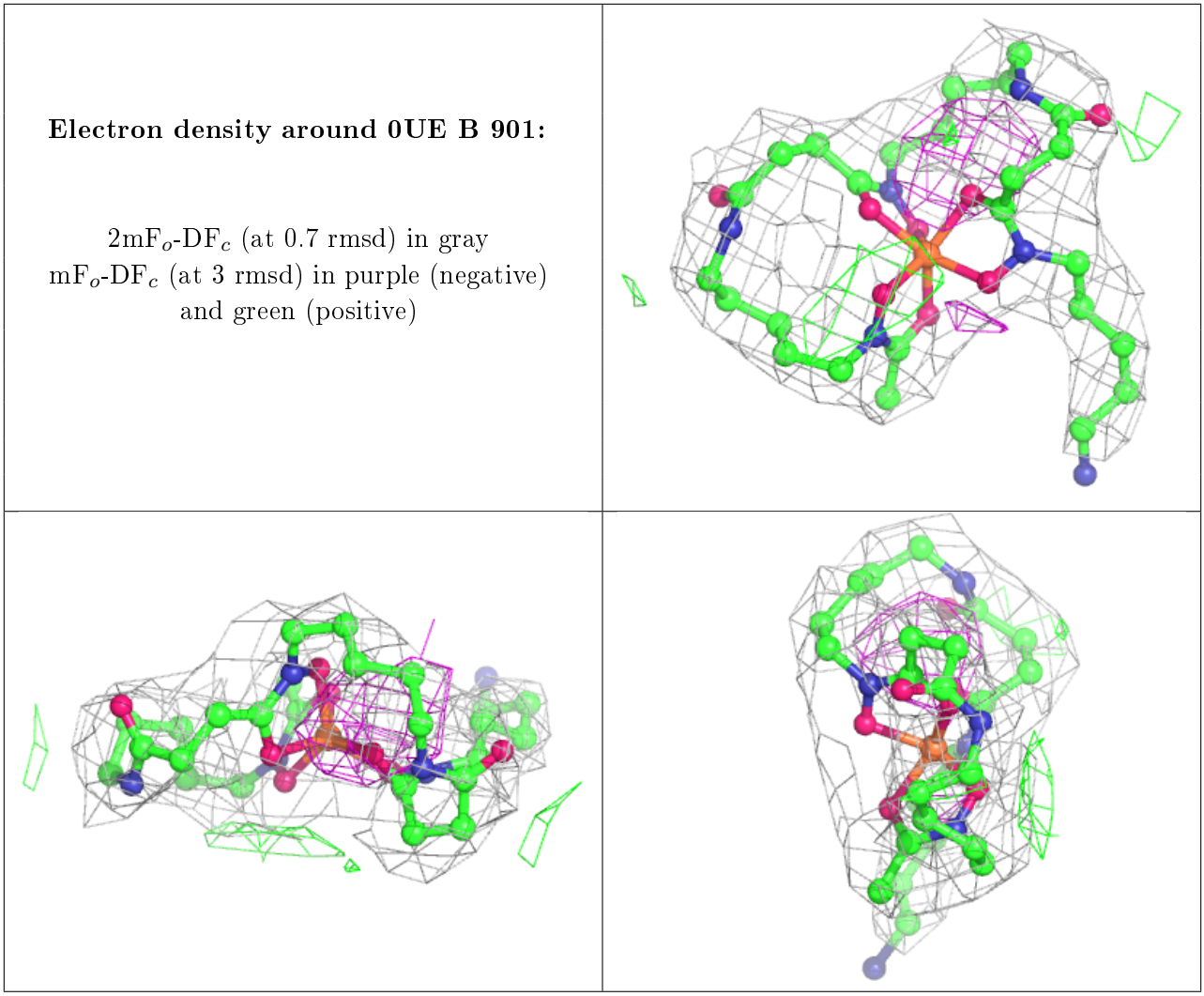






Electron density around 0UE B 901:

$2mF_o$-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

There are no such residues in this entry.