Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2022 – 10:13 pm BST

PDB ID	:	7ZEA
Title	:	Crystal Structure of truncated aspartate transcarbamoylase from Plasmodium falciparum with bound inhibitor O-benzylhydroxylamine
Authors	:	Wang, C.; Zhang, B.
Deposited on	:	2022-03-30
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

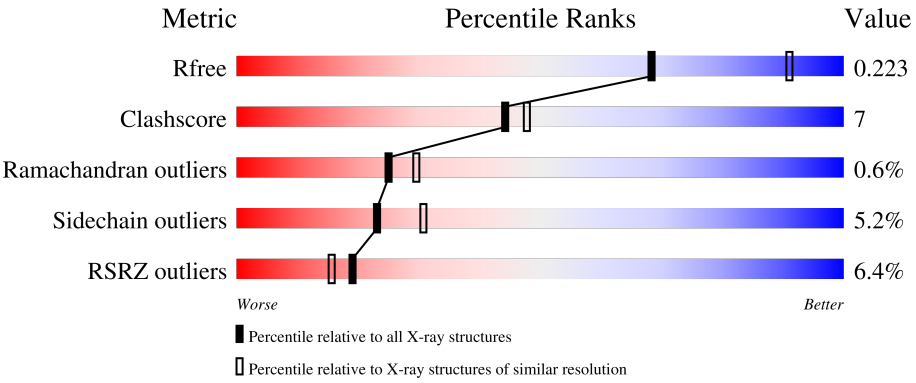
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.45 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	349	7% 76% 15% 7%
1	B	349	5% 80% 15%
1	C	349	6% 82% 11% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16442 atoms, of which 8162 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 Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	324	Total	C	H	N	O	S	83	0	0
			5248	1674	2632	428	506	8			
1	B	346	Total	C	H	N	O	S	88	0	0
			5629	1801	2814	462	544	8			
1	C	332	Total	C	H	N	O	S	85	0	0
			5384	1720	2698	441	517	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	376	SER	-	expression tag	UNP A0A5K1K910
A	377	ALA	-	expression tag	UNP A0A5K1K910
A	378	TRP	-	expression tag	UNP A0A5K1K910
A	379	SER	-	expression tag	UNP A0A5K1K910
A	380	HIS	-	expression tag	UNP A0A5K1K910
A	381	PRO	-	expression tag	UNP A0A5K1K910
A	382	GLN	-	expression tag	UNP A0A5K1K910
A	383	PHE	-	expression tag	UNP A0A5K1K910
A	384	GLU	-	expression tag	UNP A0A5K1K910
A	385	LYS	-	expression tag	UNP A0A5K1K910
B	376	SER	-	expression tag	UNP A0A5K1K910
B	377	ALA	-	expression tag	UNP A0A5K1K910
B	378	TRP	-	expression tag	UNP A0A5K1K910
B	379	SER	-	expression tag	UNP A0A5K1K910
B	380	HIS	-	expression tag	UNP A0A5K1K910
B	381	PRO	-	expression tag	UNP A0A5K1K910
B	382	GLN	-	expression tag	UNP A0A5K1K910
B	383	PHE	-	expression tag	UNP A0A5K1K910
B	384	GLU	-	expression tag	UNP A0A5K1K910
B	385	LYS	-	expression tag	UNP A0A5K1K910
C	376	SER	-	expression tag	UNP A0A5K1K910
C	377	ALA	-	expression tag	UNP A0A5K1K910
C	378	TRP	-	expression tag	UNP A0A5K1K910

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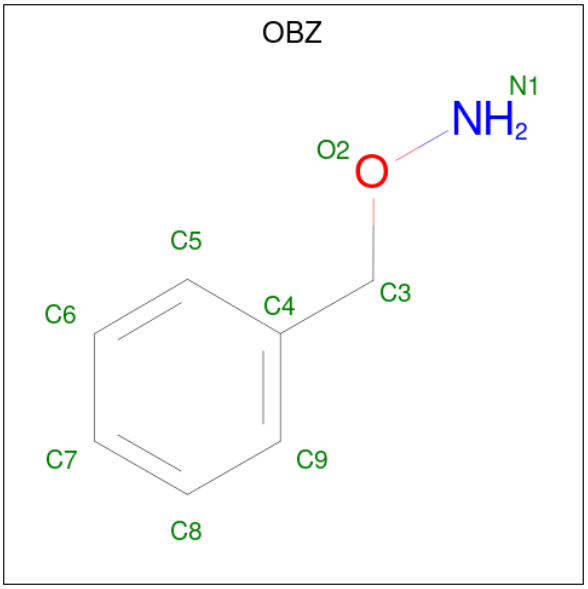
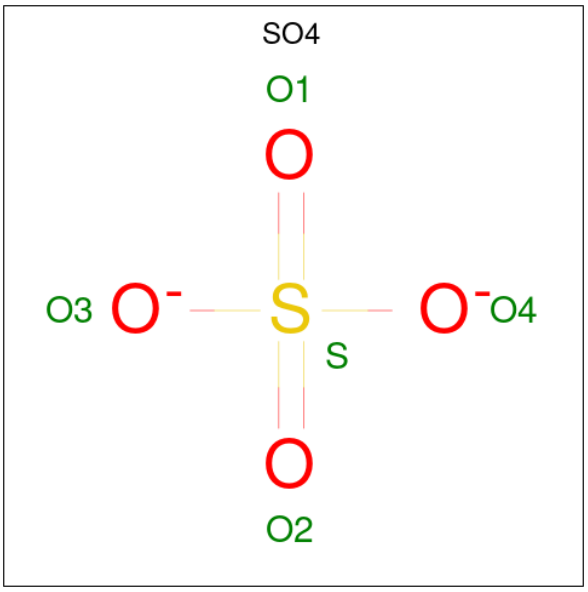
Chain	Residue	Modelled	Actual	Comment	Reference
C	379	SER	-	expression tag	UNP A0A5K1K910
C	380	HIS	-	expression tag	UNP A0A5K1K910
C	381	PRO	-	expression tag	UNP A0A5K1K910
C	382	GLN	-	expression tag	UNP A0A5K1K910
C	383	PHE	-	expression tag	UNP A0A5K1K910
C	384	GLU	-	expression tag	UNP A0A5K1K910
C	385	LYS	-	expression tag	UNP A0A5K1K910

- Molecule 2 is O-benzylhydroxylamine (three-letter code: OBZ) (formula: C_7H_9NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			18	7	9	1	1		
2	B	1	Total	C	H	N	O	0	0
			18	7	9	1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is water.

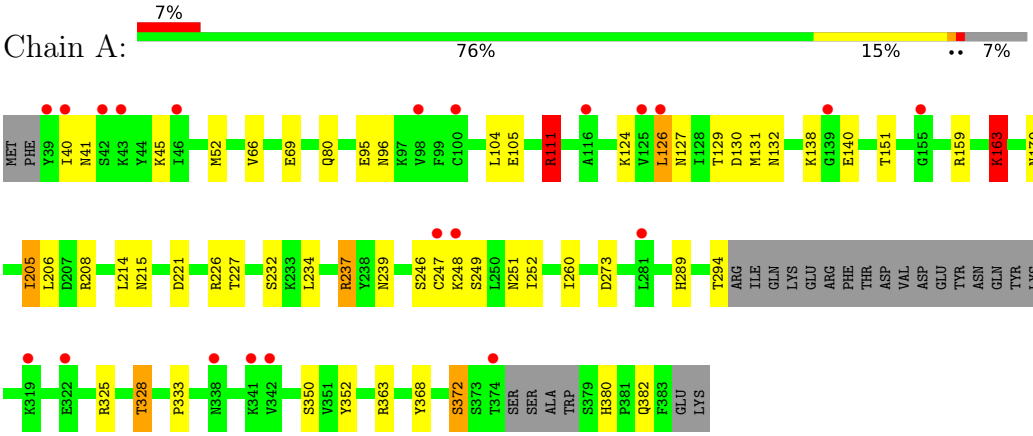
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	48	Total O 48 48	0	0
5	B	53	Total O 53 53	0	0
5	C	33	Total O 33 33	0	0

3 Residue-property plots (i)

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

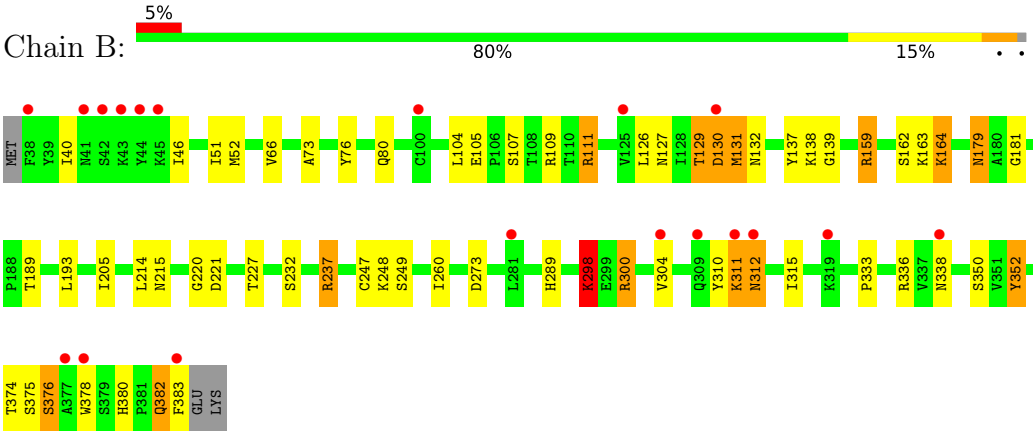
• Molecule 1: Aspartate carbamoyltransferase

Chain A:



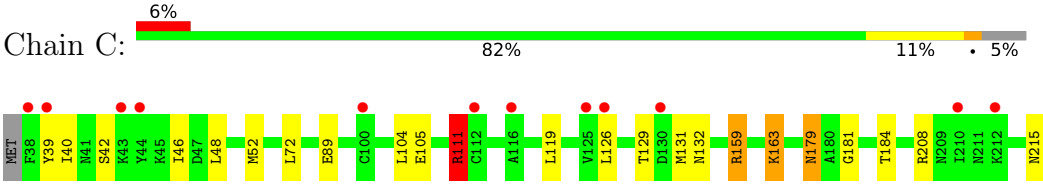
• Molecule 1: Aspartate carbamoyltransferase

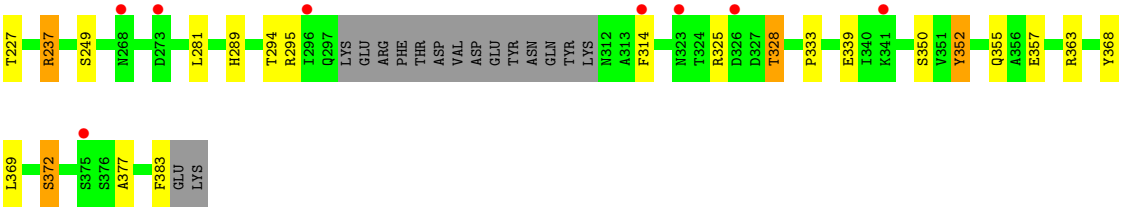
Chain B:



• Molecule 1: Aspartate carbamoyltransferase

Chain C:




T227
R237
S249
N268
D273
L281
H289
T294
R295
I296
Q297
LYS
GLU
ARG
PHE
THR
ASP
VAL
ASP
GLU
TYR
ASN
GLN
TYR
LYS
N312
A313
F314
N323
T324
R325
D326
D327
T328
P333
E339
I340
K341
S350
V351
Y352
Q355
A356
E357
R363
Y368
L369
S372
S375
S376
A377
F383
GLU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.03Å 104.51Å 87.30Å 90.00° 117.47° 90.00°	Depositor
Resolution (Å)	45.28 – 2.45 45.24 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.28-2.45) 96.3 (45.24-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.223 0.185 , 0.223	Depositor DCC
R_{free} test set	2367 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -h-l,k,h 0.004 for l,k,-h-l 0.019 for h,-k,-h-l 0.021 for -h-l,-k,l 0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16442	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: NA, SO4, OBZ

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	0.84	2/2664 (0.1%)	1.04	11/3598 (0.3%)
1	B	0.82	0/2871	1.02	8/3880 (0.2%)
1	C	0.79	0/2738	1.00	6/3700 (0.2%)
All	All	0.82	2/8273 (0.0%)	1.02	25/11178 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	GLU	CD-OE1	9.64	1.36	1.25
1	A	69	GLU	CD-OE2	8.34	1.34	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	111	ARG	NE-CZ-NH1	-9.69	115.46	120.30
1	C	111	ARG	NE-CZ-NH1	-8.61	116.00	120.30
1	A	363	ARG	NE-CZ-NH2	8.17	124.38	120.30
1	B	383	PHE	CA-C-O	8.00	136.89	120.10
1	C	237	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	A	126	LEU	N-CA-CB	-7.49	95.42	110.40
1	B	298	LYS	CB-CA-C	7.02	124.44	110.40
1	C	237	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	363	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	A	126	LEU	CB-CA-C	6.51	122.57	110.20
1	A	237	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	C	111	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	B	336	ARG	CG-CD-NE	5.89	124.17	111.80
1	A	111	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	B	363	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	A	363	ARG	NE-CZ-NH1	-5.79	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	LYS	N-CA-CB	-5.73	100.28	110.60
1	B	363	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	A	111	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	C	363	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	A	163	LYS	CB-CA-C	5.48	121.35	110.40
1	A	237	ARG	CB-CG-CD	5.27	125.30	111.60
1	B	237	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	111	ARG	CG-CD-NE	-5.16	100.97	111.80
1	B	159	ARG	CG-CD-NE	5.04	122.39	111.80

There are no chirality outliers.

There are no planarity outliers.

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	2616	2632	2623	34	0
1	B	2815	2814	2807	48	5
1	C	2686	2698	2690	29	0
2	A	9	9	9	1	0
2	B	9	9	9	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
5	A	48	0	0	4	0
5	B	53	0	0	3	0
5	C	33	0	0	0	0
All	All	8280	8162	8138	107	5

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 7.

All (107) 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:109:ARG:HD2	5:B:532:HOH:O	1.54	1.08
1:B:215:ASN:H	1:B:289:HIS:HD2	1.18	0.92
1:C:215:ASN:H	1:C:289:HIS:HD2	1.23	0.86
1:A:215:ASN:H	1:A:289:HIS:HD2	1.21	0.84
1:A:163:LYS:H	1:A:163:LYS:HD3	1.43	0.84
1:B:298:LYS:HE2	1:B:304:VAL:HG22	1.70	0.71
1:B:375:SER:HB2	1:B:380:HIS:CE1	2.28	0.68
1:C:368:TYR:O	1:C:372:SER:HB2	1.94	0.68
1:B:107:SER:OG	5:B:501:HOH:O	2.11	0.67
1:A:111:ARG:NH1	1:B:127:ASN:O	2.25	0.67
1:B:80:GLN:HE21	1:B:382:GLN:HA	1.60	0.67
1:A:368:TYR:O	1:A:372:SER:HB2	1.94	0.66
1:B:137:TYR:O	1:B:139:GLY:N	2.29	0.66
1:A:208:ARG:NH1	1:A:237:ARG:O	2.26	0.65
1:C:215:ASN:H	1:C:289:HIS:CD2	2.11	0.65
1:C:208:ARG:NH1	1:C:237:ARG:O	2.28	0.65
1:B:315:ILE:HG12	1:B:338:ASN:O	1.98	0.64
1:B:52:MET:HE3	1:B:380:HIS:CE1	2.33	0.64
1:C:163:LYS:HG3	1:C:184:THR:CG2	2.28	0.64
1:A:95:GLU:O	5:A:501:HOH:O	2.15	0.64
1:C:163:LYS:HG3	1:C:184:THR:HG23	1.79	0.63
1:A:95:GLU:O	1:A:96:ASN:HB2	1.98	0.62
1:B:52:MET:CE	1:B:380:HIS:CE1	2.82	0.62
1:A:163:LYS:HD3	1:A:163:LYS:N	2.14	0.62
1:C:39:TYR:OH	1:C:377:ALA:O	2.19	0.61
1:A:215:ASN:H	1:A:289:HIS:CD2	2.11	0.61
1:B:215:ASN:H	1:B:289:HIS:CD2	2.09	0.60
1:C:281:LEU:HD11	1:C:314:PHE:HA	1.84	0.59
1:A:140:GLU:OE1	2:A:401:OBZ:H3	2.02	0.58
1:B:163:LYS:HE2	1:B:186:GLU:OE2	2.03	0.58
1:B:163:LYS:HG3	1:B:184:THR:CG2	2.34	0.57
1:C:52:MET:HE1	1:C:368:TYR:HE2	1.71	0.56
1:B:310:TYR:C	1:B:311:LYS:O	2.41	0.56
1:C:89:GLU:OE1	1:C:383:PHE:HE1	1.88	0.56
1:B:237:ARG:HD2	5:B:516:HOH:O	2.05	0.56
1:B:179:ASN:ND2	1:B:181:GLY:H	2.04	0.55
1:B:40:ILE:CG2	1:B:46:ILE:HD11	2.36	0.55
1:A:179:ASN:ND2	1:A:181:GLY:H	2.04	0.55
1:C:48:LEU:HG	1:C:52:MET:CE	2.38	0.54
1:A:52:MET:CE	1:A:380:HIS:CE1	2.91	0.54
1:A:52:MET:HE1	1:A:380:HIS:ND1	2.23	0.54
1:C:179:ASN:ND2	1:C:181:GLY:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:MET:HE1	1:B:380:HIS:ND1	2.23	0.53
1:B:375:SER:CB	1:B:380:HIS:HE1	2.22	0.53
1:B:375:SER:HB2	1:B:380:HIS:HE1	1.73	0.52
1:A:294:THR:O	5:A:502:HOH:O	2.19	0.51
1:B:40:ILE:HG22	1:B:46:ILE:HD11	1.93	0.51
1:C:46:ILE:HD12	1:C:72:LEU:HB3	1.92	0.50
1:A:127:ASN:O	1:C:111:ARG:NH1	2.36	0.50
1:A:227:THR:HG21	1:A:333:PRO:HG3	1.94	0.50
1:C:48:LEU:HG	1:C:52:MET:HE3	1.93	0.50
1:A:163:LYS:H	1:A:163:LYS:CD	2.15	0.50
1:B:227:THR:HG21	1:B:333:PRO:HG3	1.94	0.50
1:A:129:THR:O	1:A:131:MET:N	2.45	0.49
1:B:52:MET:HE1	1:B:368:TYR:HE2	1.78	0.49
1:B:163:LYS:HB2	1:B:184:THR:HG23	1.94	0.49
1:B:129:THR:HG22	1:B:130:ASP:H	1.78	0.49
1:B:51:ILE:HG21	1:B:73:ALA:HB2	1.94	0.48
1:B:105:GLU:OE1	1:B:159:ARG:HD3	2.13	0.48
1:B:163:LYS:HG3	1:B:184:THR:OG1	2.13	0.48
1:B:376:SER:HB3	1:B:378:TRP:CE2	2.48	0.48
1:A:251:ASN:OD1	1:A:252:ILE:HG22	2.14	0.47
1:A:80:GLN:HE21	1:A:382:GLN:HA	1.79	0.47
1:C:227:THR:HG21	1:C:333:PRO:HG3	1.97	0.47
1:A:234:LEU:HA	1:A:237:ARG:HD3	1.97	0.47
1:B:80:GLN:NE2	1:B:382:GLN:HA	2.27	0.46
1:C:129:THR:O	1:C:131:MET:N	2.48	0.46
1:B:129:THR:O	1:B:131:MET:N	2.48	0.46
1:B:350:SER:HB2	1:B:352:TYR:CE1	2.51	0.46
1:B:300:ARG:HA	1:B:300:ARG:HD3	1.64	0.46
1:B:232:SER:HB3	1:B:260:ILE:HD11	1.98	0.46
1:A:325:ARG:O	1:A:328:THR:HG23	2.17	0.45
1:B:46:ILE:HD13	1:B:76:TYR:HB2	1.97	0.45
1:A:325:ARG:HB2	1:A:328:THR:HG22	1.99	0.45
1:C:52:MET:HE2	1:C:369:LEU:HD23	1.99	0.45
1:C:350:SER:HB2	1:C:352:TYR:CE1	2.51	0.44
1:B:189:THR:HB	1:B:363:ARG:HH21	1.82	0.44
1:B:312:ASN:HD22	1:B:312:ASN:N	2.13	0.44
1:C:163:LYS:HE2	1:C:184:THR:HG21	2.00	0.44
1:B:221:ASP:OD1	1:B:221:ASP:C	2.56	0.44
1:A:105:GLU:OE1	1:A:159:ARG:HD3	2.17	0.43
1:C:221:ASP:OD1	1:C:221:ASP:C	2.57	0.43
1:A:151:THR:HB	1:C:357:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:SER:HB2	1:A:352:TYR:CE1	2.53	0.43
1:B:52:MET:HE1	1:B:368:TYR:CE2	2.53	0.43
1:A:221:ASP:OD1	1:A:221:ASP:C	2.57	0.43
1:B:51:ILE:HG21	1:B:73:ALA:CB	2.49	0.43
1:B:52:MET:CE	1:B:380:HIS:ND1	2.82	0.43
1:C:104:LEU:O	1:C:132:ASN:HA	2.19	0.43
1:B:162:SER:OG	1:B:164:LYS:HD2	2.19	0.43
1:A:127:ASN:ND2	5:A:506:HOH:O	2.46	0.42
1:B:220:GLY:O	1:B:310:TYR:OH	2.27	0.42
1:C:294:THR:O	1:C:339:GLU:HG2	2.19	0.42
1:A:66:VAL:O	1:A:237:ARG:NH2	2.47	0.42
1:A:104:LEU:O	1:A:132:ASN:HA	2.20	0.42
1:C:325:ARG:O	1:C:328:THR:HG23	2.19	0.42
1:A:232:SER:HB3	1:A:260:ILE:HD11	2.01	0.41
1:A:205:ILE:HD12	1:A:206:LEU:N	2.35	0.41
1:B:66:VAL:O	1:B:237:ARG:NH2	2.44	0.41
1:B:193:LEU:C	1:B:193:LEU:HD12	2.40	0.41
1:B:163:LYS:HG3	1:B:184:THR:HG23	2.02	0.41
1:A:124:LYS:HD3	1:C:119:LEU:HD22	2.02	0.41
1:A:226:ARG:NH1	5:A:508:HOH:O	2.53	0.41
1:B:104:LEU:O	1:B:132:ASN:HA	2.21	0.41
1:C:89:GLU:OE1	1:C:383:PHE:CE1	2.71	0.41
1:C:105:GLU:OE1	1:C:159:ARG:HD2	2.21	0.40
1:C:352:TYR:O	1:C:355:GLN:HB3	2.20	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LYS:HZ2	1:B:378:TRP:CE2[2_646]	1.24	0.36
1:B:298:LYS:NZ	1:B:378:TRP:CE2[2_646]	2.07	0.13
1:B:298:LYS:NZ	1:B:378:TRP:NE1[2_646]	2.10	0.10
1:B:298:LYS:HZ2	1:B:378:TRP:CZ2[2_646]	1.60	0.00
1:B:298:LYS:HZ2	1:B:378:TRP:NE1[2_646]	1.60	0.00

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	318/349 (91%)	299 (94%)	17 (5%)	2 (1%)	25 29
1	B	344/349 (99%)	326 (95%)	14 (4%)	4 (1%)	13 13
1	C	328/349 (94%)	308 (94%)	20 (6%)	0	100 100
All	All	990/1047 (95%)	933 (94%)	51 (5%)	6 (1%)	25 29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	LYS
1	B	138	LYS
1	B	311	LYS
1	A	130	ASP
1	B	130	ASP
1	B	248	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	304/328 (93%)	287 (94%)	17 (6%)	21 27
1	B	325/328 (99%)	306 (94%)	19 (6%)	20 26
1	C	311/328 (95%)	298 (96%)	13 (4%)	30 39
All	All	940/984 (96%)	891 (95%)	49 (5%)	23 31

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	41	ASN
1	A	45	LYS
1	A	111	ARG
1	A	126	LEU
1	A	138	LYS
1	A	163	LYS
1	A	187	HIS
1	A	205	ILE
1	A	214	LEU
1	A	239	ASN
1	A	246	SER
1	A	247	CYS
1	A	249	SER
1	A	273	ASP
1	A	328	THR
1	A	372	SER
1	B	111	ARG
1	B	126	LEU
1	B	129	THR
1	B	131	MET
1	B	164	LYS
1	B	179	ASN
1	B	187	HIS
1	B	205	ILE
1	B	214	LEU
1	B	247	CYS
1	B	249	SER
1	B	273	ASP
1	B	298	LYS
1	B	300	ARG
1	B	312	ASN
1	B	352	TYR
1	B	374	THR
1	B	376	SER
1	B	382	GLN
1	C	40	ILE
1	C	42	SER
1	C	111	ARG
1	C	126	LEU
1	C	159	ARG
1	C	163	LYS

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Mol	Chain	Res	Type
1	C	179	ASN
1	C	226	ARG
1	C	249	SER
1	C	295	ARG
1	C	328	THR
1	C	352	TYR
1	C	372	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	127	ASN
1	A	165	ASN
1	A	179	ASN
1	A	199	HIS
1	A	239	ASN
1	A	243	ASN
1	A	280	ASN
1	A	289	HIS
1	A	323	ASN
1	A	338	ASN
1	B	80	GLN
1	B	165	ASN
1	B	179	ASN
1	B	243	ASN
1	B	280	ASN
1	B	289	HIS
1	B	297	GLN
1	B	312	ASN
1	B	323	ASN
1	B	338	ASN
1	B	382	GLN
1	C	80	GLN
1	C	165	ASN
1	C	179	ASN
1	C	199	HIS
1	C	224	ASN
1	C	243	ASN
1	C	268	ASN
1	C	280	ASN
1	C	289	HIS

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Mol	Chain	Res	Type
1	C	323	ASN
1	C	338	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OBZ	A	401	-	7,9,9	0.12	0	9,10,10	0.16	0
3	SO4	B	402	-	4,4,4	0.31	0	6,6,6	0.34	0
2	OBZ	B	401	-	7,9,9	0.08	0	9,10,10	0.48	0
3	SO4	A	402	-	4,4,4	0.31	0	6,6,6	0.18	0

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
2	OBZ	A	401	-	-	0/2/3/3	0/1/1/1
2	OBZ	B	401	-	-	2/2/3/3	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

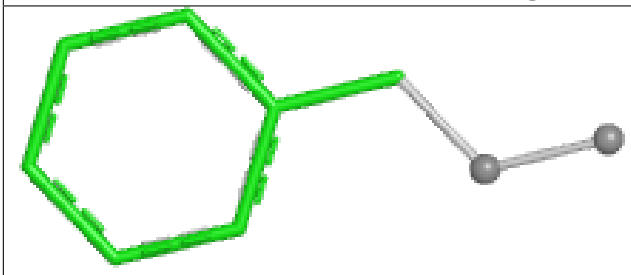
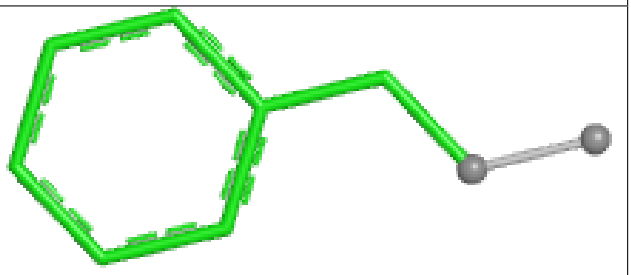
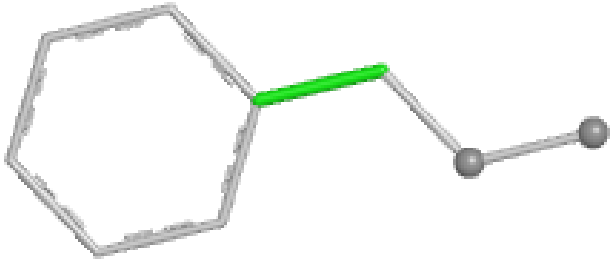
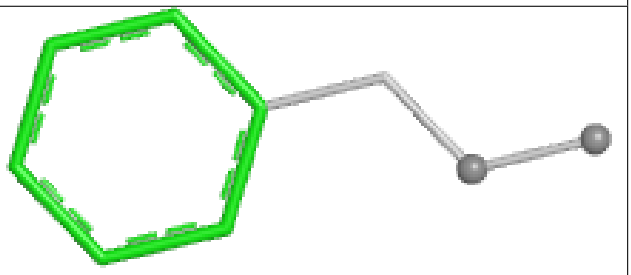
Mol	Chain	Res	Type	Atoms
2	B	401	OBZ	O2-C3-C4-C5
2	B	401	OBZ	O2-C3-C4-C9

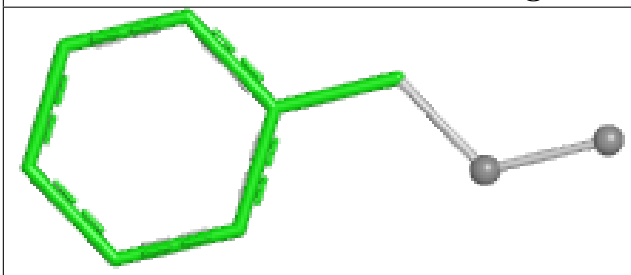
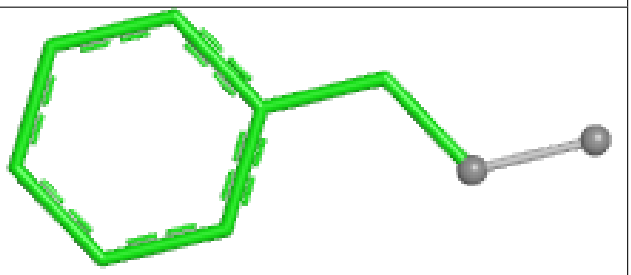
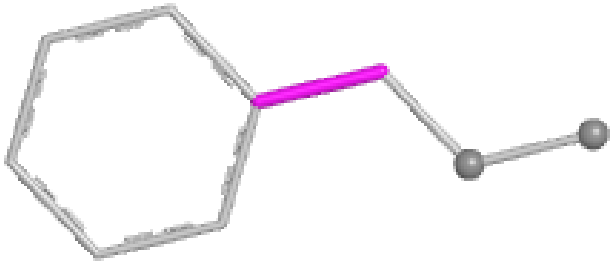
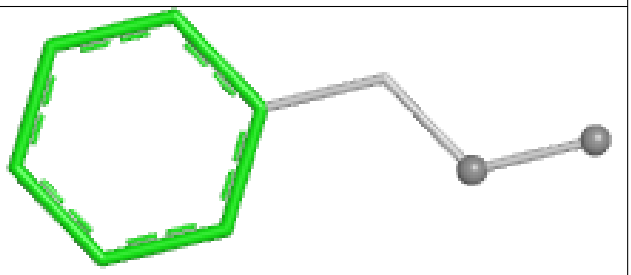
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	OBZ	1	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 OBZ A 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OBZ B 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 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	324/349 (92%)	0.46	25 (7%)	13	10	33, 53, 92, 101	0
1	B	346/349 (99%)	0.26	19 (5%)	25	21	32, 50, 94, 108	0
1	C	332/349 (95%)	0.36	20 (6%)	21	18	33, 57, 90, 113	0
All	All	1002/1047 (95%)	0.36	64 (6%)	19	16	32, 53, 92, 113	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	LYS	4.7
1	A	313	ALA	4.6
1	B	312	ASN	4.6
1	A	139	GLY	4.5
1	A	39	TYR	4.1
1	A	314	PHE	3.8
1	B	378	TRP	3.7
1	A	312	ASN	3.7
1	C	375	SER	3.5
1	A	247	CYS	3.5
1	C	273	ASP	3.2
1	B	338	ASN	3.1
1	C	39	TYR	3.0
1	C	130	ASP	3.0
1	B	377	ALA	2.9
1	A	338	ASN	2.9
1	C	323	ASN	2.9
1	C	43	LYS	2.9
1	B	44	TYR	2.9
1	B	125	VAL	2.9
1	C	44	TYR	2.9
1	A	342	VAL	2.8
1	A	341	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	43	LYS	2.7
1	A	100	CYS	2.6
1	B	45	LYS	2.6
1	B	42	SER	2.6
1	A	40	ILE	2.5
1	A	322	GLU	2.5
1	C	38	PHE	2.5
1	C	112	CYS	2.5
1	B	100	CYS	2.5
1	A	315	ILE	2.5
1	B	383	PHE	2.4
1	B	309	GLN	2.4
1	A	126	LEU	2.4
1	B	319	LYS	2.4
1	A	46	ILE	2.4
1	B	38	PHE	2.4
1	B	130	ASP	2.4
1	A	281	LEU	2.4
1	C	125	VAL	2.3
1	C	210	ILE	2.3
1	A	42	SER	2.3
1	C	341	LYS	2.3
1	B	281	LEU	2.3
1	C	296	ILE	2.3
1	C	268	ASN	2.3
1	A	248	LYS	2.3
1	B	41	ASN	2.3
1	A	125	VAL	2.2
1	C	212	LYS	2.2
1	C	116	ALA	2.2
1	A	374	THR	2.2
1	C	100	CYS	2.2
1	B	304	VAL	2.1
1	C	314	PHE	2.1
1	A	116	ALA	2.1
1	B	43	LYS	2.1
1	C	326	ASP	2.1
1	B	311	LYS	2.0
1	A	98	VAL	2.0
1	A	155	GLY	2.0
1	C	126	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

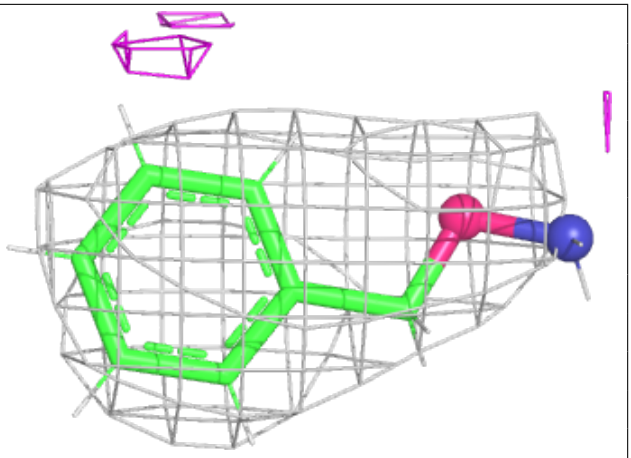
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

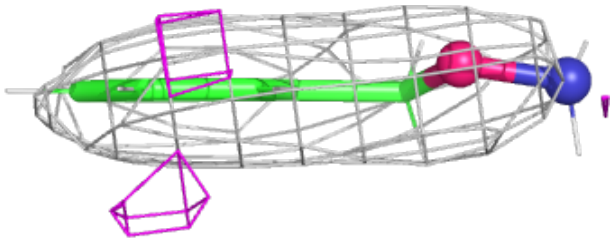
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OBZ	B	401	9/9	0.88	0.24	76,81,97,98	0
2	OBZ	A	401	9/9	0.94	0.24	81,86,100,101	0
4	NA	A	403	1/1	0.94	0.36	43,43,43,43	0
3	SO4	B	402	5/5	0.96	0.23	49,53,68,72	0
3	SO4	A	402	5/5	0.96	0.21	48,51,56,58	0

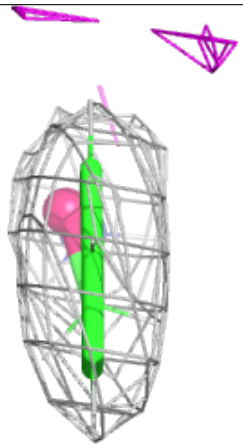
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OBZ B 401:

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

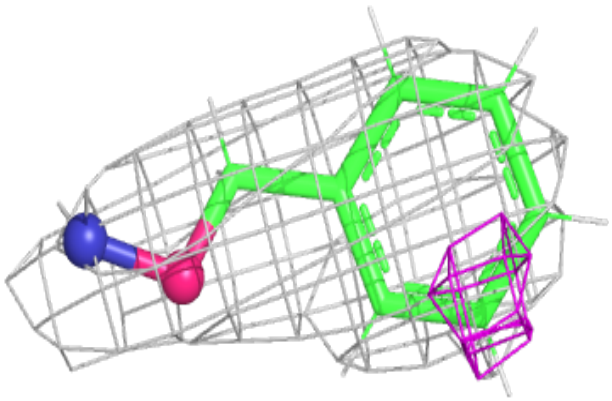


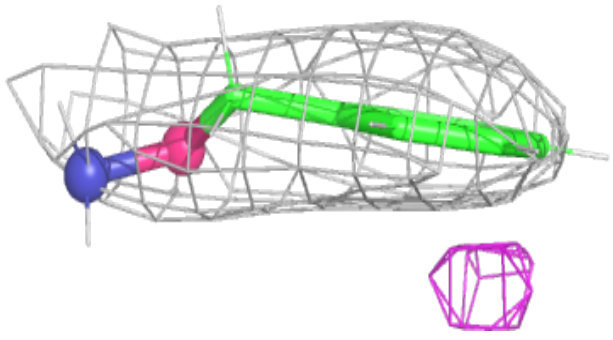


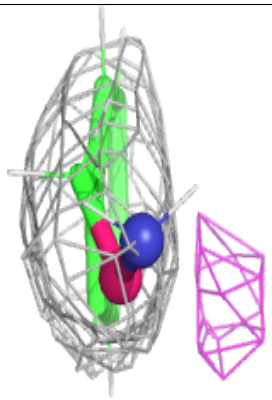


Electron density around OBZ A 401:

$2mF_o$-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.