



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 06:25 PM EDT

PDB ID : 9MY6  
Title : Structure of the BasE double mutant V336A/S247C, an NRPS adenylation domain in the acinetobactin biosynthetic pathway bound to 4-fluoro salicylic Acid  
Authors : Ahmed, S.F.; Gulick, A.M.  
Deposited on : 2025-01-21  
Resolution : 2.07 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

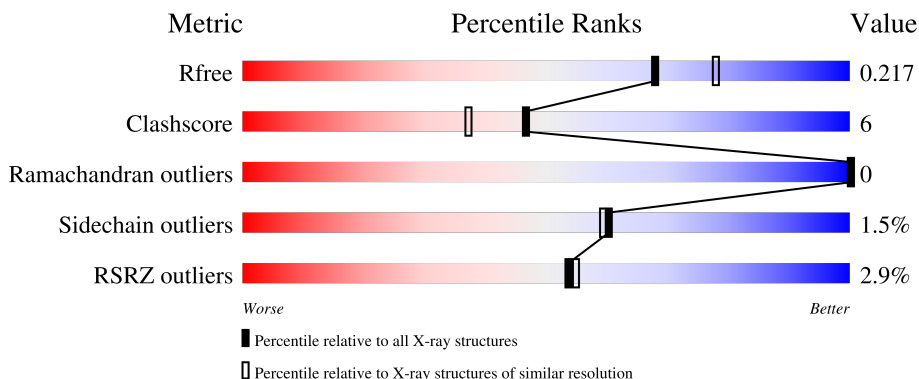
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

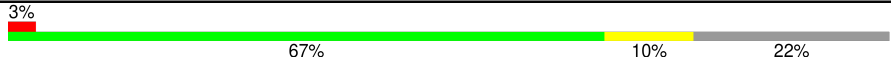

The reported resolution of this entry is 2.07 Å.

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))
$R_{free}$	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)

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  $\geq 3$ , 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	562	
1	B	562	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7070 atoms, of which 34 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 (2,3-dihydroxybenzoyl)adenylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	436	Total	C	N	O	S	0	2	0
			3385	2160	577	632	16			
1	A	436	Total	C	N	O	S	0	2	0
			3389	2160	583	630	16			

There are 54 discrepancies between the modelled and reference sequences:

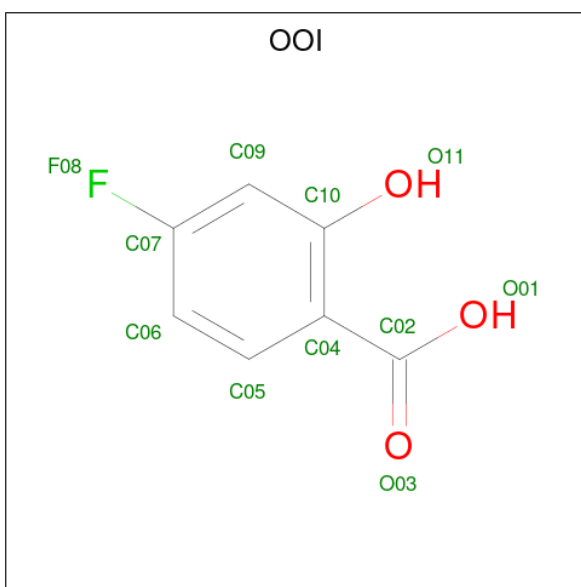
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP A0A505MWF2
B	-18	GLY	-	expression tag	UNP A0A505MWF2
B	-17	SER	-	expression tag	UNP A0A505MWF2
B	-16	SER	-	expression tag	UNP A0A505MWF2
B	-15	HIS	-	expression tag	UNP A0A505MWF2
B	-14	HIS	-	expression tag	UNP A0A505MWF2
B	-13	HIS	-	expression tag	UNP A0A505MWF2
B	-12	HIS	-	expression tag	UNP A0A505MWF2
B	-11	HIS	-	expression tag	UNP A0A505MWF2
B	-10	SER	-	expression tag	UNP A0A505MWF2
B	-9	SER	-	expression tag	UNP A0A505MWF2
B	-8	GLY	-	expression tag	UNP A0A505MWF2
B	-7	GLU	-	expression tag	UNP A0A505MWF2
B	-6	ASN	-	expression tag	UNP A0A505MWF2
B	-5	LEU	-	expression tag	UNP A0A505MWF2
B	-4	TYR	-	expression tag	UNP A0A505MWF2
B	-3	PHE	-	expression tag	UNP A0A505MWF2
B	-2	GLN	-	expression tag	UNP A0A505MWF2
B	-1	GLY	-	expression tag	UNP A0A505MWF2
B	0	HIS	-	expression tag	UNP A0A505MWF2
B	45	LEU	PRO	engineered mutation	UNP A0A505MWF2
B	68	THR	SER	conflict	UNP A0A505MWF2
B	149	ASP	GLU	conflict	UNP A0A505MWF2
B	247	CYS	SER	engineered mutation	UNP A0A505MWF2
B	336	ALA	VAL	engineered mutation	UNP A0A505MWF2

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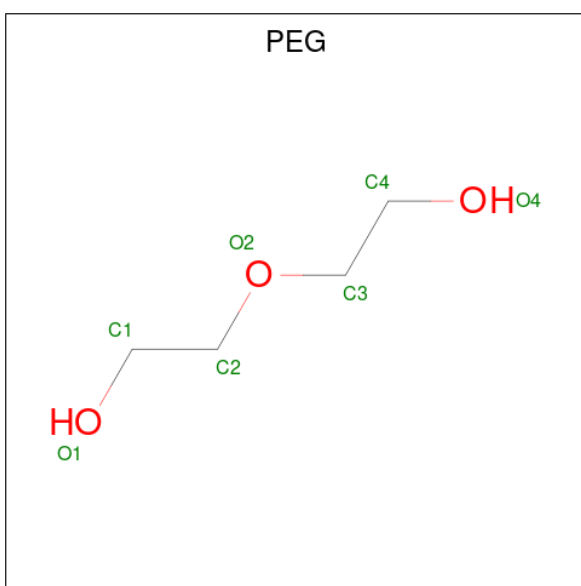
Chain	Residue	Modelled	Actual	Comment	Reference
B	378	ARG	LYS	conflict	UNP A0A505MWF2
B	385	ILE	VAL	conflict	UNP A0A505MWF2
A	-19	MET	-	initiating methionine	UNP A0A505MWF2
A	-18	GLY	-	expression tag	UNP A0A505MWF2
A	-17	SER	-	expression tag	UNP A0A505MWF2
A	-16	SER	-	expression tag	UNP A0A505MWF2
A	-15	HIS	-	expression tag	UNP A0A505MWF2
A	-14	HIS	-	expression tag	UNP A0A505MWF2
A	-13	HIS	-	expression tag	UNP A0A505MWF2
A	-12	HIS	-	expression tag	UNP A0A505MWF2
A	-11	HIS	-	expression tag	UNP A0A505MWF2
A	-10	SER	-	expression tag	UNP A0A505MWF2
A	-9	SER	-	expression tag	UNP A0A505MWF2
A	-8	GLY	-	expression tag	UNP A0A505MWF2
A	-7	GLU	-	expression tag	UNP A0A505MWF2
A	-6	ASN	-	expression tag	UNP A0A505MWF2
A	-5	LEU	-	expression tag	UNP A0A505MWF2
A	-4	TYR	-	expression tag	UNP A0A505MWF2
A	-3	PHE	-	expression tag	UNP A0A505MWF2
A	-2	GLN	-	expression tag	UNP A0A505MWF2
A	-1	GLY	-	expression tag	UNP A0A505MWF2
A	0	HIS	-	expression tag	UNP A0A505MWF2
A	45	LEU	PRO	engineered mutation	UNP A0A505MWF2
A	68	THR	SER	conflict	UNP A0A505MWF2
A	149	ASP	GLU	conflict	UNP A0A505MWF2
A	247	CYS	SER	engineered mutation	UNP A0A505MWF2
A	336	ALA	VAL	engineered mutation	UNP A0A505MWF2
A	378	ARG	LYS	conflict	UNP A0A505MWF2
A	385	ILE	VAL	conflict	UNP A0A505MWF2

- Molecule 2 is 4-fluorosalicylic acid (three-letter code: OOI) (formula:  $C_7H_5FO_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	H	O	0	0
			15	7	1	4	3		
2	A	1	Total	C	F	H	O	0	0
			15	7	1	4	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).

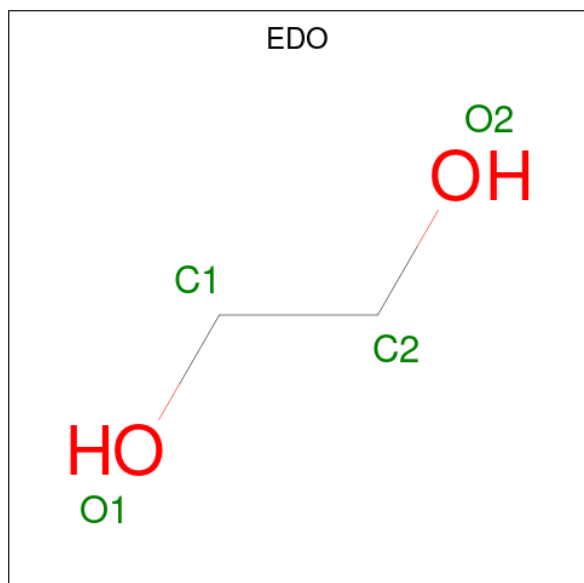


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	Ca 3	0	0
4	A	5	Total 5	Ca 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	108	Total 108	O 108	0	0
6	A	106	Total 106	O 106	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.42Å 141.25Å 148.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.78 – 2.07 63.78 – 2.07	Depositor EDS
% Data completeness (in resolution range)	95.1 (63.78-2.07) 95.1 (63.78-2.07)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.191 , 0.218 0.193 , 0.217	Depositor DCC
$R_{free}$ test set	82246 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PEG, OOI, EDO

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	0.50	0/3475	0.66	0/4732
1	B	0.54	0/3471	0.67	0/4728
All	All	0.52	0/6946	0.67	0/9460

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3389	0	3298	45	0
1	B	3385	0	3291	37	0
2	A	11	4	0	0	0
2	B	11	4	0	1	0
3	A	7	10	10	2	0
3	B	7	10	10	1	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
5	A	4	6	6	0	0
6	A	106	0	0	3	0
6	B	108	0	0	3	0
All	All	7036	34	6615	75	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 6.

All (75) 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:381:PRO:HG2	1:B:384:GLU:HG3	1.59	0.85
1:B:17:GLN:HE21	1:B:21:ASN:HD21	1.35	0.72
1:B:119:ALA:O	1:B:123:GLN:HG3	1.92	0.69
1:A:289:ALA:HA	1:A:292:MET:HE2	1.74	0.67
1:A:235[B]:CYS:SG	1:A:260:VAL:HG13	2.35	0.66
1:B:213:ASP:HB2	1:B:394:TYR:HA	1.77	0.66
1:A:308:LYS:NZ	6:A:702:HOH:O	2.31	0.64
1:B:437:LYS:HD2	1:A:433:VAL:HA	1.79	0.63
1:B:437:LYS:HE2	1:A:316:SER:HB2	1.80	0.63
1:B:382:GLU:HA	1:B:382:GLU:OE2	2.00	0.61
1:A:215:ASP:O	1:A:219:ARG:HG3	2.01	0.60
1:A:90:GLU:OE2	1:A:170:LEU:HD11	2.02	0.59
1:B:235[B]:CYS:SG	1:B:260:VAL:HG13	2.43	0.59
1:B:319:GLU:O	1:B:323:ARG:HG3	2.02	0.58
1:B:292:MET:HG2	1:A:115:TYR:CZ	2.39	0.57
1:A:235[A]:CYS:HA	1:A:244:MET:HE1	1.87	0.56
1:A:64:THR:O	1:A:68:THR:HG23	2.04	0.56
1:A:213:ASP:HB2	1:A:394:TYR:HA	1.87	0.56
1:A:10:ARG:HB3	6:A:791:HOH:O	2.05	0.56
1:B:437:LYS:NZ	1:A:316:SER:HA	2.21	0.56
1:A:235[B]:CYS:HA	1:A:244:MET:HE1	1.88	0.55
1:B:148[A]:HIS:CG	1:B:153:SER:HG	2.26	0.54
1:A:106:LEU:HD11	1:A:196:LEU:HD21	1.90	0.54
1:A:73:LYS:NZ	3:A:602:PEG:O2	2.40	0.52
1:A:235[B]:CYS:SG	1:A:260:VAL:CG1	2.98	0.52
1:A:52:ARG:NH1	1:A:90:GLU:OE2	2.42	0.51
1:B:342:GLY:HA3	1:B:395:THR:HA	1.92	0.51
1:A:248:PRO:HD2	1:A:311:GLN:NE2	2.25	0.51
1:B:387:MET:HG2	1:B:436:ILE:HG21	1.93	0.50
1:A:72:GLU:OE1	1:A:177:ALA:HB1	2.11	0.50
1:B:437:LYS:HG3	1:A:433:VAL:O	2.12	0.49
1:A:234:LEU:HB2	1:A:280:VAL:HG11	1.94	0.48
1:A:371:LYS:HD3	1:A:415:TYR:CE2	2.49	0.48
1:A:425:THR:HB	1:A:426:PRO:HD2	1.94	0.47
1:B:133:ARG:HB2	1:B:161:ASN:O	2.14	0.47
1:B:105:VAL:O	1:B:193:PHE:HB2	2.14	0.47
1:A:265:ASN:HB2	1:A:266:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:SER:HB2	6:A:757:HOH:O	2.14	0.47
1:A:162:HIS:HB2	1:A:166:ASP:HB2	1.97	0.47
1:B:10:ARG:CG	6:B:804:HOH:O	2.63	0.46
1:B:107:ASN:HB3	1:B:240:PRO:HB3	1.98	0.46
1:B:10:ARG:HG3	6:B:804:HOH:O	2.16	0.46
1:B:64:THR:O	1:B:68:THR:HG23	2.15	0.46
1:B:69:ARG:HD3	1:B:177:ALA:HA	1.96	0.46
1:B:115:TYR:CE1	1:A:292:MET:HG2	2.51	0.45
1:B:215:ASP:O	1:B:219:ARG:HG3	2.16	0.45
1:A:289:ALA:HA	1:A:292:MET:CE	2.43	0.45
1:B:410:PHE:O	3:B:602:PEG:H41	2.16	0.45
1:A:41:HIS:HB2	1:A:44:SER:OG	2.17	0.45
1:B:265:ASN:HB2	1:B:266:PRO:CD	2.47	0.45
1:B:410:PHE:HA	1:B:415:TYR:O	2.17	0.44
1:B:234:LEU:HB2	1:B:280:VAL:HG11	1.99	0.44
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.76	0.44
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.90	0.44
1:A:69:ARG:HD2	1:A:172:TRP:O	2.17	0.43
1:A:19:TYR:CE2	1:A:393:PRO:HA	2.53	0.43
1:A:62:LEU:HD22	1:A:173:ILE:HG22	1.99	0.43
1:B:437:LYS:HD2	1:A:433:VAL:CA	2.48	0.43
1:B:437:LYS:HZ1	1:A:316:SER:HA	1.82	0.43
2:B:601:OOI:O03	2:B:601:OOI:O11	2.33	0.43
6:B:745:HOH:O	1:A:201:THR:HG22	2.19	0.43
1:A:133:ARG:HG3	1:A:163:GLN:HG2	2.00	0.43
1:B:239:ALA:N	1:B:240:PRO:CD	2.83	0.42
1:B:122:LYS:HD2	1:B:122:LYS:HA	1.57	0.42
1:B:77:LYS:HE3	1:B:185:SER:O	2.20	0.41
1:B:159:MET:O	1:B:162:HIS:HB3	2.19	0.41
1:A:73:LYS:HZ1	3:A:602:PEG:C3	2.33	0.41
1:A:337:PHE:CG	1:A:432:VAL:HG21	2.55	0.41
1:B:300:TYR:O	1:B:301:LYS:C	2.59	0.41
1:A:69:ARG:HA	1:A:177:ALA:HB2	2.02	0.41
1:A:62:LEU:HB3	1:A:173:ILE:HG23	2.03	0.40
1:A:248:PRO:CD	1:A:311:GLN:NE2	2.84	0.40
1:B:311:GLN:HA	1:B:334:GLN:O	2.22	0.40
1:A:234:LEU:HD21	1:A:271:CYS:HB2	2.02	0.40
1:A:425:THR:OG1	1:A:427:ASP:OD1	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/562 (78%)	428 (98%)	8 (2%)	0	100	100
1	B	436/562 (78%)	428 (98%)	8 (2%)	0	100	100
All	All	872/1124 (78%)	856 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	363/487 (74%)	358 (99%)	5 (1%)	62	62
1	B	363/487 (74%)	357 (98%)	6 (2%)	56	54
All	All	726/974 (74%)	715 (98%)	11 (2%)	60	59

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	175	THR
1	B	214	TYR
1	B	339	MET
1	B	387	MET
1	B	396	PHE
1	B	413	ASP
1	A	180	PHE
1	A	273	SER

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Mol	Chain	Res	Type
1	A	354	GLU
1	A	396	PHE
1	A	427	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	GLN
1	A	311	GLN
1	A	334	GLN
1	A	405	HIS
1	A	408	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	OOI	A	601	-	11,11,11	1.15	1 (9%)	15,15,15	1.49	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	A	602	-	6,6,6	0.30	0	5,5,5	0.15	0
2	OOI	B	601	-	11,11,11	1.27	2 (18%)	15,15,15	1.72	2 (13%)
3	PEG	B	602	-	6,6,6	0.35	0	5,5,5	0.16	0
5	EDO	A	603	-	3,3,3	0.58	0	2,2,2	0.35	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	OOI	A	601	-	-	0/4/4/4	0/1/1/1
3	PEG	A	602	-	-	3/4/4/4	-
2	OOI	B	601	-	-	0/4/4/4	0/1/1/1
3	PEG	B	602	-	-	3/4/4/4	-
5	EDO	A	603	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	OOI	O11-C10	2.84	1.42	1.36
2	B	601	OOI	O11-C10	2.26	1.40	1.36
2	B	601	OOI	O01-C02	-2.09	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	OOI	C10-C04-C02	-3.75	116.15	120.00
2	A	601	OOI	C05-C04-C10	3.33	122.33	118.15
2	B	601	OOI	C05-C04-C10	2.50	121.29	118.15
2	A	601	OOI	O03-C02-C04	-2.11	116.94	121.97
2	A	601	OOI	O01-C02-C04	2.01	120.99	115.28

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	PEG	O1-C1-C2-O2
3	B	602	PEG	O2-C3-C4-O4
3	A	602	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	A	603	EDO	O1-C1-C2-O2
3	A	602	PEG	C1-C2-O2-C3
3	B	602	PEG	C1-C2-O2-C3
3	A	602	PEG	C4-C3-O2-C2

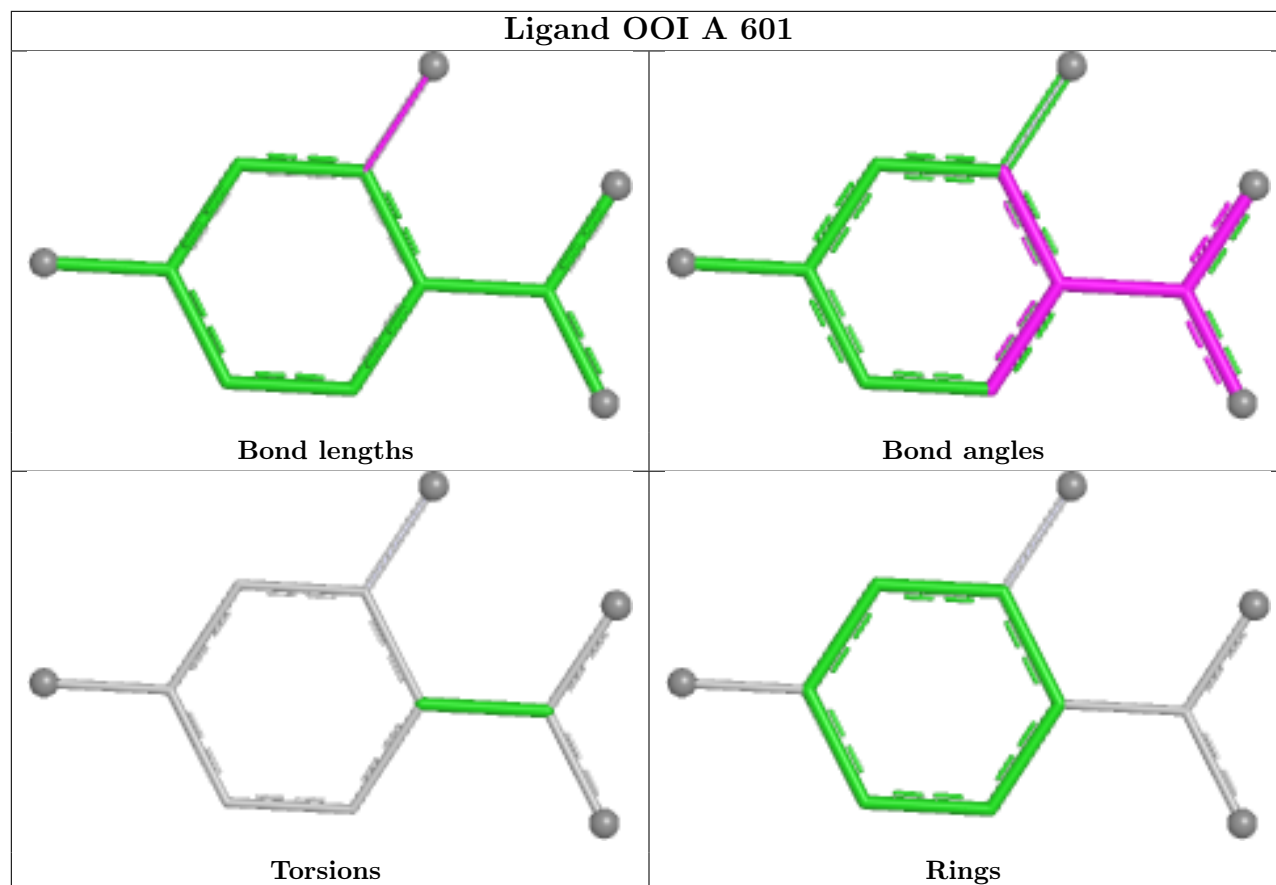
There are no ring outliers.

3 monomers are involved in 4 short contacts:

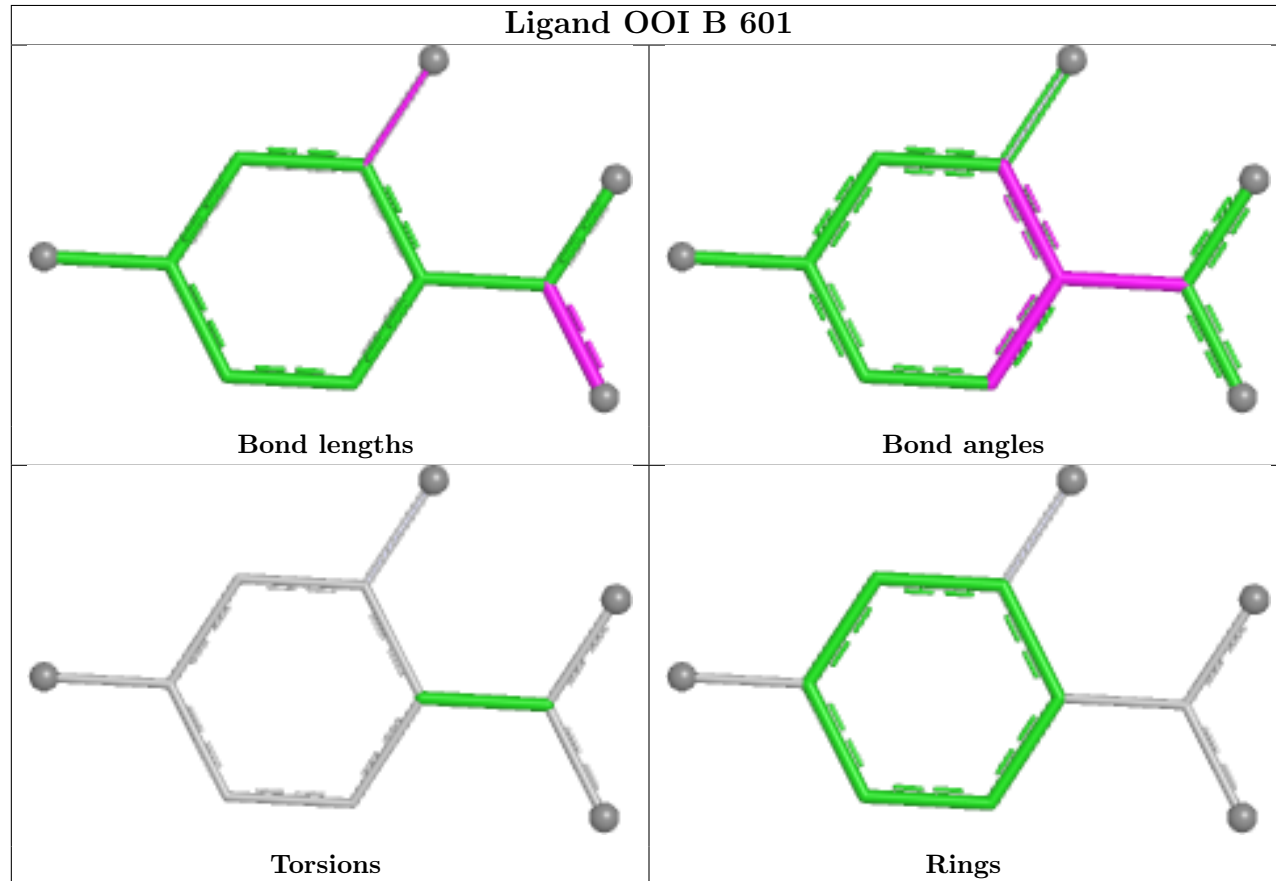
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	PEG	2	0
2	B	601	OOI	1	0
3	B	602	PEG	1	0

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 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.

## Ligand OOI A 601



## Ligand OOI B 601





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	436/562 (77%)	0.26	15 (3%)	48	50	32, 52, 71, 82	2 (0%)
1	B	436/562 (77%)	0.17	10 (2%)	61	62	26, 48, 72, 84	2 (0%)
All	All	872/1124 (77%)	0.21	25 (2%)	54	55	26, 50, 72, 84	4 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	GLY	4.6
1	B	438	ASP	4.5
1	A	270	ASN	4.3
1	A	199	GLY	4.2
1	B	148[A]	HIS	3.6
1	A	148[A]	HIS	3.4
1	A	178	GLU	3.3
1	B	3	LYS	3.1
1	A	269	LEU	3.0
1	B	150	VAL	2.8
1	A	298	ALA	2.7
1	B	437	LYS	2.7
1	B	427	ASP	2.6
1	B	115	TYR	2.6
1	A	271	CYS	2.4
1	A	438	ASP	2.4
1	B	376	GLN	2.4
1	A	142	GLN	2.4
1	A	182	ASP	2.4
1	A	437	LYS	2.3
1	B	149	ASP	2.3
1	A	149	ASP	2.2
1	A	201	THR	2.1
1	A	200	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	151	ASN	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](#)

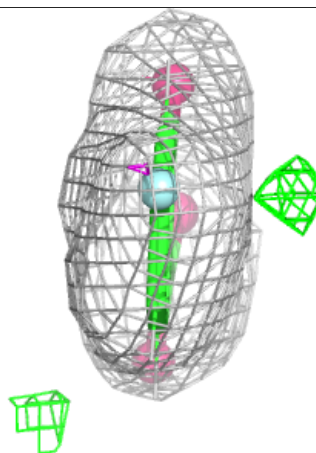
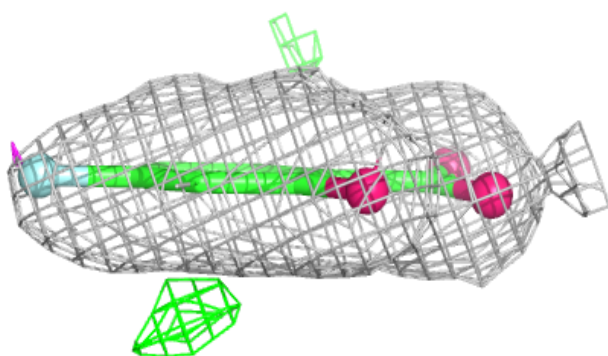
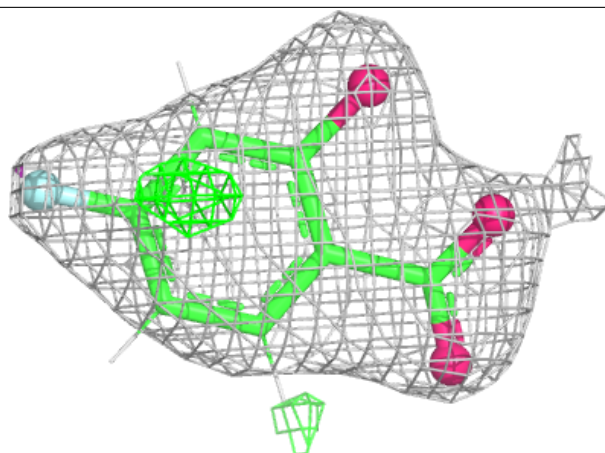
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEG	A	602	7/7	0.74	0.17	72,86,88,88	0
3	PEG	B	602	7/7	0.79	0.14	61,73,77,80	0
5	EDO	A	603	4/4	0.87	0.12	58,70,75,77	0
4	CA	A	607	1/1	0.89	0.10	88,88,88,88	0
4	CA	B	604	1/1	0.90	0.15	74,74,74,74	0
2	OOI	A	601	11/11	0.91	0.12	41,43,52,53	15
2	OOI	B	601	11/11	0.94	0.09	37,39,46,48	15
4	CA	A	604	1/1	0.96	0.06	74,74,74,74	0
4	CA	A	606	1/1	0.96	0.05	54,54,54,54	0
4	CA	B	605	1/1	0.97	0.10	63,63,63,63	0
4	CA	A	608	1/1	0.98	0.07	54,54,54,54	0
4	CA	B	603	1/1	0.98	0.04	44,44,44,44	0
4	CA	A	605	1/1	0.99	0.04	60,60,60,60	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.

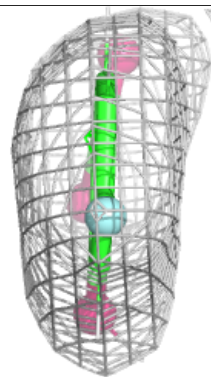
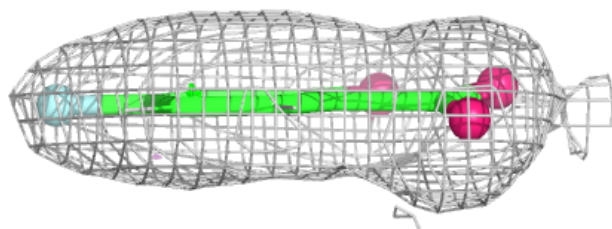
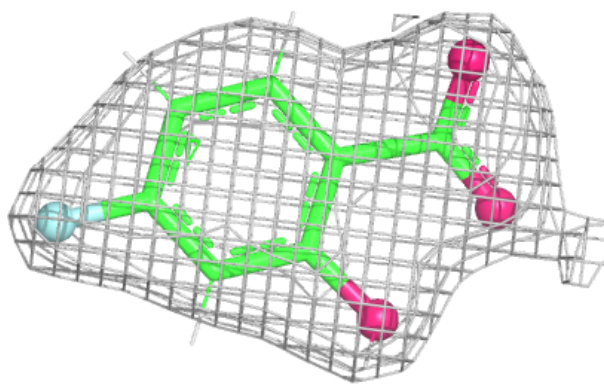
**Electron density around OOI A 601:**

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



**Electron density around OOI B 601:**

$2mF_o-DF_c$  (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.