

# wwPDB X-ray Structure Validation Summary Report (i)

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:	7ZB2
:	apo macrocyclase OphP
:	Song, H.; Naismith, J.H.
:	2022-03-23
:	1.94  Å(reported)
	: : : :

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.94 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	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	AAA	745	2% 	7%	
1	BBB	745	% •	70/	
1	ada	740	2%	1%	•
	CCC	745	90%	7%	•
1	DDD	745	89%	7%	·
1	EEE	745	90%	7%	·

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Mol	Chain	Length	Quality of chain			
1	FFF	745	<sup>2%</sup> 89%	7%	•	•
1	GGG	745	3% 	7%	•	,
1	HHH	745	3% 90%	7%		•



# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 47221 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.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace	
1		794	Total	С	Ν	Ο	S	0	2	0	
1		124	5833	3726	983	1098	26	0	5	0	
1	BBB	718	Total	С	Ν	Ο	$\mathbf{S}$	0	9	0	
1		110	5778	3693	971	1088	26	0		0	
1	CCC	720	Total	С	Ν	Ο	S	0	1	0	
1	000	120	5780	3696	971	1087	26	0	T	0	
1	מממ	717	Total	С	Ν	Ο	$\mathbf{S}$	0	1	0	
1		111	5760	3678	971	1085	26	0	T	U	
1	FFF	791	Total	С	Ν	Ο	$\mathbf{S}$	0	9	0	
1		121	5795	3700	976	1093	26	0	2	0	
1	FFF	718	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0	
1	LTT	110	5760	3681	968	1085	26	0	0	0	
1	CCC	714	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0	
1	999	114	5730	3661	961	1082	26	0	0	0	
1	ннн	793	Total	С	N	Ō	S	0	0	0	
1	111111	120	5784	3694	971	1093	26			U	

• Molecule 1 is a protein called OphP S580A.

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Na 1 1	0	0
2	BBB	2	Total Na 2 2	0	0
2	DDD	2	Total Na 2 2	0	0
2	EEE	3	Total Na 3 3	0	0
2	FFF	2	Total Na 2 2	0	0
2	GGG	3	Total Na 3 3	0	0





• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	CCC	1	TotalCO633	0	0
3	DDD	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	EEE	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	ННН	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	CCC	2	Total Mg 2 2	0	0
4	FFF	1	Total Mg 1 1	0	0

• Molecule 5 is THREONINE (three-letter code: THR) (formula:  $C_4H_9NO_3$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	EEE	1	Total 7	С 4	N 1	O 2	0	0
5	FFF	1	Total 7	С 4	N 1	0 2	0	0

• Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	EEE	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	GGG	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0



• Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	FFF	1	Total 8	С 4	N 1	O 3	0	0
7	GGG	1	Total 8	С 4	N 1	O 3	0	0

• Molecule 8 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:  $C_{11}H_{26}N_2O_6$ ).





Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
8	HHH	1	Total 19	C 11	N 2	0 6	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	192	Total O 192 192	0	0
9	BBB	110	Total         O           110         110	0	0
9	CCC	104	Total O 104 104	0	0
9	DDD	141	Total         O           141         141	0	0
9	EEE	57	$\begin{array}{cc} \text{Total} & \text{O} \\ 57 & 57 \end{array}$	0	0
9	FFF	80	Total O 80 80	0	0
9	GGG	97	Total         O           97         97	0	0
9	ННН	117	Total O 117 117	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: OphP S580A







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	69.86Å 113.43Å 186.32Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$83.97^{\circ}$ $82.09^{\circ}$ $76.93^{\circ}$	Depositor
Bosolution(A)	66.08 - 1.94	Depositor
Resolution (A)	66.00 - 1.94	EDS
% Data completeness	97.6 (66.08-1.94)	Depositor
(in resolution range)	97.6 (66.00-1.94)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.30 (at 1.94 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D	0.212 , $0.241$	Depositor
$n, n_{free}$	0.212 , $0.243$	DCC
$R_{free}$ test set	19701  reflections  (4.96%)	wwPDB-VP
Wilson B-factor $(Å^2)$	32.9	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$   <  L  > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	47221	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 14.78% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, B3P, TRS, GOL, EDO, NA

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).

Mal	Chain	Bo	nd lengths	B	ond angles
	Unain	$ RMSZ  \qquad \# Z  > 5$		RMSZ	# Z  > 5
1	AAA	0.66	0/6005	0.78	3/8146~(0.0%)
1	BBB	0.66	1/5947~(0.0%)	0.77	1/8067~(0.0%)
1	CCC	0.64	0/5949	0.75	1/8068~(0.0%)
1	DDD	0.66	0/5927	0.78	0/8038
1	EEE	0.65	0/5963	0.76	1/8087~(0.0%)
1	FFF	0.66	0/5928	0.77	2/8041~(0.0%)
1	GGG	0.67	0/5897	0.79	3/7999~(0.0%)
1	HHH	0.66	0/5954	0.78	2/8078~(0.0%)
All	All	0.66	1/47570~(0.0%)	0.77	13/64524~(0.0%)

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	<b>#Planarity outliers</b>
1	$\mathbf{FFF}$	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	259	GLU	CD-OE1	-5.44	1.19	1.25

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	AAA	435	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	BBB	435	ARG	NE-CZ-NH1	-8.03	116.29	120.30
1	HHH	203	ARG	NE-CZ-NH1	-7.35	116.62	120.30
1	$\mathbf{FFF}$	435	ARG	NE-CZ-NH1	6.87	123.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	GGG	115	ARG	CB-CG-CD	-6.73	94.10	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	$\mathbf{FFF}$	144	ASN	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	AAA	5833	0	5561	40	1
1	BBB	5778	0	5515	44	0
1	CCC	5780	0	5524	36	0
1	DDD	5760	0	5505	56	1
1	EEE	5795	0	5531	37	0
1	FFF	5760	0	5501	39	3
1	GGG	5730	0	5472	37	1
1	HHH	5784	0	5516	42	2
2	AAA	1	0	0	0	0
2	BBB	2	0	0	0	0
2	DDD	2	0	0	0	0
2	EEE	3	0	0	0	0
2	FFF	2	0	0	0	0
2	GGG	3	0	0	0	0
3	BBB	6	0	8	0	0
3	CCC	6	0	8	0	0
3	DDD	6	0	8	1	0
3	EEE	6	0	8	1	0
3	HHH	6	0	8	0	0
4	CCC	2	0	0	0	0
4	FFF	1	0	0	0	0
5	EEE	7	0	6	1	0
5	FFF	7	0	6	0	0
6	EEE	4	0	6	3	0
6	GGG	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	$\mathbf{FFF}$	8	0	12	0	0
7	GGG	8	0	12	0	0
8	HHH	19	0	26	1	0
9	AAA	192	0	0	2	0
9	BBB	110	0	0	5	0
9	CCC	104	0	0	1	0
9	DDD	141	0	0	1	0
9	EEE	57	0	0	0	0
9	$\mathbf{FFF}$	80	0	0	1	0
9	GGG	97	0	0	2	0
9	HHH	117	0	0	2	0
All	All	47221	0	44239	295	4

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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 3.

The worst 5 of 295 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:HHH:103:ASP:HB3	1:HHH:106:GLN:HE22	1.13	1.09
1:EEE:140:SER:OG	1:EEE:145:ALA:HB2	1.61	1.00
1:HHH:103:ASP:CB	1:HHH:106:GLN:HE22	1.74	1.00
1:DDD:381:ARG:HG2	1:HHH:566:ASN:OD1	1.63	0.97
1:EEE:138:LEU:O	1:EEE:188:ARG:O	1.83	0.96

All (4) 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:FFF:188:ARG:NH1	1:GGG:79:LYS:O[1_546]	2.07	0.13
1:AAA:196:ASN:OD1	1:HHH:44:GLU:OE1[1_554]	2.13	0.07
1:FFF:296:HIS:O	1:HHH:296:HIS:ND1[1_655]	2.16	0.04
1:DDD:474:THR:OG1	1:FFF:567:LYS:NZ[1_565]	2.19	0.01



## 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	Perce	ntiles
1	AAA	723/745~(97%)	702 (97%)	18 (2%)	3~(0%)	34	24
1	BBB	714/745~(96%)	695~(97%)	18 (2%)	1 (0%)	51	43
1	CCC	715/745~(96%)	695~(97%)	19 (3%)	1 (0%)	51	43
1	DDD	712/745~(96%)	691~(97%)	19 (3%)	2~(0%)	41	32
1	EEE	717/745~(96%)	696~(97%)	20 (3%)	1 (0%)	51	43
1	FFF	712/745~(96%)	692~(97%)	17 (2%)	3~(0%)	34	24
1	GGG	708/745~(95%)	691 (98%)	15 (2%)	2(0%)	41	32
1	HHH	719/745~(96%)	701 (98%)	17 (2%)	1 (0%)	51	43
All	All	5720/5960 (96%)	5563 (97%)	143 (2%)	14 (0%)	47	39

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	168	SER
1	FFF	145	ALA
1	FFF	146	ALA
1	GGG	168	SER
1	AAA	700	GLY

#### 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 Outlier		Percentiles	
1	AAA	629/644~(98%)	619~(98%)	10 (2%)	62 52	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	BBB	624/644~(97%)	619~(99%)	5 (1%)	81 78
1	CCC	623/644~(97%)	619~(99%)	4 (1%)	86 85
1	DDD	622/644~(97%)	617~(99%)	5(1%)	81 78
1	EEE	626/644~(97%)	618~(99%)	8 (1%)	69 62
1	$\mathbf{FFF}$	622/644~(97%)	616~(99%)	6 (1%)	76 71
1	GGG	620/644~(96%)	612~(99%)	8 (1%)	69 62
1	HHH	624/644~(97%)	617~(99%)	7(1%)	73 67
All	All	4990/5152~(97%)	4937 (99%)	53 (1%)	76 67

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5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	307	LYS
1	FFF	186	GLN
1	HHH	226	ASP
1	EEE	308[A]	ASN
1	FFF	38	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 28 ligands modelled in this entry, 16 are monoatomic - leaving 12 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).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
3	GOL	DDD	801	-	$5,\!5,\!5$	0.16	0	$5,\!5,\!5$	0.43	0
3	GOL	HHH	801	-	$5,\!5,\!5$	0.16	0	$5,\!5,\!5$	0.53	0
3	GOL	CCC	801	-	$5,\!5,\!5$	0.15	0	$5,\!5,\!5$	0.34	0
3	GOL	EEE	802	-	$5,\!5,\!5$	0.16	0	$5,\!5,\!5$	0.49	0
5	THR	EEE	801	-	$5,\!6,\!7$	0.50	0	6,7,9	1.07	0
7	TRS	FFF	802	-	7,7,7	0.19	0	9,9,9	0.22	0
7	TRS	GGG	802	-	7,7,7	0.18	0	9,9,9	0.22	0
6	EDO	GGG	801	-	3,3,3	0.20	0	2,2,2	0.16	0
5	THR	FFF	801	-	$5,\!6,\!7$	0.59	0	6,7,9	0.57	0
3	GOL	BBB	801	-	$5,\!5,\!5$	0.10	0	$5,\!5,\!5$	0.34	0
8	B3P	HHH	802	-	18,18,18	0.24	0	21,23,23	0.68	0
6	EDO	EEE	803	-	3,3,3	0.18	0	2,2,2	0.24	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
3	GOL	DDD	801	-	-	0/4/4/4	-
3	GOL	HHH	801	-	-	2/4/4/4	-
3	GOL	CCC	801	-	-	0/4/4/4	-
3	GOL	EEE	802	-	-	2/4/4/4	-
5	THR	EEE	801	-	-	0/5/6/8	-
7	TRS	$\mathbf{FFF}$	802	-	-	7/9/9/9	-
7	TRS	GGG	802	-	-	9/9/9/9	-
6	EDO	GGG	801	-	-	1/1/1/1	-
5	THR	FFF	801	-	-	0/5/6/8	-
3	GOL	BBB	801	-	-	2/4/4/4	-
8	B3P	HHH	802	-	-	9/28/28/28	-
6	EDO	EEE	803	-	-	1/1/1/1	-

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	801	GOL	C1-C2-C3-O3
3	BBB	801	GOL	O2-C2-C3-O3
3	EEE	802	GOL	C1-C2-C3-O3
3	HHH	801	GOL	O1-C1-C2-C3
7	FFF	802	TRS	C3-C-C1-O1

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DDD	801	GOL	1	0
3	EEE	802	GOL	1	0
5	EEE	801	THR	1	0
8	HHH	802	B3P	1	0
6	EEE	803	EDO	3	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 similar rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.













## 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	AAA	724/745~(97%)	-0.03	16 (2%) 62 69	24, 35, 66, 130	0
1	BBB	718/745~(96%)	-0.02	11 (1%) 73 79	29, 40, 69, 133	0
1	CCC	720/745~(96%)	0.01	13 (1%) 68 74	25, 40, 75, 121	0
1	DDD	717/745~(96%)	0.07	20 (2%) 53 60	24, 39, 74, 144	0
1	EEE	721/745~(96%)	0.22	26 (3%) 42 50	30, 49, 83, 138	0
1	$\mathbf{FFF}$	718/745~(96%)	0.05	16 (2%) 62 69	29, 43, 74, 129	0
1	GGG	714/745~(95%)	0.09	20 (2%) 53 60	30, 42, 78, 123	0
1	HHH	723/745~(97%)	0.08	22 (3%) 50 57	27, 44, 76, 128	0
All	All	5755/5960~(96%)	0.06	144 (2%) 57 64	24, 41, 76, 144	0

The worst 5 of 144 RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	BBB	3	PHE	10.5
1	AAA	3	PHE	9.3
1	AAA	702	PHE	9.2
1	FFF	166	HIS	8.5
1	BBB	2	SER	7.9

## 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
5	THR	FFF	801	7/8	0.59	0.28	75,102,115,129	0
2	NA	DDD	803	1/1	0.64	0.18	64,64,64,64	0
2	NA	EEE	804	1/1	0.67	0.35	62,62,62,62	0
5	THR	EEE	801	7/8	0.68	0.23	83,108,120,125	0
3	GOL	EEE	802	6/6	0.76	0.16	41,61,73,77	0
3	GOL	CCC	801	6/6	0.82	0.18	40,58,64,70	0
8	B3P	HHH	802	19/19	0.83	0.20	49,69,83,86	0
7	TRS	GGG	802	8/8	0.84	0.17	45,63,74,80	0
3	GOL	HHH	801	6/6	0.84	0.26	41,61,72,79	0
2	NA	AAA	801	1/1	0.85	0.28	$55,\!55,\!55,\!55$	0
3	GOL	DDD	801	6/6	0.85	0.15	36,49,56,64	0
2	NA	GGG	805	1/1	0.87	0.19	46,46,46,46	0
7	TRS	FFF	802	8/8	0.89	0.14	50,65,72,75	0
3	GOL	BBB	801	6/6	0.89	0.16	46,57,66,71	0
6	EDO	EEE	803	4/4	0.89	0.30	42,50,52,64	0
2	NA	BBB	803	1/1	0.90	0.26	46,46,46,46	0
2	NA	GGG	804	1/1	0.90	0.13	46,46,46,46	0
2	NA	EEE	806	1/1	0.91	0.26	49,49,49,49	0
2	NA	GGG	803	1/1	0.91	0.12	48,48,48,48	0
2	NA	DDD	802	1/1	0.91	0.42	54,54,54,54	0
6	EDO	GGG	801	4/4	0.92	0.10	47,50,51,57	0
4	MG	CCC	803	1/1	0.93	0.11	42,42,42,42	0
2	NA	BBB	802	1/1	0.94	0.26	47,47,47,47	0
4	MG	CCC	802	1/1	0.94	0.08	43,43,43,43	0
2	NA	FFF	804	1/1	0.95	0.16	44,44,44,44	0
2	NA	EEE	805	1/1	0.95	0.13	61,61,61,61	0
4	MG	FFF	803	1/1	0.97	0.17	43,43,43,43	0
2	NA	FFF	805	1/1	0.98	0.24	$53,\!53,\!53,\!53$	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.

























## 6.5 Other polymers (i)

There are no such residues in this entry.

