



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:46 PM UTC

PDB ID : 5O8Y / pdb_00005o8y
Title : Conformational dynamism for DNA interaction in Salmonella typhimurium RcsB response regulator.
Authors : Casino, P.; Marina, A.; Miguel-Romero, L.; Huesa, J.
Deposited on : 2017-06-14
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

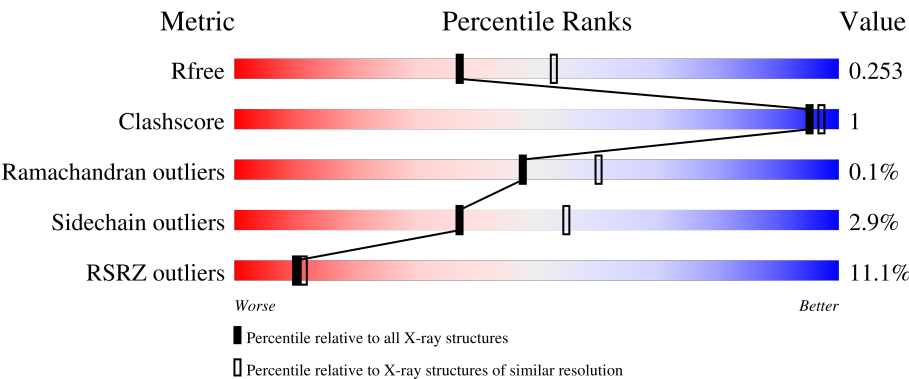
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	216	9% 92% 5%
1	C	216	9% 89% 6%
1	D	216	13% 90% 5% 5%
1	F	216	6% 90% 5%
1	G	216	18% 88% 7%

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Mol	Chain	Length	Quality of chain
1	H	216	9% 92%

2 Entry composition [i](#)

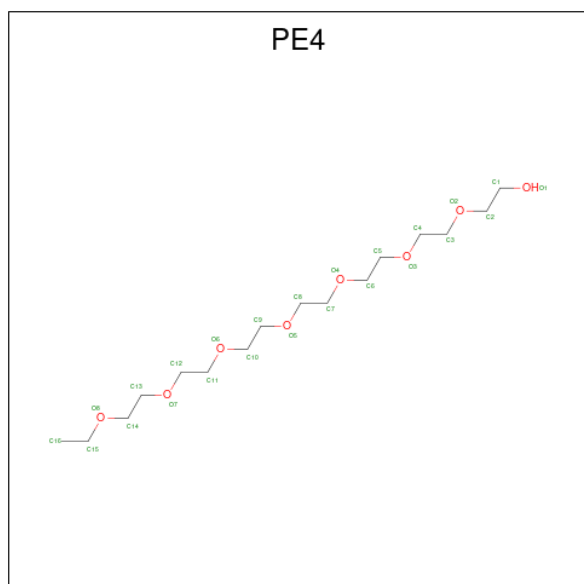
There are 4 unique types of molecules in this entry. The entry contains 9583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transcriptional regulatory protein RcsB.

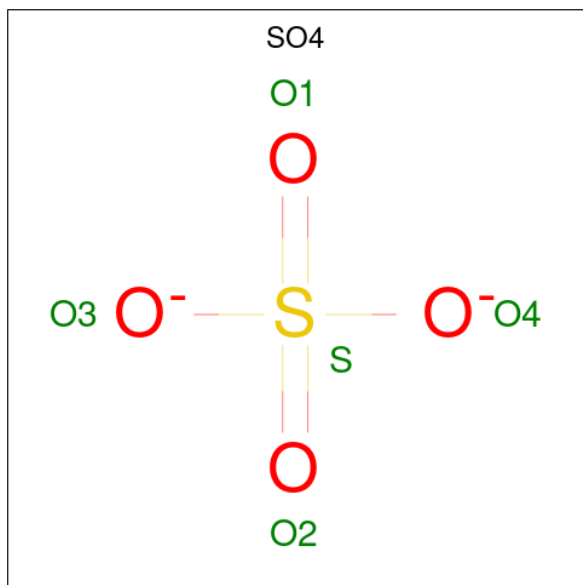
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1570	1010	263	292	5			
1	C	207	Total	C	N	O	S	0	0	0
			1558	1001	258	294	5			
1	D	206	Total	C	N	O	S	0	1	0
			1527	983	254	285	5			
1	G	207	Total	C	N	O	S	0	1	0
			1561	1005	262	289	5			
1	F	207	Total	C	N	O	S	0	2	0
			1586	1019	267	295	5			
1	H	208	Total	C	N	O	S	0	0	0
			1572	1010	262	294	6			

- Molecule 2 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	16	8		
2	C	1	Total	C	O	0	0
			24	16	8		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

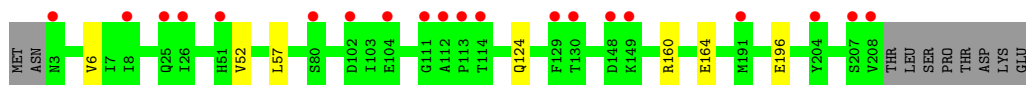


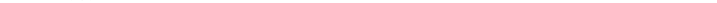
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

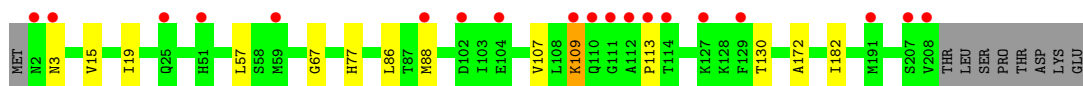
- Molecule 4 is water.

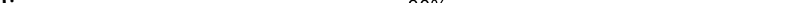
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	C	26	Total 26	O 26	0	0
4	D	14	Total 14	O 14	0	0
4	G	25	Total 25	O 25	0	0
4	F	10	Total 10	O 10	0	0
4	H	6	Total 6	O 6	0	0

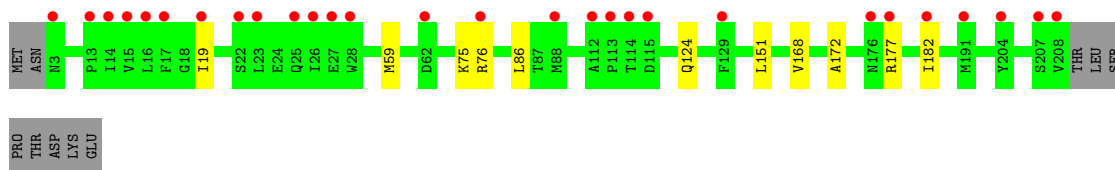
- Molecule 1: Transcriptional regulatory protein RcsB

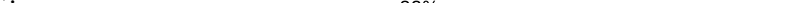


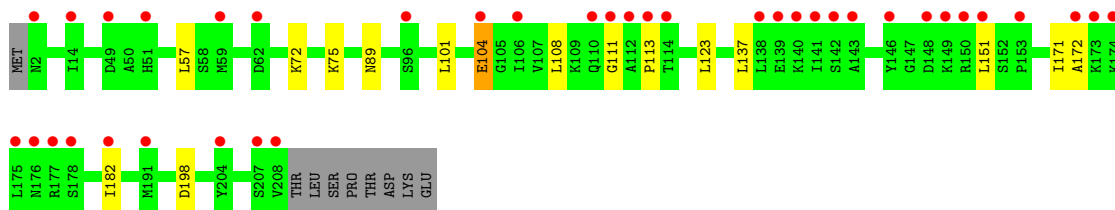
- Chain C:  9% 89% 6%

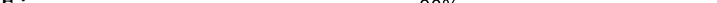


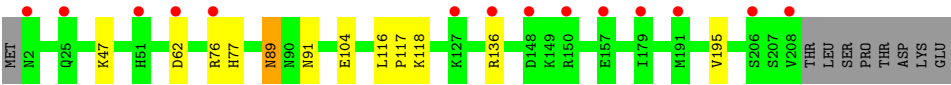
- Chain D:  13% 90% 5% 5%



- Chain G:  18% 88% 7%



- Chain F:  6% 90% 5% .



● Molecule 1: Transcriptional regulatory protein RcsB



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.83Å 108.83Å 306.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.56 – 2.30 102.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (102.56-2.30) 100.0 (102.56-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.223 , 0.253 0.225 , 0.253	Depositor DCC
R_{free} test set	4361 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9583	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PE4

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	0.58	0/1593	0.79	0/2154
1	C	0.59	0/1581	0.81	0/2143
1	D	0.58	0/1552	0.80	0/2105
1	F	0.60	0/1615	0.83	0/2184
1	G	0.61	0/1587	0.84	0/2148
1	H	0.61	0/1595	0.81	0/2160
All	All	0.60	0/9523	0.81	0/12894

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	1570	0	1642	2	0
1	C	1558	0	1597	7	0
1	D	1527	0	1572	3	0
1	F	1586	0	1657	3	0
1	G	1561	0	1623	7	0
1	H	1572	0	1629	3	0
2	A	24	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	34	0	0
3	A	15	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	F	10	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	A	30	0	0	0	0
4	C	26	0	0	0	0
4	D	14	0	0	0	0
4	F	10	0	0	0	0
4	G	25	0	0	0	0
4	H	6	0	0	1	0
All	All	9583	0	9788	23	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 1.

All (23) 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:G:171:ILE:HG22	1:G:182:ILE:HD13	1.77	0.66
1:G:104:GLU:HG2	1:G:123:LEU:HD13	1.78	0.65
1:C:15:VAL:HG21	1:C:109:LYS:HD2	1.78	0.65
1:C:172:ALA:HA	1:C:182:ILE:CD1	2.30	0.61
1:G:172:ALA:HA	1:G:182:ILE:HD12	1.82	0.61
1:C:19:ILE:HD11	1:C:86:LEU:CD2	2.30	0.61
1:D:168:VAL:O	1:D:182:ILE:HD11	2.08	0.52
1:C:19:ILE:HD11	1:C:86:LEU:HD22	1.92	0.51
1:G:198:ASP:HB3	1:H:91:ASN:HD21	1.77	0.50
1:C:86:LEU:HD12	1:C:107:VAL:O	2.12	0.50
1:G:108:LEU:HD11	1:G:137:LEU:HD12	1.95	0.49
1:H:20:ARG:NH2	4:H:401:HOH:O	2.46	0.49
1:A:6:VAL:HG22	1:A:52:VAL:CG1	2.43	0.48
1:D:19:ILE:HD11	1:D:86:LEU:CD2	2.45	0.46
1:F:89:ASN:HD22	1:F:91:ASN:H	1.63	0.46
1:H:10:ASP:HA	1:H:56:ASP:HB2	1.98	0.45
1:D:172:ALA:HB1	1:D:177:ARG:O	2.18	0.43
1:A:160:ARG:O	1:A:164:GLU:HG2	2.19	0.43
1:C:77:HIS:HE1	1:F:77:HIS:ND1	2.17	0.42
1:G:111:GLY:C	1:G:113:PRO:HD2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LEU:O	1:C:67:GLY:HA2	2.19	0.41
1:G:72:LYS:HG3	1:G:101:LEU:HD22	2.03	0.40
1:F:116:LEU:HB3	1:F:117:PRO:HD3	2.04	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	204/216 (94%)	201 (98%)	3 (2%)	0	100	100
1	C	205/216 (95%)	201 (98%)	3 (2%)	1 (0%)	24	31
1	D	205/216 (95%)	202 (98%)	3 (2%)	0	100	100
1	F	207/216 (96%)	203 (98%)	4 (2%)	0	100	100
1	G	206/216 (95%)	200 (97%)	6 (3%)	0	100	100
1	H	206/216 (95%)	202 (98%)	4 (2%)	0	100	100
All	All	1233/1296 (95%)	1209 (98%)	23 (2%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	113	PRO

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	173/189 (92%)	170 (98%)	3 (2%)	53	72
1	C	169/189 (89%)	165 (98%)	4 (2%)	43	62
1	D	164/189 (87%)	159 (97%)	5 (3%)	36	53
1	F	175/189 (93%)	166 (95%)	9 (5%)	21	32
1	G	170/189 (90%)	165 (97%)	5 (3%)	37	55
1	H	172/189 (91%)	167 (97%)	5 (3%)	37	55
All	All	1023/1134 (90%)	992 (97%)	31 (3%)	37	53

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	124	GLN
1	A	196	GLU
1	C	3	ASN
1	C	88	MET
1	C	109	LYS
1	C	130	THR
1	D	59	MET
1	D	75	LYS
1	D	76	ARG
1	D	124	GLN
1	D	151	LEU
1	G	57	LEU
1	G	75	LYS
1	G	89	ASN
1	G	104	GLU
1	G	151	LEU
1	F	47	LYS
1	F	62	ASP
1	F	76[A]	ARG
1	F	76[B]	ARG
1	F	89	ASN
1	F	104	GLU
1	F	118	LYS
1	F	136	ARG
1	F	195	VAL
1	H	6	VAL
1	H	66	ASP
1	H	75	LYS
1	H	96	SER

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Mol	Chain	Res	Type
1	H	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	C	30	ASN
1	C	77	HIS
1	D	124	GLN
1	D	203	ASN
1	G	3	ASN
1	G	44	ASN
1	G	89	ASN
1	G	185	GLN
1	G	203	ASN
1	F	25	GLN
1	F	89	ASN
1	F	91	ASN
1	F	203	ASN
1	H	3	ASN
1	H	91	ASN
1	H	203	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	SO4	C	302	-	4,4,4	0.37	0	6,6,6	0.21	0
3	SO4	G	301	-	4,4,4	0.39	0	6,6,6	0.13	0
2	PE4	A	301	-	23,23,23	0.44	0	22,22,22	0.32	0
3	SO4	C	303	-	4,4,4	0.44	0	6,6,6	0.09	0
3	SO4	F	301	-	4,4,4	0.34	0	6,6,6	0.19	0
3	SO4	H	301	-	4,4,4	0.27	0	6,6,6	0.22	0
3	SO4	A	303	-	4,4,4	0.45	0	6,6,6	0.16	0
3	SO4	D	301	-	4,4,4	0.42	0	6,6,6	0.18	0
2	PE4	C	301	-	23,23,23	0.48	0	22,22,22	0.34	0
3	SO4	A	304	-	4,4,4	0.45	0	6,6,6	0.12	0
3	SO4	A	302	-	4,4,4	0.45	0	6,6,6	0.31	0
3	SO4	F	302	-	4,4,4	0.46	0	6,6,6	0.16	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	PE4	C	301	-	-	9/21/21/21	-
2	PE4	A	301	-	-	10/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	PE4	O3-C5-C6-O4
2	C	301	PE4	O6-C11-C12-O7
2	A	301	PE4	O6-C11-C12-O7
2	A	301	PE4	O2-C3-C4-O3
2	C	301	PE4	O2-C3-C4-O3

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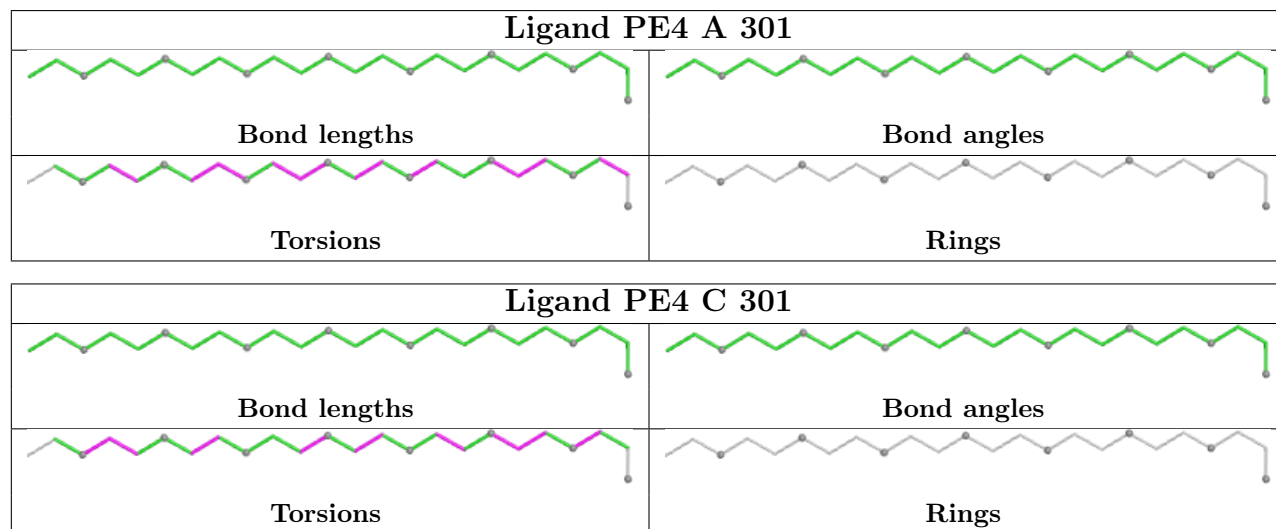
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Mol	Chain	Res	Type	Atoms
2	A	301	PE4	O4-C7-C8-O5
2	C	301	PE4	O7-C13-C14-O8
2	C	301	PE4	O4-C7-C8-O5
2	A	301	PE4	O6-C10-C9-O5
2	A	301	PE4	O1-C1-C2-O2
2	A	301	PE4	C10-C9-O5-C8
2	A	301	PE4	C12-C11-O6-C10
2	A	301	PE4	O7-C13-C14-O8
2	A	301	PE4	C3-C4-O3-C5
2	C	301	PE4	C10-C9-O5-C8
2	C	301	PE4	C3-C4-O3-C5
2	C	301	PE4	C13-C14-O8-C15
2	C	301	PE4	C1-C2-O2-C3
2	A	301	PE4	C5-C6-O4-C7

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	206/216 (95%)	0.64	20 (9%)	13 15	34, 46, 75, 99	0
1	C	207/216 (95%)	0.69	19 (9%)	14 16	32, 48, 73, 103	0
1	D	206/216 (95%)	0.75	28 (13%)	7 7	26, 49, 86, 96	1 (0%)
1	F	207/216 (95%)	0.65	14 (6%)	23 25	26, 50, 73, 92	2 (0%)
1	G	207/216 (95%)	0.98	38 (18%)	3 4	32, 51, 91, 101	1 (0%)
1	H	208/216 (96%)	0.73	19 (9%)	15 16	33, 49, 73, 89	0
All	All	1241/1296 (95%)	0.74	138 (11%)	10 11	26, 49, 80, 103	4 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	ALA	7.8
1	C	208	VAL	6.2
1	G	111	GLY	6.2
1	F	2	ASN	6.2
1	H	208	VAL	6.0
1	F	208	VAL	5.9
1	G	208	VAL	5.8
1	D	14	ILE	5.5
1	C	2	ASN	5.5
1	A	208	VAL	5.5
1	A	3	ASN	5.4
1	G	113	PRO	5.4
1	D	208	VAL	5.4
1	G	112	ALA	5.2
1	G	2	ASN	4.8
1	H	204	TYR	4.8
1	C	113	PRO	4.7
1	A	112	ALA	4.6
1	A	113	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	114	THR	4.5
1	G	148	ASP	4.2
1	G	149	LYS	4.0
1	C	111	GLY	4.0
1	G	176	ASN	3.9
1	H	177	ARG	3.8
1	A	114	THR	3.8
1	F	51	HIS	3.8
1	A	111	GLY	3.8
1	D	17	PHE	3.7
1	H	147	GLY	3.6
1	D	204	TYR	3.6
1	G	182	ILE	3.6
1	G	191	MET	3.4
1	A	207	SER	3.4
1	A	204	TYR	3.4
1	G	175	LEU	3.4
1	H	140	LYS	3.4
1	H	149	LYS	3.4
1	D	182	ILE	3.3
1	G	142	SER	3.3
1	G	143	ALA	3.2
1	D	113	PRO	3.2
1	A	51	HIS	3.2
1	H	148	ASP	3.2
1	D	15	VAL	3.1
1	D	62	ASP	3.1
1	D	115	ASP	3.1
1	C	109	LYS	3.1
1	C	102	ASP	3.0
1	G	62	ASP	3.0
1	F	191	MET	3.0
1	G	153	PRO	3.0
1	G	150	ARG	3.0
1	A	129	PHE	2.9
1	C	207	SER	2.9
1	D	114	THR	2.9
1	D	3	ASN	2.9
1	G	204	TYR	2.9
1	H	191	MET	2.8
1	H	207	SER	2.8
1	G	173	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	141	ILE	2.8
1	D	16	LEU	2.8
1	G	178[A]	SER	2.8
1	D	27	GLU	2.7
1	G	151	LEU	2.7
1	F	25	GLN	2.7
1	A	191	MET	2.7
1	D	191	MET	2.7
1	D	207	SER	2.6
1	H	198	ASP	2.6
1	D	22	SER	2.6
1	G	96	SER	2.6
1	C	25	GLN	2.6
1	G	146	TYR	2.6
1	A	80	SER	2.6
1	A	104	GLU	2.6
1	H	135	SER	2.6
1	H	62	ASP	2.5
1	G	139	GLU	2.5
1	G	49	ASP	2.5
1	D	25	GLN	2.5
1	H	27	GLU	2.4
1	H	139	GLU	2.4
1	A	26	ILE	2.4
1	C	191	MET	2.4
1	A	25	GLN	2.4
1	F	136	ARG	2.4
1	C	104	GLU	2.4
1	G	14	ILE	2.4
1	F	148	ASP	2.3
1	A	8	ILE	2.3
1	F	179	ILE	2.3
1	G	177	ARG	2.3
1	C	3	ASN	2.3
1	D	112	ALA	2.3
1	H	142	SER	2.3
1	G	106	ILE	2.3
1	G	110	GLN	2.3
1	G	59	MET	2.3
1	G	104	GLU	2.3
1	D	177	ARG	2.3
1	G	114	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	149	LYS	2.3
1	G	140	LYS	2.3
1	C	129	PHE	2.2
1	F	62	ASP	2.2
1	H	150	ARG	2.2
1	D	26	ILE	2.2
1	D	129	PHE	2.2
1	C	51	HIS	2.2
1	C	110	GLN	2.2
1	D	28	TRP	2.2
1	C	59	MET	2.2
1	H	88	MET	2.2
1	D	13	PRO	2.2
1	G	174	LYS	2.2
1	G	172	ALA	2.2
1	F	206	SER	2.2
1	A	148	ASP	2.1
1	D	176	ASN	2.1
1	D	76	ARG	2.1
1	D	23	LEU	2.1
1	A	102	ASP	2.1
1	G	51	HIS	2.1
1	G	207	SER	2.1
1	D	88	MET	2.1
1	F	76[A]	ARG	2.1
1	F	150	ARG	2.1
1	F	157	GLU	2.0
1	G	138	LEU	2.0
1	D	19	ILE	2.0
1	H	126	GLY	2.0
1	C	88	MET	2.0
1	A	130	THR	2.0
1	H	132	GLU	2.0
1	C	127	LYS	2.0
1	F	127	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

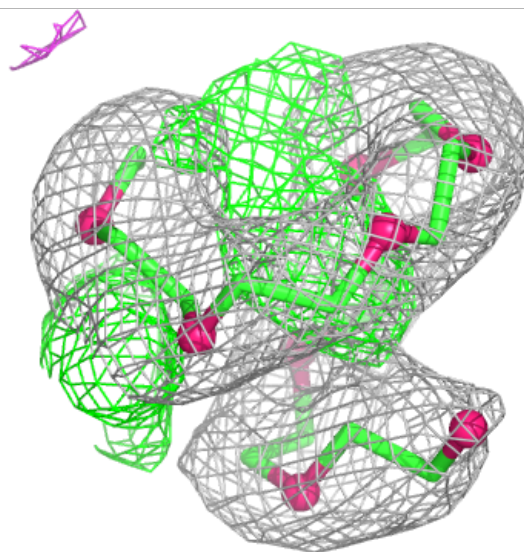
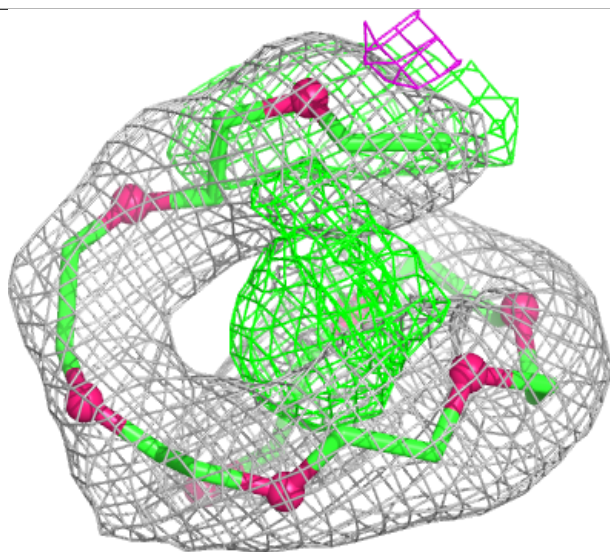
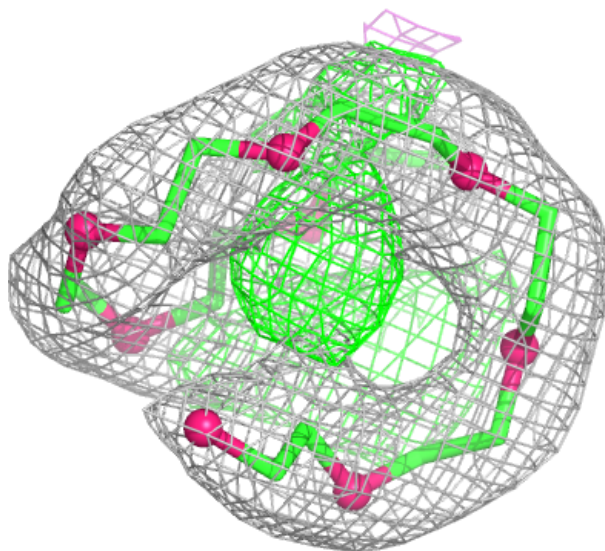
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	304	5/5	0.74	0.17	79,83,85,87	0
3	SO4	C	303	5/5	0.74	0.13	87,92,94,94	0
2	PE4	A	301	24/24	0.86	0.21	59,66,70,72	0
3	SO4	D	301	5/5	0.87	0.11	81,82,84,85	0
3	SO4	F	302	5/5	0.87	0.09	74,77,81,82	0
2	PE4	C	301	24/24	0.88	0.17	54,58,63,66	0
3	SO4	C	302	5/5	0.89	0.12	96,96,98,102	0
3	SO4	A	303	5/5	0.89	0.09	71,74,75,80	0
3	SO4	A	302	5/5	0.97	0.07	43,44,47,47	0
3	SO4	H	301	5/5	0.97	0.08	54,55,57,63	0
3	SO4	G	301	5/5	0.98	0.05	48,51,55,55	0
3	SO4	F	301	5/5	0.98	0.06	46,48,50,51	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.

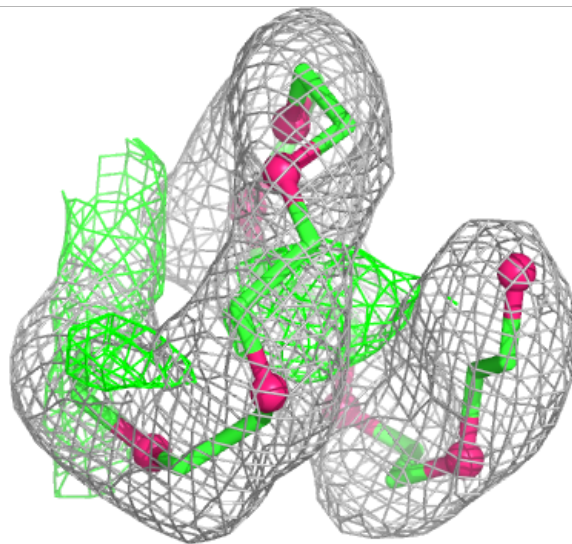
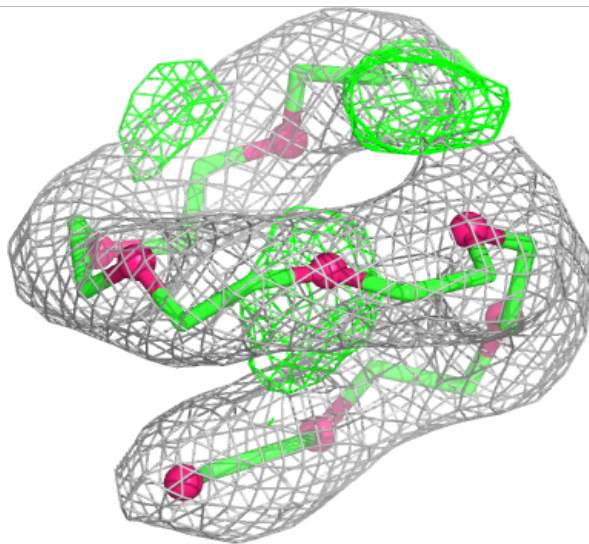
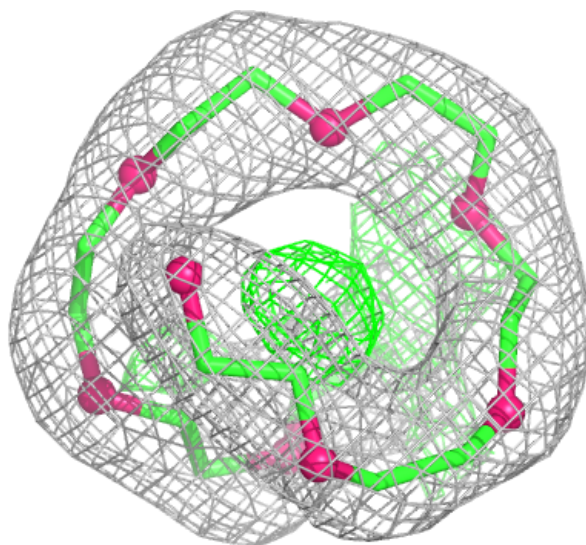
Electron density around PE4 A 301:

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



Electron density around PE4 C 301:

$2mF_o-DF_c$ (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.