

wwPDB X-ray Structure Validation Summary Report (i)

Jan 13, 2024 - 06:00 pm GMT

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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:

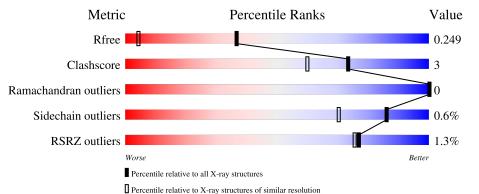
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.40 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	А	210	% • 89%	10%
1	В	210	2% 88 %	10% ••
1	С	210	91%	8%
1	D	210	% 90%	9%



2 Entry composition (i)

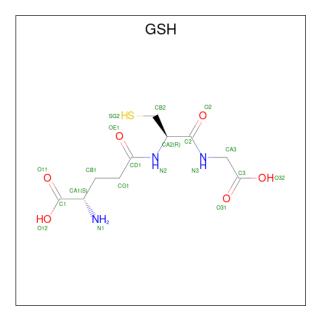
There are 6 unique types of molecules in this entry. The entry contains 7649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	Atoms				ZeroOcc	AltConf	Trace		
1	٨	А	209	Total	С	Ν	0	\mathbf{S}	0	2	0
	A	209	1652	1060	274	310	8	0		0	
1	В	208	Total	С	Ν	0	S	0	1	0	
	D	208	1659	1064	275	312	8	0	4	U	
1	С	209	Total	С	Ν	0	S	0	2	0	
	U	209	1652	1060	274	310	8	0	2	0	
1	П	209	Total	С	Ν	0	S	0	3	0	
		209	1658	1063	275	312	8	0	5	U	

• Molecule 1 is a protein called Glutathione S-transferase P.

• Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



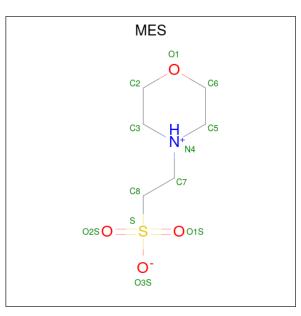
Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf
2	А	1	Total 20	C 10			S 1	0	0
2	В	1	Total 20	C 10	N 3	O 6	S 1	0	0



α \cdot \cdot \cdot	C		
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		1	1 0

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
2	С	1	Total C N O S	0	0	
		1	20 10 3 6 1	0	0	
2	Л	1	Total C N O S	0	0	
	D	D	1	20 10 3 6 1	0	0

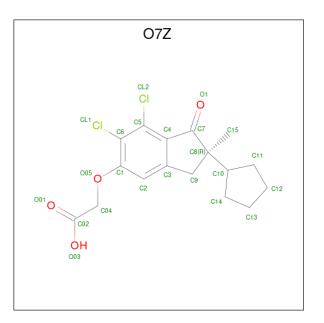
• Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C N O S	0	0
5	Л	1	12 6 1 4 1	0	0
3	В	1	Total C N O S	0	0
0	D	1	12 6 1 4 1	0	0
3	В	1	Total C N O S	0	0
0	D	1	12 6 1 4 1	0	0
3	С	1	Total C N O S	0	0
0	U	1	12 6 1 4 1	0	0
3	D	1	Total C N O S	0	0
0	D	1	12 6 1 4 1	0	0
3	р	1	Total C N O S	0	0
5	D	1	12 6 1 4 1	0	0

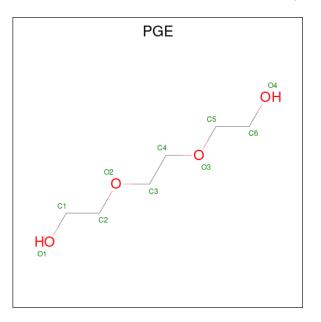
• Molecule 4 is 2-[[6,7-bis(chloranyl)-2-cyclopentyl-2-methyl-1-oxidanylidene-3 {H}-inden-5-y l]oxy]ethanoic acid (three-letter code: O7Z) (formula: $C_{17}H_{18}Cl_2O_4$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 5 & 2 & 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 2 3 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 5 2 3 \end{array}$	0	0

• Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	Total C O 10 6 4	0	0
5	D	1	Total C O 10 6 4	0	0

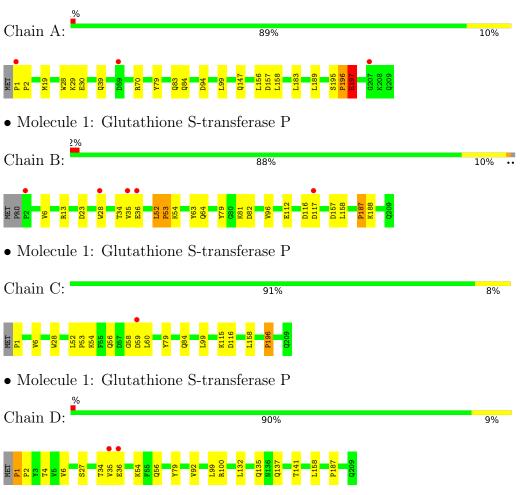
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	206	Total O 206 206	0	0
6	В	212	Total O 212 212	0	0
6	С	207	Total O 207 207	0	0
6	D	216	Total O 216 216	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: Glutathione S-transferase P



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	68.64Å 72.18Å 88.62Å	Deneiten
a, b, c, α , β , γ	90.00° 90.14° 90.00°	Depositor
Resolution (Å)	55.97 - 1.40	Depositor
Resolution (A)	$55.97 \ - \ 1.40$	EDS
% Data completeness	95.0 (55.97-1.40)	Depositor
(in resolution range)	94.4~(55.97-1.40)	EDS
R _{merge}	0.13	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.45 (at 1.40 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
D D	0.217 , 0.251	Depositor
R, R_{free}	0.219 , 0.249	DCC
R_{free} test set	7891 reflections (4.91%)	wwPDB-VP
Wilson B-factor $(Å^2)$	16.4	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 43.2	EDS
L-test for twinning ²	$< L > = 0.47, < L^2 > = 0.29$	Xtriage
	0.000 for -k,-h,-l	
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
	0.179 for h,-k,-l	
F_o, F_c correlation	0.97	EDS
Total number of atoms	7649	wwPDB-VP
Average B, all atoms $(Å^2)$	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 38.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8230e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities 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: PGE, GSH, MES, O7Z

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	Mol Chain		nd lengths	Bond angles	
IVIOI			# Z > 5	RMSZ	# Z > 5
1	А	0.80	6/1687~(0.4%)	0.80	6/2287~(0.3%)
1	В	0.99	8/1693~(0.5%)	0.87	11/2294~(0.5%)
1	С	0.83	5/1687~(0.3%)	0.65	0/2287
1	D	0.89	6/1693~(0.4%)	0.67	0/2295
All	All	0.88	25/6760~(0.4%)	0.75	17/9163~(0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	D	35	VAL	C-N	-19.64	0.88	1.34
1	В	116	ASP	C-N	-18.62	0.91	1.34
1	С	115	LYS	C-N	-18.31	0.92	1.34
1	D	34	THR	C-N	-14.30	1.01	1.34
1	А	196	PRO	C-N	-12.96	1.04	1.34

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	196	PRO	O-C-N	9.33	137.63	122.70
1	А	29	LYS	O-C-N	8.47	136.26	122.70
1	В	35	VAL	O-C-N	7.85	135.26	122.70
1	А	28	TRP	C-N-CA	7.84	141.31	121.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	36	GLU	O-C-N	-7.26	111.08	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	197	GLU	Mainchain

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	А	1652	0	1652	14	0
1	В	1659	0	1656	9	0
1	С	1652	0	1652	9	0
1	D	1658	0	1656	13	0
2	А	20	0	15	0	0
2	В	20	0	15	0	0
2	С	20	0	15	1	0
2	D	20	0	15	0	0
3	А	12	0	12	0	0
3	В	24	0	24	1	0
3	С	12	0	12	1	0
3	D	24	0	24	2	0
4	А	5	0	0	0	0
4	В	5	0	0	0	0
4	D	5	0	0	2	0
5	С	10	0	14	1	0
5	D	10	0	14	2	0
6	А	206	0	0	1	0
6	В	212	0	0	2	0
6	С	207	0	0	2	0
6	D	216	0	0	1	0
All	All	7649	0	6776	45	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 3.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:PRO:N	1:B:187:PRO:CA	1.69	1.42
1:C:196:PRO:N	1:C:196:PRO:CA	1.67	1.35
1:A:196:PRO:N	1:A:196:PRO:CA	1.67	1.29
2:C:301:GSH:SG2	6:C:557:HOH:O	2.35	0.83
1:D:1:PRO:H2	1:D:2:PRO:HD2	1.46	0.80

The worst 5 of 45 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	Perce	entiles
1	А	209/210~(100%)	205~(98%)	4 (2%)	0	100	100
1	В	210/210~(100%)	205~(98%)	5 (2%)	0	100	100
1	С	209/210~(100%)	203~(97%)	6 (3%)	0	100	100
1	D	210/210~(100%)	205~(98%)	5 (2%)	0	100	100
All	All	838/840 (100%)	818 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	Analysed Rotameric Outliers		Percentiles		
1	А	178/177~(101%)	177~(99%)	1 (1%)	86 70		
1	В	179/177~(101%)	178 (99%)	1 (1%)	86 70		
1	С	178/177~(101%)	177~(99%)	1 (1%)	86 70		
1	D	179/177~(101%)	178 (99%)	1 (1%)	86 70		
All	All	714/708~(101%)	710 (99%)	4 (1%)	86 70		

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	79	TYR
1	В	79	TYR
1	С	79	TYR
1	D	79	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	147	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

15 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	Bo	ond leng	ths	В	ond ang	les
WIOI	Type		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	PGE	С	303	-	$9,\!9,\!9$	0.53	0	8,8,8	0.39	0
3	MES	А	302	-	$12,\!12,\!12$	4.28	7 (58%)	$14,\!16,\!16$	2.03	5 (35%)
3	MES	С	302	-	12,12,12	4.26	7 (58%)	$14,\!16,\!16$	1.87	4 (28%)
3	MES	D	302	-	12,12,12	4.28	7 (58%)	14,16,16	1.51	3 (21%)
4	O7Z	А	303	-	4,4,25	0.98	0	4,4,38	1.31	0
2	GSH	D	301	-	$18,\!19,\!19$	1.97	3 (16%)	$23,\!24,\!24$	1.36	3 (13%)
2	GSH	В	301	-	18,19,19	2.00	3 (16%)	23,24,24	1.37	3 (13%)
4	O7Z	D	305	-	4,4,25	0.97	0	4,4,38	1.44	1 (25%)
2	GSH	С	301	-	18,19,19	1.89	2 (11%)	23,24,24	1.20	2 (8%)
3	MES	В	303	-	12,12,12	4.40	6 (50%)	14,16,16	1.67	6 (42%)
3	MES	D	303	-	12,12,12	4.30	<mark>6 (50%)</mark>	14,16,16	1.45	2 (14%)
5	PGE	D	304	-	$9,\!9,\!9$	0.50	0	8,8,8	0.35	0
4	O7Z	В	304	-	4,4,25	0.88	0	4,4,38	1.56	1 (25%)
3	MES	В	302	-	12,12,12	4.27	7 (58%)	14,16,16	1.53	4 (28%)
2	GSH	А	301	-	18,19,19	1.86	3 (16%)	23,24,24	1.47	3 (13%)

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
5	PGE	С	303	-	-	3/7/7/7	-
3	MES	А	302	-	-	2/6/14/14	0/1/1/1
3	MES	С	302	-	-	0/6/14/14	0/1/1/1
3	MES	D	302	-	-	2/6/14/14	0/1/1/1
4	O7Z	А	303	-	-	2/2/2/33	-
2	GSH	D	301	-	-	0/24/24/24	-
2	GSH	В	301	-	-	1/24/24/24	-
4	O7Z	D	305	-	-	2/2/2/33	-
2	GSH	С	301	-	-	2/24/24/24	-
3	MES	В	303	-	-	5/6/14/14	0/1/1/1
3	MES	D	303	-	-	1/6/14/14	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	D	304	-	-	2/7/7/7	-
4	O7Z	В	304	-	-	2/2/2/33	-
3	MES	В	302	-	-	5/6/14/14	0/1/1/1
2	GSH	А	301	-	-	0/24/24/24	-

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The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	В	303	MES	C7-N4	-8.79	1.27	1.47
3	D	303	MES	C7-N4	-8.72	1.27	1.47
3	D	302	MES	C7-N4	-8.53	1.27	1.47
3	В	302	MES	C7-N4	-8.49	1.27	1.47
3	С	302	MES	C7-N4	-8.39	1.28	1.47

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	301	GSH	CA2-CB2-SG2	-4.07	109.62	114.19
2	А	301	GSH	CB2-CA2-N2	-3.91	105.71	111.28
3	А	302	MES	C5-N4-C3	3.72	117.20	108.83
2	D	301	GSH	CB2-CA2-N2	-3.71	105.99	111.28
3	А	302	MES	C6-C5-N4	3.54	115.47	110.10

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	302	MES	C7-C8-S-O2S
3	В	302	MES	C7-C8-S-O3S
3	В	303	MES	N4-C7-C8-S
3	В	303	MES	C7-C8-S-O2S
3	D	303	MES	N4-C7-C8-S

There are no ring outliers.

7 monomers are involved in 8 short contacts:

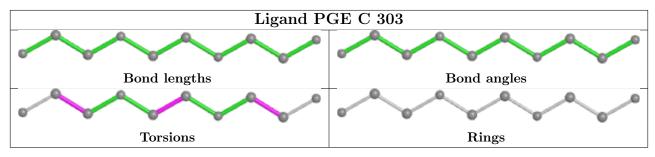
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	С	303	PGE	1	0
3	С	302	MES	1	0
4	D	305	O7Z	2	0



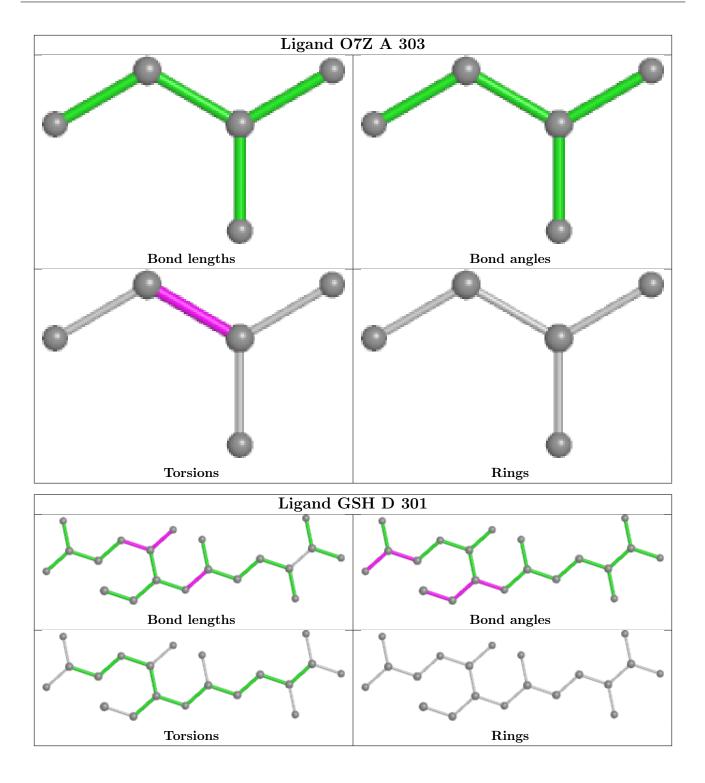
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	301	GSH	1	0
3	D	303	MES	2	0
5	D	304	PGE	2	0
3	В	302	MES	1	0

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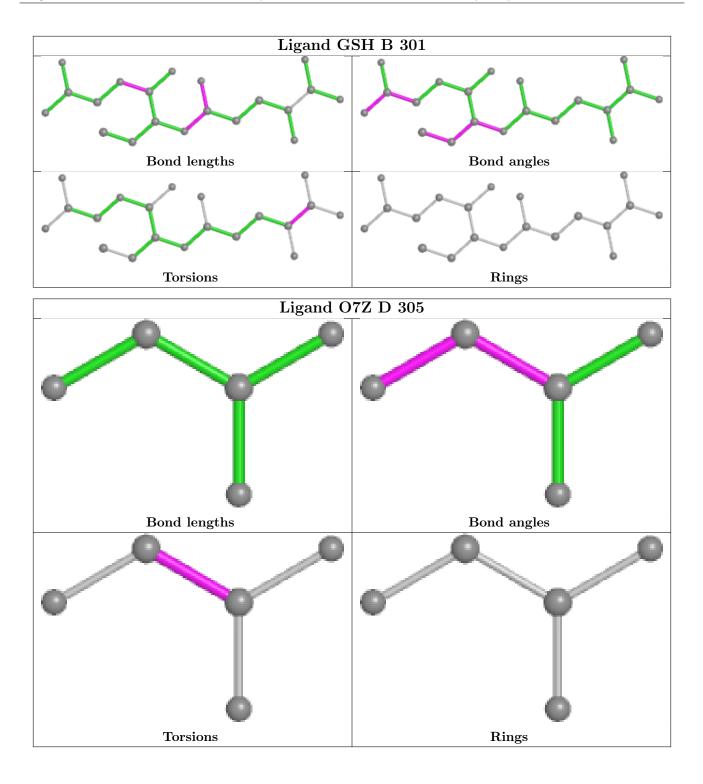
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





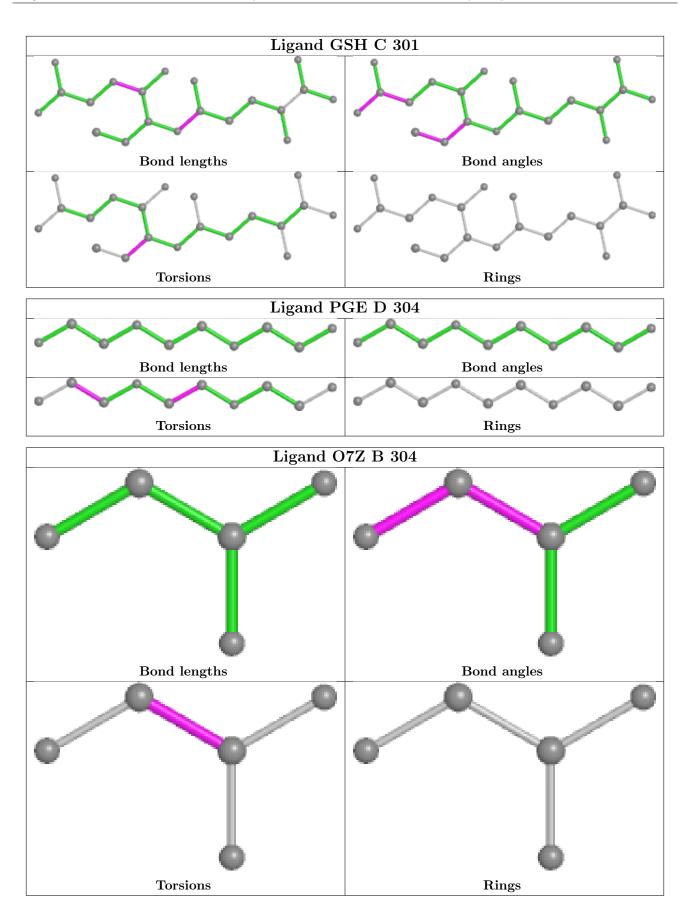




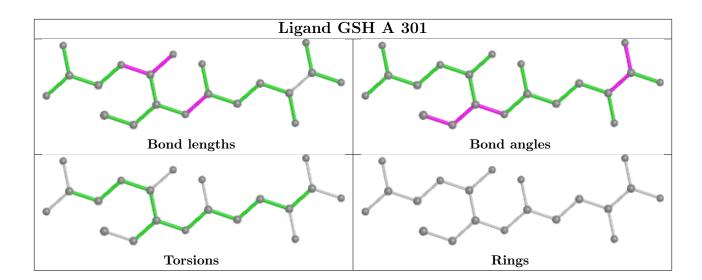












5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	5
1	В	5
1	А	2
1	С	2

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	100:ARG	С	101[B]:CYS	Ν	1.20
1	А	197:GLU	С	198:TYR	Ν	1.19
1	D	1:PRO	С	2:PRO	Ν	1.19
1	В	81:LYS	С	82:ASP	Ν	1.18
1	В	157:ASP	С	158:LEU	Ν	1.15



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	$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$
1	А	209/210~(99%)	-0.28	3 (1%) 75 74	12, 19, 31, 44	0
1	В	208/210~(99%)	-0.19	5 (2%) 59 58	10, 20, 36, 47	0
1	С	209/210~(99%)	-0.23	1 (0%) 91 89	12, 20, 33, 41	0
1	D	209/210~(99%)	-0.25	2 (0%) 82 80	12, 19, 32, 39	0
All	All	835/840~(99%)	-0.24	11 (1%) 77 75	10, 19, 32, 47	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1	PRO	5.2
1	В	35	VAL	4.8
1	В	36	GLU	4.5
1	D	35	VAL	4.1
1	D	36	GLU	3.5

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.

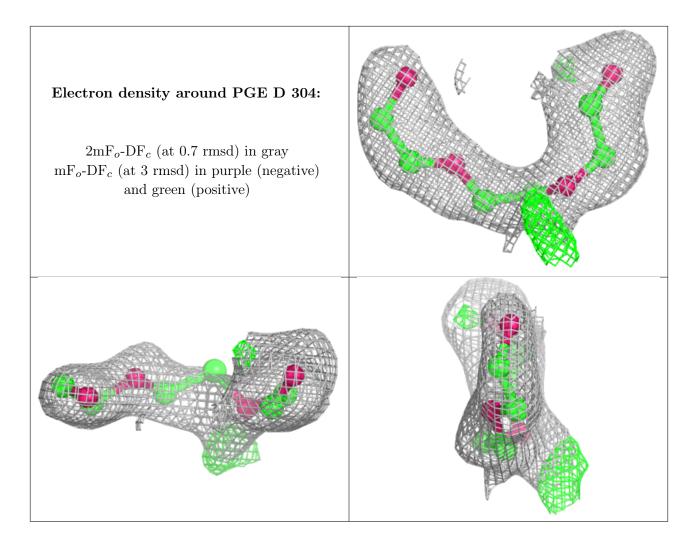


6Y1E

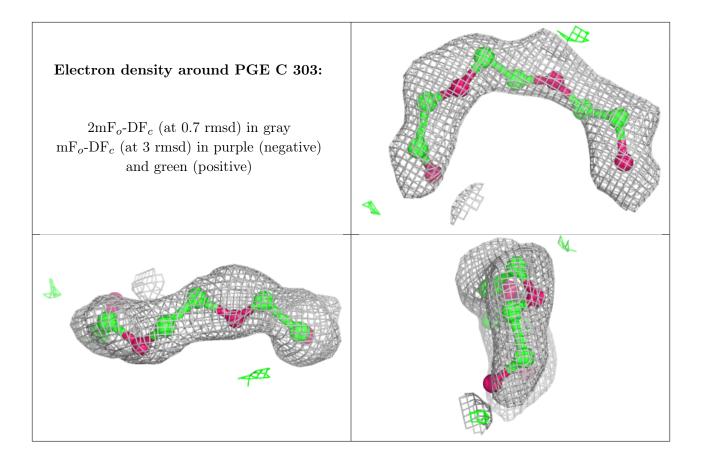
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
5	PGE	D	304	10/10	0.67	0.15	32,38,45,45	0
5	PGE	С	303	10/10	0.78	0.15	33,39,47,49	0
3	MES	В	303	12/12	0.83	0.16	28,39,45,52	0
4	O7Z	А	303	5/23	0.85	0.16	23,31,36,44	0
4	O7Z	D	305	5/23	0.86	0.13	$29,\!30,\!39,\!42$	0
3	MES	В	302	12/12	0.87	0.10	$20,\!27,\!37,\!38$	0
3	MES	D	303	12/12	0.89	0.20	30,38,44,51	0
4	O7Z	В	304	5/23	0.91	0.11	$27,\!30,\!38,\!47$	0
2	GSH	С	301	20/20	0.92	0.07	11,18,24,32	0
2	GSH	В	301	20/20	0.93	0.09	14,19,31,32	0
2	GSH	А	301	20/20	0.93	0.07	$12,\!17,\!25,\!30$	0
3	MES	С	302	12/12	0.94	0.08	22,26,40,43	0
3	MES	D	302	12/12	0.94	0.09	18,27,40,41	0
2	GSH	D	301	20/20	0.95	0.07	14,18,26,32	0
3	MES	А	302	12/12	0.95	0.12	20,27,37,39	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.

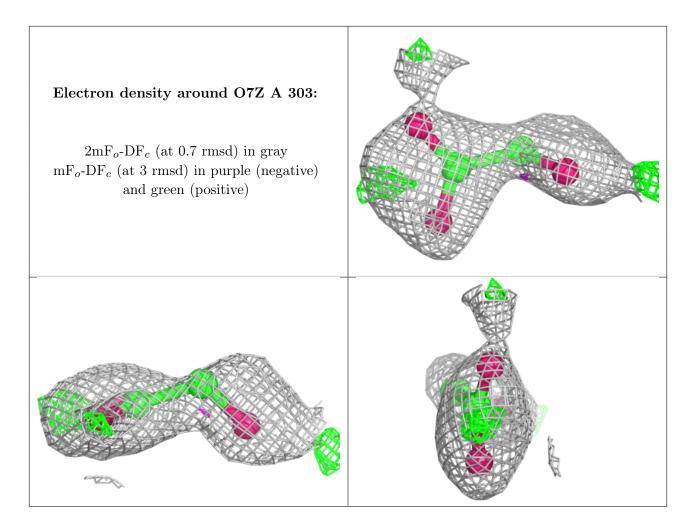




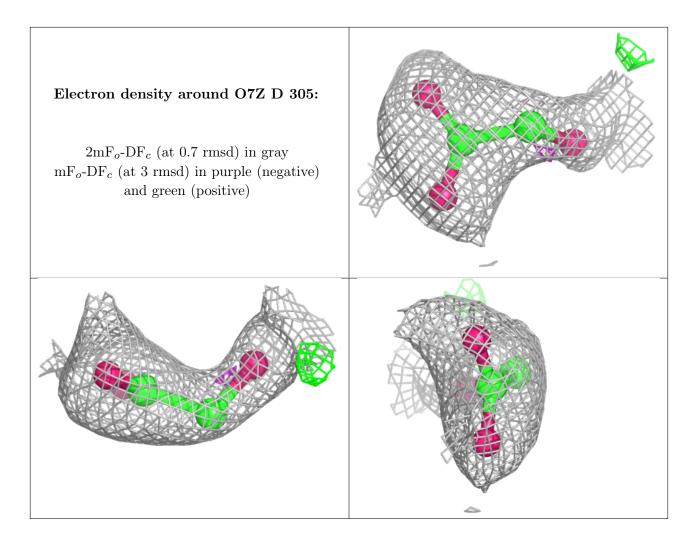




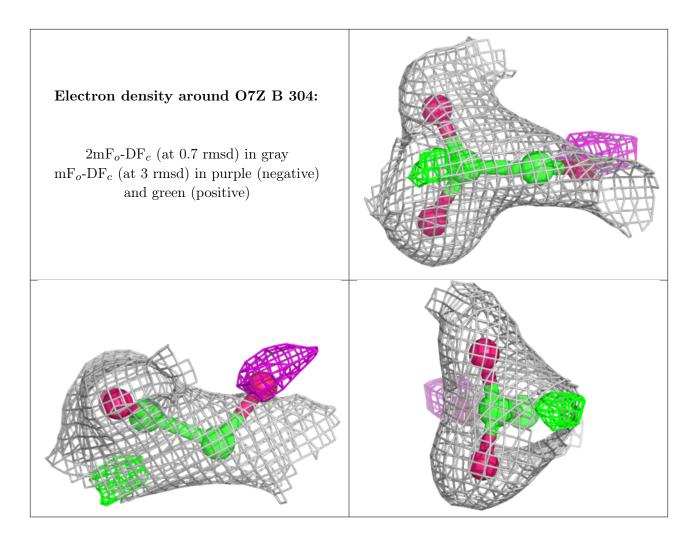




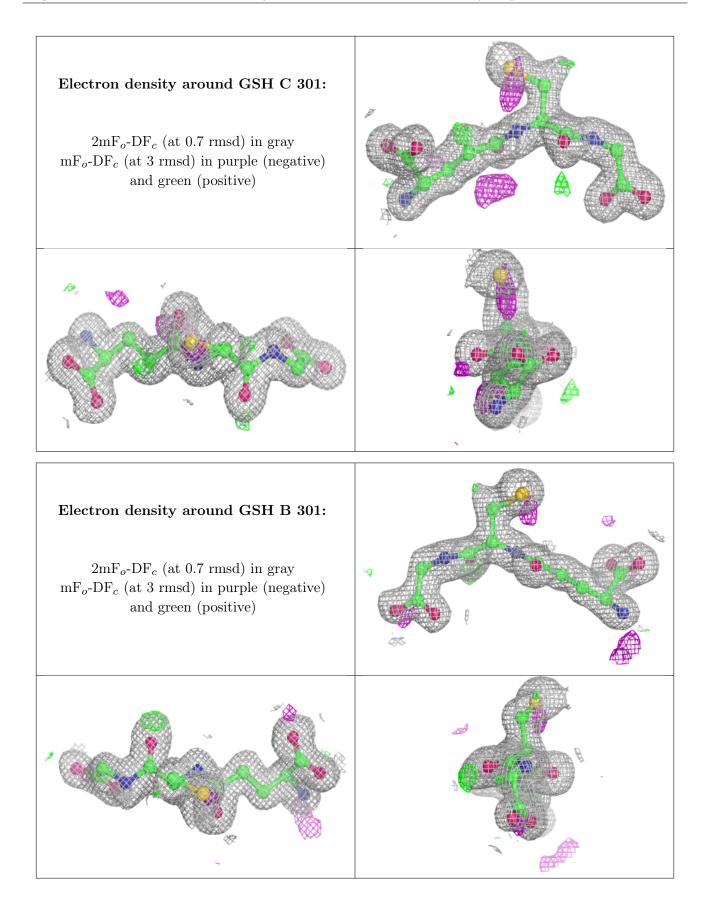




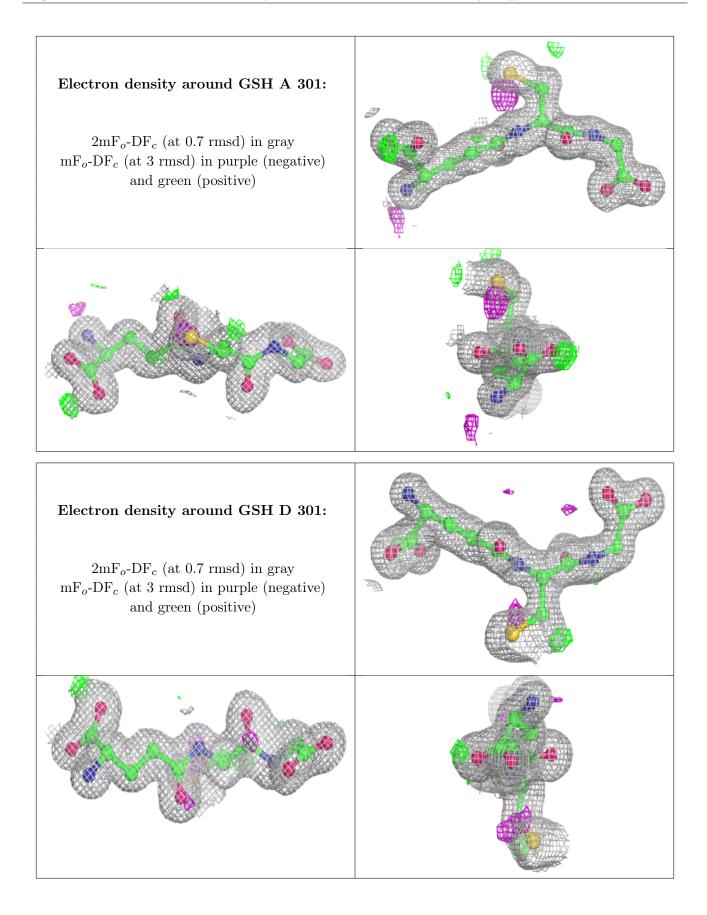














6.5 Other polymers (i)

There are no such residues in this entry.

