



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:22 AM UTC

PDB ID : 3VB0 / pdb\_00003vb0  
Title : Crystal structure of 2,2',3-trihydroxybiphenyl 1,2-dioxygenase from dibenzofuran-degrading *Sphingomonas wittichii* strain RW1  
Authors : Koksal, M.; Kumar, P.; Bolin, J.T.  
Deposited on : 2011-12-30  
Resolution : 2.10 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

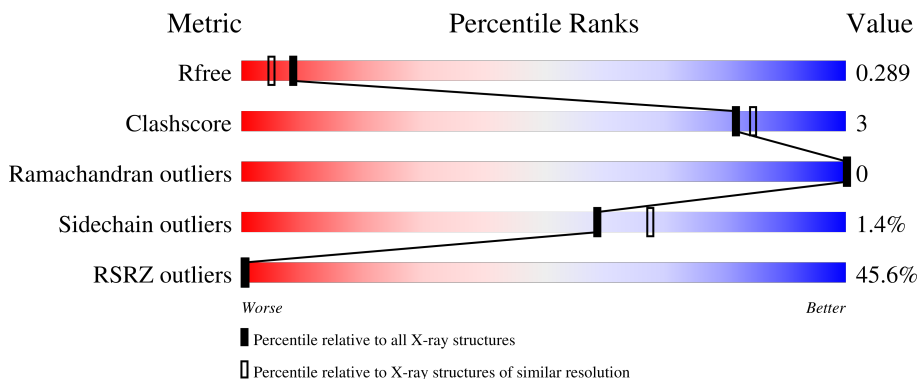
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	294	 8% 89% 9%
1	B	294	 9% 88% 10%
1	C	294	 78% 97%
1	D	294	 85% 98%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	P6G	B	302	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9162 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.

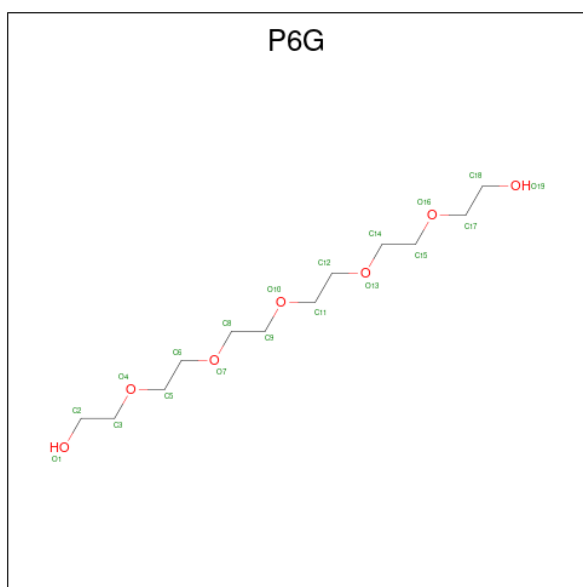
- Molecule 1 is a protein called Glyoxalase/bleomycin resistance protein/dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	2238	1429	384	415	10	0	0	0
1	B	289	2238	1429	384	415	10	0	0	0
1	C	289	2238	1429	384	415	10	0	0	0
1	D	289	2238	1429	384	415	10	0	0	0

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		
3	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

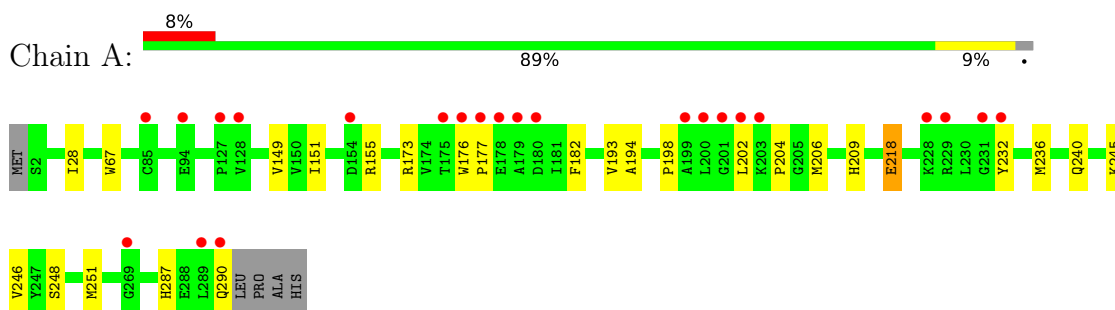
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	77	Total 77	O 77	0	0
5	B	80	Total 80	O 80	0	0
5	C	1	Total 1	O 1	0	0

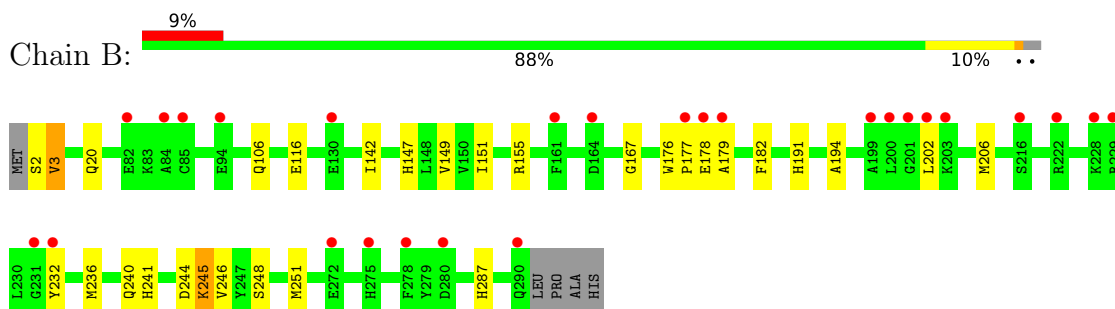
### 3 Residue-property plots [i](#)

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.

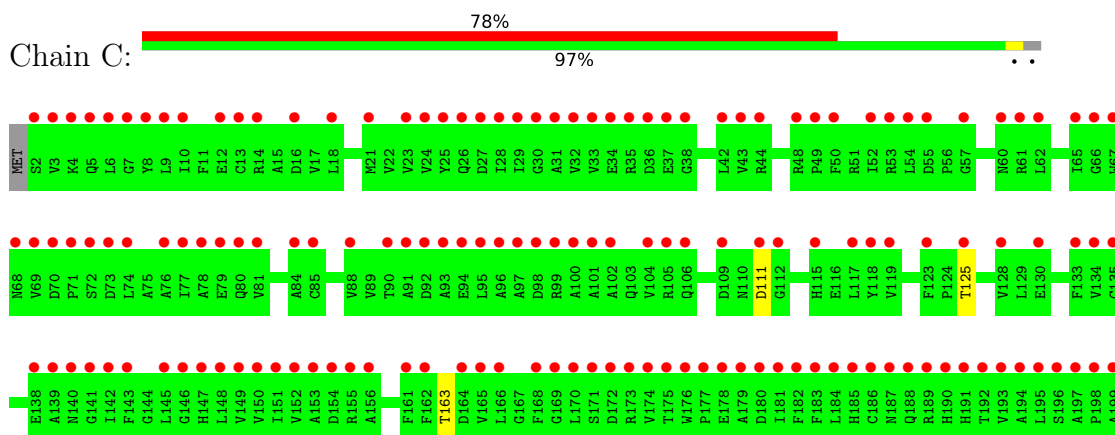
- Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase

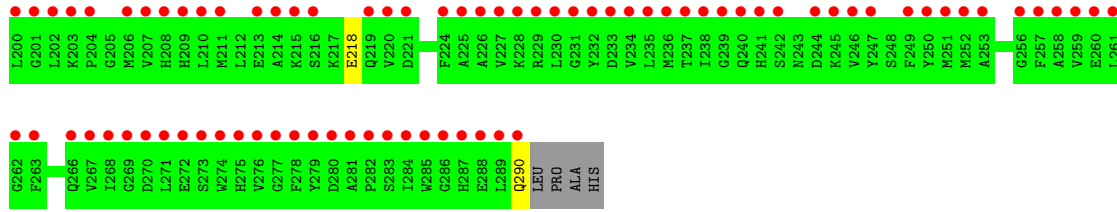


- Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase

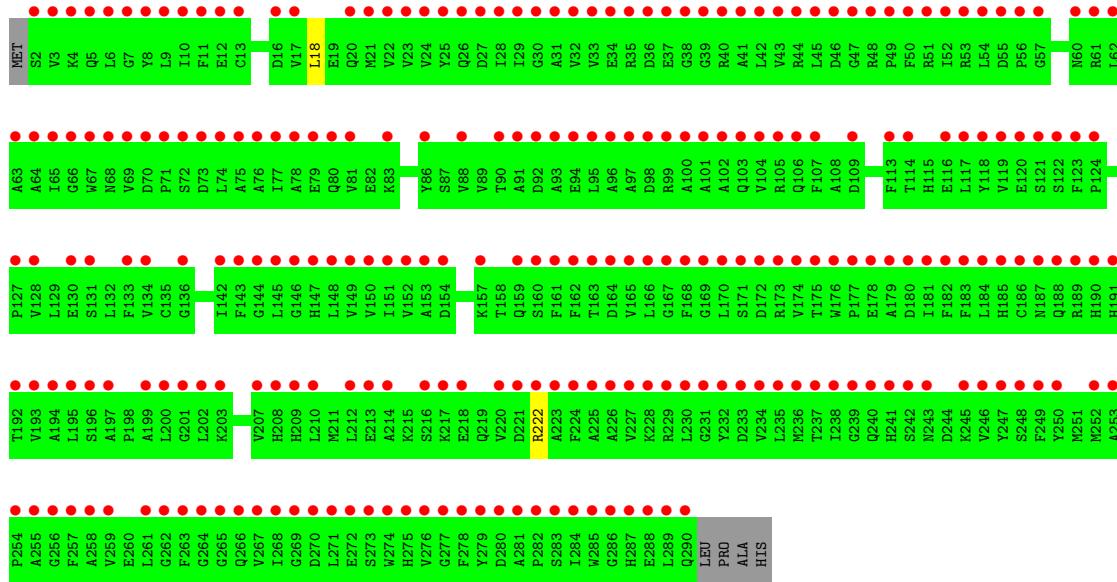
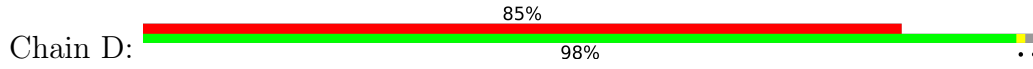


- Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase





● Molecule 1: Glyoxalase/bleomycin resistance protein/dioxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.59Å 131.59Å 103.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.85 – 2.10 92.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (92.85-2.10) 98.0 (92.85-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.254 , 0.289 0.254 , 0.289	Depositor DCC
$R_{free}$ test set	2647 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.169	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 70.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.40$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.87 % 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 2.9012e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P6G, FE2, SO4

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	0.64	0/2291	0.79	0/3111
1	B	0.67	1/2291 (0.0%)	0.79	0/3111
1	C	0.41	0/2291	0.71	0/3111
1	D	0.40	0/2291	0.71	0/3111
All	All	0.54	1/9164 (0.0%)	0.75	0/12444

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	VAL	CA-CB	5.64	1.59	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2238	0	2173	19	0
1	B	2238	0	2173	26	0
1	C	2238	0	2173	0	0
1	D	2238	0	2173	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	19	0	26	2	0
3	B	19	0	26	9	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	77	0	0	0	0
5	B	80	0	0	0	0
5	C	1	0	0	0	0
All	All	9162	0	8744	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.

All (45) 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:251:MET:HE3	3:B:302:P6G:H62	1.54	0.89
1:B:251:MET:HE3	3:B:302:P6G:C6	2.14	0.77
1:B:236:MET:HE3	1:B:287:HIS:HB3	1.70	0.74
1:A:232:TYR:CZ	3:A:302:P6G:H31	2.29	0.68
1:B:251:MET:CE	3:B:302:P6G:H62	2.23	0.67
1:B:149:VAL:HG22	1:B:194:ALA:HB3	1.80	0.63
1:B:232:TYR:CZ	3:B:302:P6G:H31	2.33	0.63
1:A:236:MET:HE3	1:A:287:HIS:HB3	1.79	0.63
1:B:176:TRP:NE1	1:B:178:GLU:HG2	2.17	0.60
1:A:202:LEU:HD22	1:A:206:MET:CE	2.32	0.59
1:A:149:VAL:HG22	1:A:194:ALA:HB3	1.86	0.56
1:B:232:TYR:CG	3:B:302:P6G:H51	2.41	0.56
1:A:173:ARG:HH11	1:A:182:PHE:HZ	1.53	0.56
1:B:202:LEU:HD22	1:B:206:MET:HE2	1.89	0.54
1:B:202:LEU:HD22	1:B:206:MET:CE	2.38	0.54
1:B:176:TRP:HB2	1:B:177:PRO:CD	2.37	0.54
1:B:246:VAL:HG12	1:B:248:SER:HB3	1.89	0.54
1:B:151:ILE:HG13	1:B:202:LEU:HB3	1.90	0.53
1:A:149:VAL:HG21	1:A:209:HIS:CE1	2.46	0.50
1:B:251:MET:CE	3:B:302:P6G:C6	2.85	0.50
1:A:218:GLU:H	1:A:218:GLU:CD	2.18	0.49
1:A:202:LEU:HD22	1:A:206:MET:HE2	1.93	0.49
1:B:236:MET:HE3	1:B:287:HIS:CB	2.42	0.48
1:B:251:MET:HE1	3:B:302:P6G:H52	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD22	1:A:206:MET:HE1	1.95	0.48
1:A:240:GLN:HA	1:A:246:VAL:O	2.14	0.47
1:B:106:GLN:HG3	1:B:116:GLU:HG2	1.97	0.47
1:B:155:ARG:HD3	1:B:182:PHE:CD2	2.51	0.46
1:B:232:TYR:CD2	3:B:302:P6G:H51	2.51	0.46
1:A:155:ARG:HD3	1:A:182:PHE:CD2	2.51	0.46
1:B:244:ASP:O	1:B:245:LYS:HB2	2.15	0.46
1:B:176:TRP:CH2	1:B:179:ALA:HB3	2.51	0.45
1:A:28:ILE:HG21	1:A:251:MET:HE1	1.98	0.45
1:B:20:GLN:HB3	3:B:302:P6G:H22	1.98	0.44
1:A:151:ILE:HG13	1:A:202:LEU:HB3	1.99	0.44
1:B:241:HIS:HB2	1:B:244:ASP:OD1	2.18	0.44
1:A:176:TRP:HB2	1:A:177:PRO:CD	2.49	0.43
1:B:2:SER:HB2	1:B:167:GLY:HA3	2.01	0.42
1:A:198:PRO:HG3	1:A:204:PRO:HD3	2.01	0.42
1:B:147:HIS:HB3	1:B:191:HIS:O	2.18	0.42
1:B:240:GLN:HA	1:B:246:VAL:O	2.19	0.42
1:A:176:TRP:HB2	1:A:177:PRO:HD2	2.00	0.42
1:A:232:TYR:CD2	3:A:302:P6G:H51	2.55	0.41
1:A:67:TRP:HH2	1:A:193:VAL:CG2	2.33	0.41
1:A:246:VAL:CG1	1:A:248:SER:HB3	2.52	0.41

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	287/294 (98%)	283 (99%)	4 (1%)	0	100	100
1	B	287/294 (98%)	281 (98%)	6 (2%)	0	100	100
1	C	287/294 (98%)	282 (98%)	5 (2%)	0	100	100
1	D	287/294 (98%)	282 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1148/1176 (98%)	1128 (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	Rotameric	Outliers	Percentiles	
1	A	231/235 (98%)	228 (99%)	3 (1%)	61	69
1	B	231/235 (98%)	228 (99%)	3 (1%)	61	69
1	C	231/235 (98%)	226 (98%)	5 (2%)	45	53
1	D	231/235 (98%)	229 (99%)	2 (1%)	70	78
All	All	924/940 (98%)	911 (99%)	13 (1%)	59	67

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	GLU
1	A	245	LYS
1	A	290	GLN
1	B	3	VAL
1	B	142	ILE
1	B	245	LYS
1	C	111	ASP
1	C	125	THR
1	C	163	THR
1	C	218	GLU
1	C	290	GLN
1	D	18	LEU
1	D	222	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	219	GLN
1	A	290	GLN
1	C	106	GLN
1	C	110	ASN
1	C	290	GLN
1	D	60	ASN
1	D	187	ASN
1	D	275	HIS

### 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	B	303	-	4,4,4	0.30	0	6,6,6	0.08	0
3	P6G	A	302	-	18,18,18	0.50	0	17,17,17	0.35	0
3	P6G	B	302	-	18,18,18	0.46	0	17,17,17	0.55	0
4	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.10	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	P6G	A	302	-	-	4/16/16/16	-
3	P6G	B	302	-	-	5/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

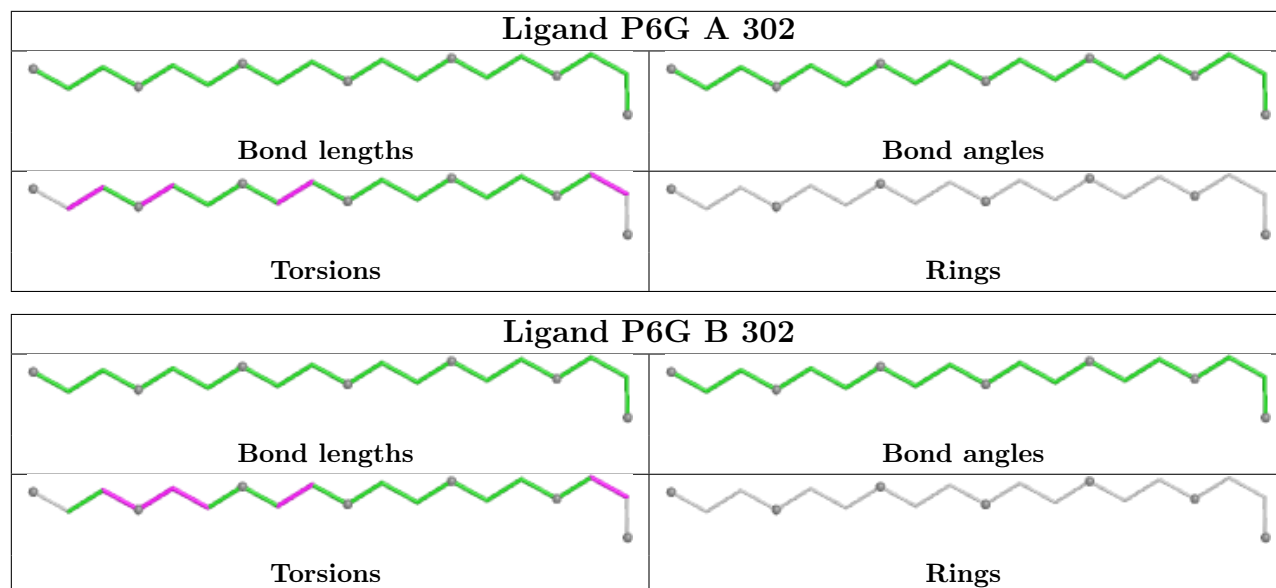
Mol	Chain	Res	Type	Atoms
3	A	302	P6G	O16-C17-C18-O19
3	A	302	P6G	O10-C11-C12-O13
3	B	302	P6G	C14-C15-O16-C17
3	B	302	P6G	C18-C17-O16-C15
3	B	302	P6G	O10-C11-C12-O13
3	B	302	P6G	O1-C2-C3-O4
3	A	302	P6G	C14-C15-O16-C17
3	B	302	P6G	O13-C14-C15-O16
3	A	302	P6G	O1-C2-C3-O4

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	P6G	2	0
3	B	302	P6G	9	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.



## 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	289/294 (98%)	0.53	23 (7%) 18 19	9, 18, 29, 36	289 (100%)
1	B	289/294 (98%)	0.68	26 (8%) 15 16	9, 18, 29, 36	289 (100%)
1	C	289/294 (98%)	4.70	228 (78%) 0 0	2, 5, 7, 9	289 (100%)
1	D	289/294 (98%)	4.38	250 (86%) 0 0	2, 4, 7, 9	289 (100%)
All	All	1156/1176 (98%)	2.57	527 (45%) 0 1	2, 9, 25, 36	1156 (100%)

All (527) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	200	LEU	16.1
1	C	231	GLY	15.1
1	C	216	SER	11.7
1	C	152	VAL	11.4
1	B	200	LEU	11.2
1	C	232	TYR	11.0
1	C	203	LYS	10.9
1	D	275	HIS	10.9
1	D	60	ASN	10.9
1	D	193	VAL	10.6
1	C	27	ASP	10.6
1	C	100	ALA	10.5
1	D	238	ILE	10.5
1	C	201	GLY	10.5
1	C	234	VAL	10.4
1	D	246	VAL	10.4
1	C	151	ILE	10.0
1	C	200	LEU	10.0
1	C	202	LEU	9.9
1	D	47	GLY	9.9
1	C	193	VAL	9.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	81	VAL	9.7
1	C	278	PHE	9.7
1	C	32	VAL	9.7
1	C	156	ALA	9.7
1	C	139	ALA	9.6
1	D	63	ALA	9.6
1	C	2	SER	9.5
1	C	96	ALA	9.2
1	C	31	ALA	9.2
1	C	10	ILE	9.2
1	D	265	GLY	9.2
1	C	91	ALA	9.1
1	C	169	GLY	9.0
1	D	178	GLU	9.0
1	C	285	TRP	8.8
1	C	154	ASP	8.8
1	C	28	ILE	8.6
1	C	230	LEU	8.6
1	D	231	GLY	8.6
1	C	49	PRO	8.5
1	C	239	GLY	8.5
1	C	267	VAL	8.5
1	C	180	ASP	8.5
1	D	148	LEU	8.5
1	D	30	GLY	8.5
1	C	214	ALA	8.4
1	C	93	ALA	8.3
1	C	257	PHE	8.2
1	C	244	ASP	8.2
1	C	199	ALA	8.2
1	C	111	ASP	8.2
1	D	91	ALA	8.2
1	D	234	VAL	8.1
1	C	226	ALA	8.1
1	C	197	ALA	8.0
1	C	153	ALA	8.0
1	D	201	GLY	7.9
1	D	166	LEU	7.9
1	D	271	LEU	7.9
1	D	276	VAL	7.9
1	A	200	LEU	7.9
1	D	267	VAL	7.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	43	VAL	7.8
1	D	61	ARG	7.7
1	C	227	VAL	7.7
1	C	146	GLY	7.7
1	C	118	TYR	7.7
1	D	12	GLU	7.6
1	C	237	THR	7.6
1	C	207	VAL	7.6
1	B	85	CYS	7.6
1	C	274	TRP	7.6
1	C	112	GLY	7.5
1	C	276	VAL	7.5
1	D	245	LYS	7.5
1	C	104	VAL	7.5
1	D	182	PHE	7.4
1	D	289	LEU	7.4
1	D	279	TYR	7.4
1	D	232	TYR	7.3
1	C	277	GLY	7.3
1	C	71	PRO	7.3
1	C	101	ALA	7.2
1	C	184	LEU	7.2
1	C	273	SER	7.2
1	C	70	ASP	7.2
1	C	176	TRP	7.2
1	C	229	ARG	7.2
1	C	233	ASP	7.2
1	C	228	LYS	7.1
1	D	65	ILE	7.1
1	D	38	GLY	7.1
1	D	29	ILE	7.1
1	D	149	VAL	7.0
1	C	95	LEU	7.0
1	D	123	PHE	6.9
1	C	74	LEU	6.9
1	C	289	LEU	6.9
1	D	67	TRP	6.9
1	D	268	ILE	6.8
1	C	275	HIS	6.8
1	D	278	PHE	6.8
1	D	269	GLY	6.8
1	D	117	LEU	6.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	273	SER	6.8
1	D	183	PHE	6.8
1	C	57	GLY	6.7
1	C	266	GLN	6.7
1	D	51	ARG	6.7
1	C	195	LEU	6.7
1	C	77	ILE	6.7
1	D	77	ILE	6.7
1	D	163	THR	6.7
1	C	250	TYR	6.6
1	D	145	LEU	6.6
1	C	38	GLY	6.6
1	D	144	GLY	6.6
1	C	253	ALA	6.6
1	C	186	CYS	6.6
1	C	170	LEU	6.6
1	C	98	ASP	6.5
1	C	194	ALA	6.5
1	C	9	LEU	6.5
1	C	290	GLN	6.5
1	C	189	ARG	6.5
1	C	187	ASN	6.5
1	D	33	VAL	6.5
1	C	269	GLY	6.4
1	C	149	VAL	6.4
1	D	122	SER	6.4
1	C	62	LEU	6.4
1	D	3	VAL	6.4
1	D	184	LEU	6.4
1	C	3	VAL	6.3
1	D	50	PHE	6.3
1	D	78	ALA	6.3
1	D	221	ASP	6.3
1	D	242	SER	6.3
1	C	135	CYS	6.2
1	C	284	ILE	6.2
1	D	247	TYR	6.2
1	C	204	PRO	6.2
1	D	208	HIS	6.2
1	D	179	ALA	6.2
1	D	220	VAL	6.2
1	D	27	ASP	6.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	177	PRO	6.1
1	C	235	LEU	6.1
1	D	62	LEU	6.1
1	D	162	PHE	6.1
1	D	22	VAL	6.1
1	C	13	CYS	6.1
1	C	97	ALA	6.1
1	D	180	ASP	6.0
1	D	228	LYS	6.0
1	D	270	ASP	6.0
1	D	97	ALA	5.9
1	C	210	LEU	5.9
1	C	271	LEU	5.9
1	C	168	PHE	5.9
1	C	90	THR	5.9
1	D	66	GLY	5.9
1	D	176	TRP	5.9
1	C	241	HIS	5.9
1	D	76	ALA	5.8
1	C	92	ASP	5.8
1	C	109	ASP	5.8
1	C	37	GLU	5.8
1	C	213	GLU	5.8
1	D	227	VAL	5.8
1	D	199	ALA	5.8
1	D	229	ARG	5.8
1	C	262	GLY	5.8
1	C	73	ASP	5.8
1	C	198	PRO	5.8
1	C	42	LEU	5.7
1	D	222	ARG	5.7
1	C	171	SER	5.7
1	C	26	GLN	5.7
1	D	23	VAL	5.7
1	D	46	ASP	5.6
1	C	165	VAL	5.6
1	D	230	LEU	5.6
1	C	287	HIS	5.6
1	C	36	ASP	5.6
1	D	187	ASN	5.6
1	D	75	ALA	5.6
1	D	31	ALA	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	254	PRO	5.6
1	D	171	SER	5.5
1	D	281	ALA	5.5
1	D	17	VAL	5.5
1	D	114	THR	5.5
1	D	64	ALA	5.5
1	C	150	VAL	5.5
1	C	166	LEU	5.5
1	C	259	VAL	5.5
1	D	192	THR	5.4
1	C	208	HIS	5.4
1	D	239	GLY	5.4
1	C	44	ARG	5.4
1	D	188	GLN	5.4
1	D	280	ASP	5.3
1	D	236	MET	5.3
1	D	274	TRP	5.3
1	D	283	SER	5.3
1	B	231	GLY	5.3
1	D	39	GLY	5.3
1	D	43	VAL	5.3
1	C	175	THR	5.3
1	D	255	ALA	5.3
1	C	30	GLY	5.3
1	D	170	LEU	5.3
1	C	99	ARG	5.2
1	C	21	MET	5.2
1	D	49	PRO	5.2
1	C	35	ARG	5.2
1	C	72	SER	5.2
1	C	258	ALA	5.2
1	D	226	ALA	5.2
1	C	164	ASP	5.2
1	D	109	ASP	5.2
1	D	2	SER	5.2
1	D	130	GLU	5.2
1	D	181	ILE	5.2
1	C	5	GLN	5.2
1	C	147	HIS	5.1
1	C	270	ASP	5.1
1	C	130	GLU	5.1
1	C	7	GLY	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	118	TYR	5.1
1	D	277	GLY	5.1
1	C	155	ARG	5.1
1	D	210	LEU	5.1
1	D	94	GLU	5.1
1	D	272	GLU	5.1
1	D	104	VAL	5.1
1	D	264	GLY	5.1
1	C	50	PHE	5.0
1	C	286	GLY	5.0
1	D	284	ILE	5.0
1	D	128	VAL	5.0
1	C	179	ALA	5.0
1	D	257	PHE	5.0
1	D	175	THR	5.0
1	C	279	TYR	5.0
1	C	34	GLU	4.9
1	D	88	VAL	4.9
1	D	165	VAL	4.9
1	C	161	PHE	4.9
1	C	251	MET	4.9
1	D	74	LEU	4.9
1	D	223	ALA	4.9
1	D	35	ARG	4.9
1	C	67	TRP	4.8
1	D	256	GLY	4.8
1	D	48	ARG	4.8
1	C	52	ILE	4.8
1	D	235	LEU	4.8
1	D	37	GLU	4.8
1	D	5	GLN	4.8
1	D	286	GLY	4.7
1	D	20	GLN	4.7
1	C	280	ASP	4.7
1	C	246	VAL	4.7
1	D	134	VAL	4.7
1	D	290	GLN	4.7
1	D	69	VAL	4.7
1	D	248	SER	4.7
1	D	237	THR	4.7
1	D	225	ALA	4.7
1	D	11	PHE	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	281	ALA	4.7
1	D	167	GLY	4.7
1	D	285	TRP	4.6
1	C	65	ILE	4.6
1	C	242	SER	4.6
1	C	206	MET	4.5
1	C	256	GLY	4.5
1	D	103	GLN	4.5
1	C	191	HIS	4.5
1	D	55	ASP	4.5
1	D	56	PRO	4.5
1	C	268	ILE	4.5
1	D	28	ILE	4.5
1	D	121	SER	4.5
1	D	113	PHE	4.5
1	D	266	GLN	4.5
1	C	33	VAL	4.5
1	D	186	CYS	4.5
1	C	174	VAL	4.4
1	D	101	ALA	4.4
1	D	95	LEU	4.4
1	C	125	THR	4.4
1	D	54	LEU	4.4
1	D	202	LEU	4.4
1	C	24	VAL	4.4
1	C	68	ASN	4.3
1	D	194	ALA	4.3
1	C	283	SER	4.3
1	D	131	SER	4.3
1	D	173	ARG	4.3
1	D	25	TYR	4.3
1	C	53	ARG	4.3
1	C	4	LYS	4.3
1	D	4	LYS	4.3
1	C	105	ARG	4.2
1	C	173	ARG	4.2
1	C	236	MET	4.2
1	D	36	ASP	4.2
1	D	8	TYR	4.2
1	C	8	TYR	4.2
1	C	12	GLU	4.1
1	D	249	PHE	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	252	MET	4.1
1	A	178	GLU	4.1
1	D	261	LEU	4.1
1	D	177	PRO	4.1
1	C	6	LEU	4.1
1	C	117	LEU	4.1
1	D	71	PRO	4.1
1	D	41	ALA	4.0
1	D	100	ALA	4.0
1	C	260	GLU	4.0
1	D	258	ALA	4.0
1	D	240	GLN	4.0
1	B	178	GLU	4.0
1	D	172	ASP	4.0
1	D	287	HIS	4.0
1	C	143	PHE	4.0
1	C	185	HIS	4.0
1	D	81	VAL	4.0
1	C	247	TYR	4.0
1	D	168	PHE	4.0
1	C	29	ILE	4.0
1	C	225	ALA	3.9
1	C	183	PHE	3.9
1	C	188	GLN	3.9
1	C	145	LEU	3.9
1	C	192	THR	3.9
1	D	24	VAL	3.9
1	C	209	HIS	3.9
1	C	172	ASP	3.9
1	C	288	GLU	3.9
1	D	159	GLN	3.9
1	C	55	ASP	3.8
1	D	93	ALA	3.8
1	D	233	ASP	3.8
1	D	7	GLY	3.8
1	C	196	SER	3.8
1	C	94	GLU	3.8
1	C	245	LYS	3.8
1	D	263	PHE	3.8
1	C	181	ILE	3.7
1	D	151	ILE	3.7
1	D	174	VAL	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	73	ASP	3.7
1	D	212	LEU	3.7
1	C	66	GLY	3.7
1	B	199	ALA	3.7
1	D	213	GLU	3.7
1	D	80	GLN	3.6
1	D	133	PHE	3.6
1	C	88	VAL	3.6
1	D	72	SER	3.6
1	D	92	ASP	3.6
1	B	275	HIS	3.6
1	D	127	PRO	3.5
1	D	241	HIS	3.5
1	B	290	GLN	3.5
1	C	219	GLN	3.5
1	C	48	ARG	3.5
1	B	202	LEU	3.5
1	D	250	TYR	3.5
1	D	157	LYS	3.5
1	D	42	LEU	3.5
1	D	169	GLY	3.5
1	D	282	PRO	3.4
1	D	40	ARG	3.4
1	C	115	HIS	3.4
1	C	142	ILE	3.4
1	C	141	GLY	3.4
1	D	224	PHE	3.4
1	C	261	LEU	3.4
1	C	23	VAL	3.4
1	D	44	ARG	3.4
1	D	99	ARG	3.4
1	B	94	GLU	3.4
1	D	102	ALA	3.4
1	D	106	GLN	3.3
1	A	231	GLY	3.3
1	A	232	TYR	3.3
1	D	52	ILE	3.3
1	B	130	GLU	3.3
1	C	272	GLU	3.3
1	A	176	TRP	3.3
1	D	160	SER	3.3
1	A	179	ALA	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	102	ALA	3.3
1	D	120	GLU	3.3
1	D	262	GLY	3.2
1	D	32	VAL	3.2
1	D	34	GLU	3.2
1	D	252	MET	3.2
1	D	70	ASP	3.2
1	A	85	CYS	3.2
1	C	128	VAL	3.2
1	C	84	ALA	3.2
1	D	96	ALA	3.2
1	C	138	GLU	3.2
1	D	119	VAL	3.2
1	C	240	GLN	3.2
1	D	6	LEU	3.2
1	D	10	ILE	3.2
1	D	124	PRO	3.2
1	C	140	ASN	3.2
1	D	191	HIS	3.1
1	A	177	PRO	3.1
1	D	218	GLU	3.1
1	C	190	HIS	3.1
1	D	13	CYS	3.1
1	B	84	ALA	3.1
1	A	202	LEU	3.1
1	C	78	ALA	3.1
1	C	282	PRO	3.0
1	B	164	ASP	3.0
1	D	68	ASN	3.0
1	C	249	PHE	3.0
1	A	94	GLU	3.0
1	D	79	GLU	3.0
1	D	21	MET	3.0
1	D	217	LYS	2.9
1	D	142	ILE	2.9
1	C	178	GLU	2.9
1	B	232	TYR	2.9
1	D	98	ASP	2.8
1	B	229	ARG	2.8
1	D	189	ARG	2.8
1	D	190	HIS	2.8
1	D	209	HIS	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	146	GLY	2.8
1	A	128	VAL	2.8
1	C	14	ARG	2.8
1	D	16	ASP	2.8
1	D	116	GLU	2.8
1	A	201	GLY	2.8
1	D	143	PHE	2.8
1	A	203	LYS	2.8
1	B	201	GLY	2.7
1	C	182	PHE	2.7
1	D	90	THR	2.7
1	C	85	CYS	2.7
1	D	243	ASN	2.7
1	C	54	LEU	2.7
1	C	61	ARG	2.7
1	D	26	GLN	2.7
1	D	214	ALA	2.7
1	D	152	VAL	2.7
1	B	272	GLU	2.6
1	B	177	PRO	2.6
1	D	259	VAL	2.6
1	D	105	ARG	2.6
1	C	211	MET	2.6
1	D	150	VAL	2.6
1	D	136	GLY	2.6
1	B	278	PHE	2.6
1	D	207	VAL	2.6
1	C	215	LYS	2.6
1	C	119	VAL	2.5
1	C	220	VAL	2.5
1	D	86	TYR	2.5
1	A	154	ASP	2.5
1	D	253	ALA	2.5
1	D	216	SER	2.5
1	C	134	VAL	2.5
1	D	288	GLU	2.5
1	C	18	LEU	2.5
1	D	45	LEU	2.5
1	A	269	GLY	2.5
1	C	69	VAL	2.5
1	B	203	LYS	2.4
1	B	222	ARG	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	57	GLY	2.4
1	D	161	PHE	2.4
1	A	180	ASP	2.4
1	B	216	SER	2.4
1	D	196	SER	2.4
1	B	179	ALA	2.4
1	D	197	ALA	2.4
1	B	82	GLU	2.4
1	A	290	GLN	2.4
1	C	80	GLN	2.4
1	D	203	LYS	2.4
1	D	9	LEU	2.3
1	A	228	LYS	2.3
1	A	199	ALA	2.3
1	A	289	LEU	2.3
1	C	60	ASN	2.3
1	B	228	LYS	2.3
1	D	83	LYS	2.3
1	D	185	HIS	2.2
1	A	127	PRO	2.2
1	A	175	THR	2.2
1	C	162	PHE	2.2
1	D	153	ALA	2.2
1	C	106	GLN	2.2
1	D	147	HIS	2.2
1	D	107	PHE	2.2
1	C	76	ALA	2.2
1	D	195	LEU	2.2
1	B	280	ASP	2.2
1	C	133	PHE	2.1
1	C	238	ILE	2.1
1	C	263	PHE	2.1
1	A	229	ARG	2.1
1	D	53	ARG	2.1
1	C	16	ASP	2.1
1	D	164	ASP	2.1
1	B	161	PHE	2.1
1	C	123	PHE	2.1
1	C	224	PHE	2.1
1	C	148	LEU	2.1
1	C	79	GLU	2.1
1	C	221	ASP	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	154	ASP	2.0
1	C	25	TYR	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

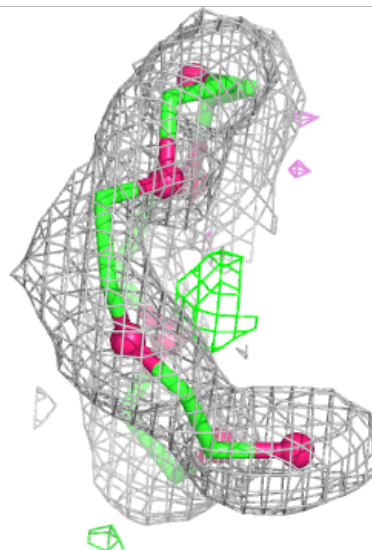
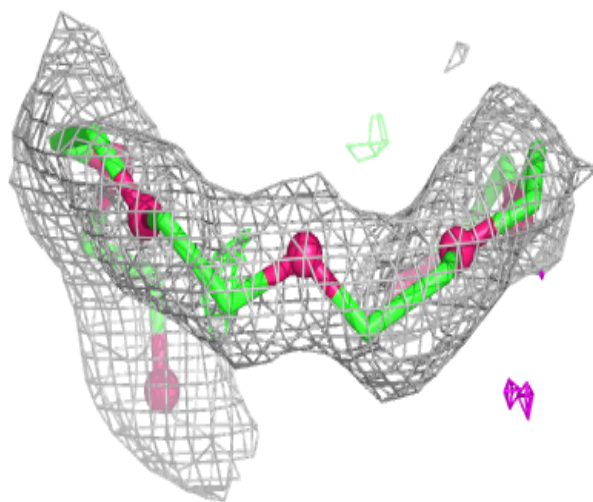
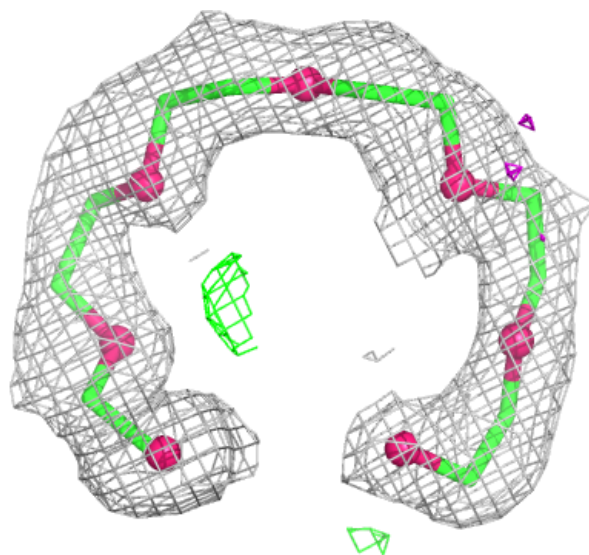
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

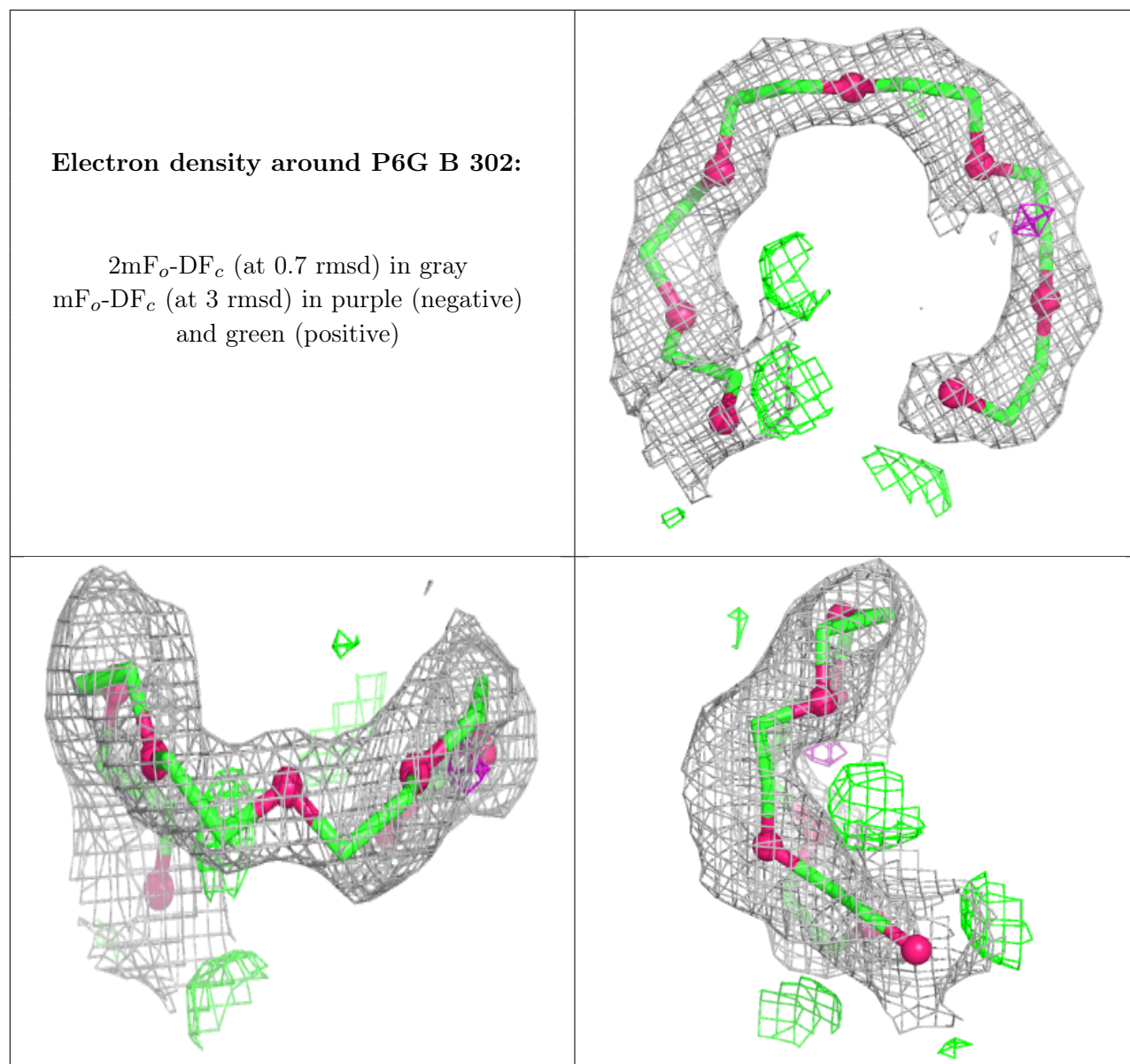
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	P6G	A	302	19/19	0.80	0.17	42,46,52,53	19
3	P6G	B	302	19/19	0.80	0.15	36,39,46,48	19
4	SO4	A	303	5/5	0.93	0.15	48,48,50,50	5
4	SO4	B	303	5/5	0.94	0.16	46,46,47,48	5
2	FE2	C	300	1/1	0.96	0.20	20,20,20,20	1
2	FE2	D	300	1/1	0.97	0.24	20,20,20,20	1
2	FE2	A	301	1/1	0.99	0.04	21,21,21,21	1
2	FE2	B	301	1/1	0.99	0.04	20,20,20,20	1

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 P6G A 302:**

$2mF_o-DF_c$  (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.