



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:57 pm BST

PDB ID : 5CEX  
Title : Crystal Structure of Fab 32H+109L, a putative precursor of the PGT121 family of potent HIV-1 antibodies  
Authors : Garces, F.; Wilson, I.A.  
Deposited on : 2015-07-07  
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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

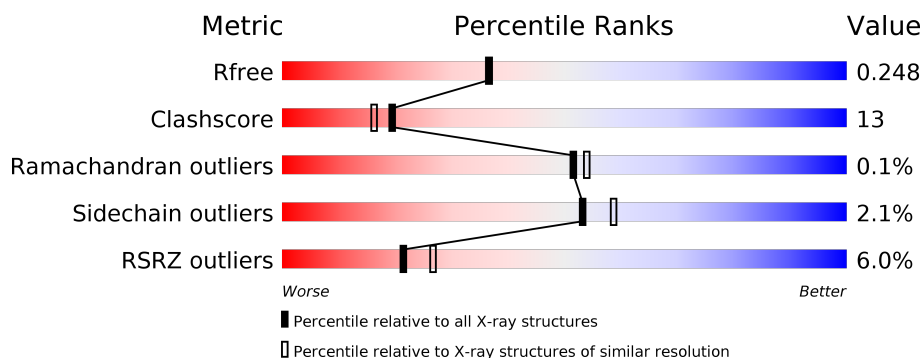
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on 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	218	<div> <div>10%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	C	218	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
2	B	236	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>•</div> </div> </div>
2	D	236	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PG4	A	301	-	-	X	-
3	PG4	C	305	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7033 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.

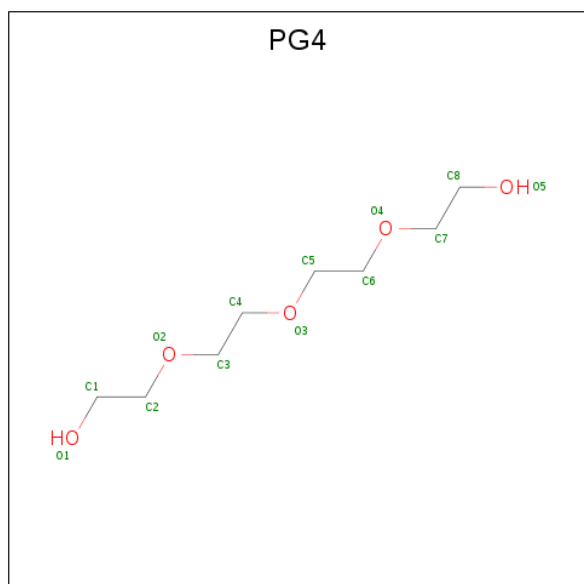
- Molecule 1 is a protein called Antibody 9H+3L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	1	0
			1567	981	268	313	5			
1	C	213	Total	C	N	O	S	0	2	0
			1620	1015	276	324	5			

- Molecule 2 is a protein called Antibody 9H+3L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1761	1116	293	347	5			
2	D	232	Total	C	N	O	S	0	1	0
			1758	1116	292	345	5			

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



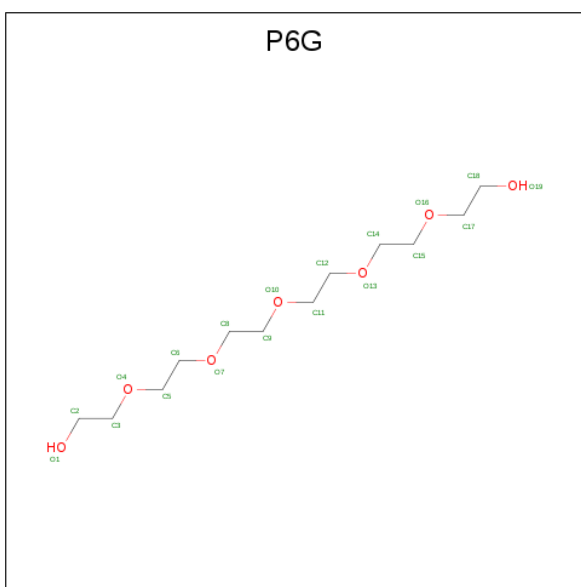
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	C	1	Total	C	O	0	0
			13	8	5		
3	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



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

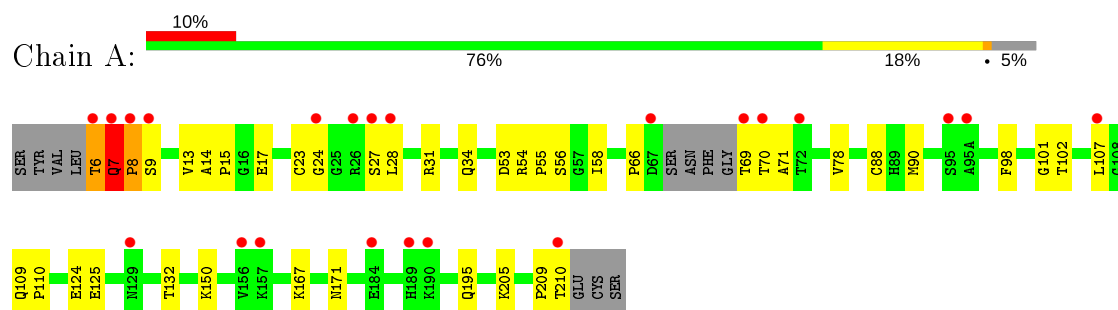
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	50	Total 50	O 50	0	0
7	B	46	Total 46	O 46	0	0
7	C	67	Total 67	O 67	0	0
7	D	53	Total 53	O 53	0	0

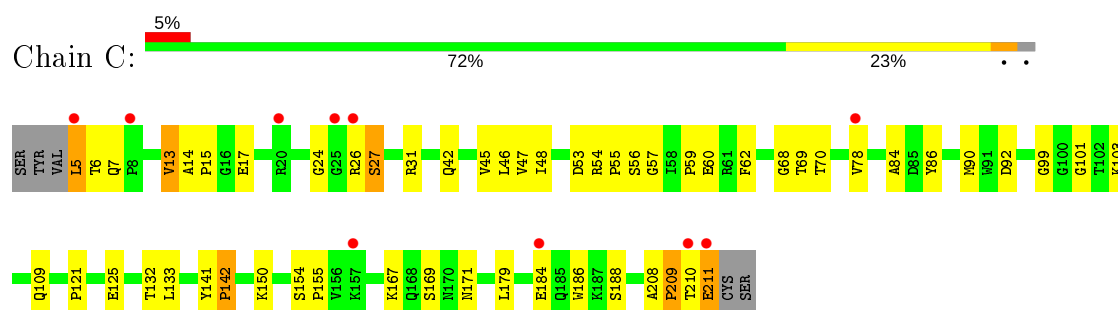
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

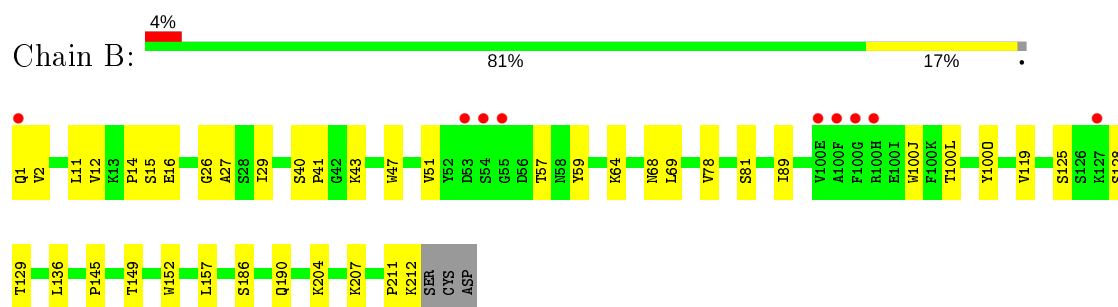
- Molecule 1: Antibody 9H+3L Fab light chain



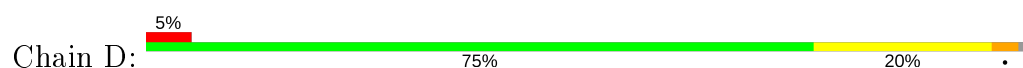
- Molecule 1: Antibody 9H+3L Fab light chain



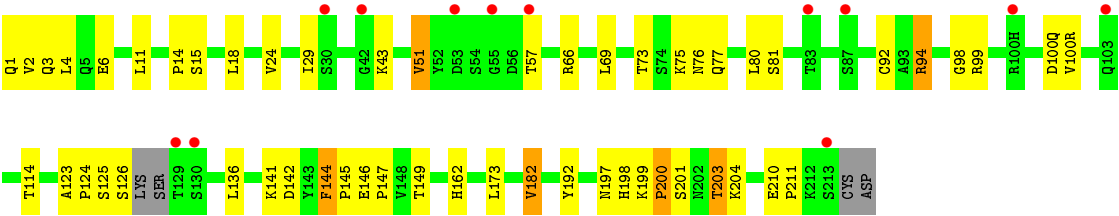
- Molecule 2: Antibody 9H+3L Fab heavy chain



- Molecule 2: Antibody 9H+3L Fab heavy chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.95Å 108.73Å 72.70Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	46.45 – 2.10 46.45 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.45-2.10) 98.0 (46.45-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.4 _1496	Depositor
R, $R_{free}$	0.200 , 0.244 0.219 , 0.248	Depositor DCC
$R_{free}$ test set	3171 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.034 for h,-k,-l 0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PG4, PGE, P6G

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	0.54	2/1609 (0.1%)	0.68	4/2197 (0.2%)
1	C	0.56	3/1664 (0.2%)	0.67	3/2274 (0.1%)
2	B	0.49	0/1808	0.62	1/2472 (0.0%)
2	D	0.61	4/1807 (0.2%)	0.74	7/2468 (0.3%)
All	All	0.55	9/6888 (0.1%)	0.68	15/9411 (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
2	D	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	142	PRO	N-CD	5.86	1.56	1.47
2	D	147	PRO	N-CD	5.21	1.55	1.47
2	D	124	PRO	N-CD	5.19	1.55	1.47
2	D	211	PRO	N-CD	5.15	1.55	1.47
1	C	209	PRO	N-CD	5.14	1.55	1.47
1	C	15	PRO	N-CD	5.13	1.55	1.47
2	D	200	PRO	N-CD	5.12	1.55	1.47
1	A	110	PRO	N-CD	5.09	1.54	1.47
1	A	8	PRO	N-CD	5.05	1.54	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ALA	O-C-N	-8.60	108.94	122.70
2	D	136	LEU	CA-CB-CG	8.58	135.03	115.30
1	A	71	ALA	CA-C-N	7.33	133.33	117.20
1	A	7	GLN	C-N-CD	5.84	140.66	128.40
2	B	136	LEU	CA-CB-CG	5.82	128.69	115.30
1	C	7	GLN	C-N-CD	5.82	140.62	128.40
2	D	182	VAL	C-N-CD	5.63	140.24	128.40
1	A	109	GLN	C-N-CD	5.55	140.05	128.40
1	C	208	ALA	C-N-CD	5.52	139.99	128.40
1	C	14	ALA	C-N-CD	5.51	139.98	128.40
2	D	123	ALA	C-N-CD	5.47	139.90	128.40
2	D	199	LYS	C-N-CD	5.47	139.89	128.40
2	D	210	GLU	C-N-CD	5.46	139.86	128.40
2	D	147	PRO	CA-N-CD	-5.38	103.97	111.50
2	D	146	GLU	C-N-CD	5.24	139.40	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	144	PHE	Peptide

## 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	1567	0	1516	42	0
1	C	1620	0	1571	66	0
2	B	1761	0	1717	43	0
2	D	1758	0	1719	37	0
3	A	13	0	18	11	0
3	C	26	0	36	12	0
4	B	6	0	8	0	0
4	C	18	0	24	5	0
5	B	19	0	26	4	0
5	C	19	0	26	7	0
6	C	10	0	14	1	0
7	A	50	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	46	0	0	1	0
7	C	67	0	0	0	0
7	D	53	0	0	2	0
All	All	7033	0	6675	173	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 13.

All (173) 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)
2:B:1:GLN:HE21	1:C:57:GLY:CA	1.55	1.17
1:A:7:GLN:HG3	1:A:101:GLY:H	1.11	1.14
2:B:1:GLN:NE2	1:C:57:GLY:HA2	1.66	1.08
2:B:1:GLN:NE2	1:C:57:GLY:CA	2.21	1.04
2:D:94:ARG:NH1	7:D:301:HOH:O	1.93	1.00
2:B:125:SER:O	2:B:129:THR:HG23	1.62	1.00
2:B:1:GLN:HE21	1:C:57:GLY:C	1.65	0.98
1:A:15:PRO:HD3	1:A:107:LEU:O	1.64	0.97
1:C:42:GLN:HE21	5:C:304:P6G:H31	1.28	0.96
1:C:45:VAL:HG13	3:C:305:PG4:H11	1.45	0.95
1:C:6:THR:O	1:C:24:GLY:HA2	1.69	0.92
1:A:7:GLN:HG3	1:A:101:GLY:N	1.85	0.90
1:A:7:GLN:CG	1:A:101:GLY:H	1.86	0.89
2:B:1:GLN:NE2	1:C:57:GLY:O	2.06	0.88
2:B:1:GLN:HG2	1:C:57:GLY:CA	2.05	0.85
1:C:27:SER:OG	1:C:92:ASP:OD1	1.95	0.85
1:A:54:ARG:HH12	3:A:301:PG4:H12	1.40	0.85
1:A:54:ARG:H	3:A:301:PG4:H52	1.43	0.82
1:C:13:VAL:CG1	1:C:78:VAL:HG21	2.10	0.82
2:B:1:GLN:HG2	1:C:57:GLY:C	2.04	0.78
1:C:53:ASP:HA	4:C:303:GOL:H31	1.66	0.76
2:D:201:SER:OG	2:D:203:THR:HG23	1.85	0.76
1:A:7:GLN:NE2	1:A:88:CYS:SG	2.60	0.74
2:B:2:VAL:HG12	2:B:27:ALA:HB2	1.67	0.74
3:A:301:PG4:H62	2:D:99:ARG:H	1.52	0.74
2:B:1:GLN:CD	1:C:57:GLY:HA2	2.07	0.74
1:C:209:PRO:O	1:C:211:GLU:HG3	1.88	0.73
2:B:125:SER:N	2:B:128:SER:OG	2.12	0.72
1:C:133[B]:LEU:HD12	1:C:179:LEU:HD23	1.71	0.71
2:D:142:ASP:HB3	2:D:173:LEU:HD13	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NH2	1:A:66:PRO:O	2.23	0.71
2:B:1:GLN:CG	1:C:57:GLY:C	2.59	0.70
1:A:7:GLN:OE1	1:A:101:GLY:HA2	1.92	0.70
2:B:89:ILE:CD1	5:B:302:P6G:H21	2.21	0.69
1:A:125:GLU:OE1	7:A:401:HOH:O	2.10	0.69
2:D:2:VAL:HG23	2:D:100(R):VAL:HG11	1.74	0.69
1:C:5:LEU:HD11	1:C:90:MET:HB3	1.74	0.69
3:A:301:PG4:H62	2:D:98:GLY:HA2	1.74	0.69
2:D:51:VAL:HG12	2:D:57:THR:HG22	1.73	0.68
1:C:57:GLY:H	3:C:306:PG4:H12	1.59	0.68
2:B:1:GLN:HG2	1:C:57:GLY:HA2	1.75	0.68
1:C:46:LEU:O	3:C:305:PG4:H22	1.93	0.67
1:C:6:THR:O	1:C:24:GLY:CA	2.43	0.67
2:B:186:SER:HB2	2:B:190:GLN:HG3	1.77	0.66
1:C:59:PRO:HB3	4:C:302:GOL:H32	1.76	0.66
2:B:125:SER:H	2:B:128:SER:HG	1.42	0.66
1:C:42:GLN:HE22	5:C:304:P6G:H92	1.60	0.65
2:B:89:ILE:HD13	5:B:302:P6G:H21	1.78	0.65
1:C:184:GLU:O	1:C:188:SER:OG	2.13	0.65
2:B:1:GLN:CG	1:C:57:GLY:HA2	2.27	0.64
1:A:54:ARG:N	3:A:301:PG4:H52	2.13	0.63
1:A:27:SER:O	1:A:69:THR:HG22	1.97	0.63
3:C:305:PG4:H52	2:D:100(Q):ASP:OD2	1.99	0.63
2:D:2:VAL:CG2	2:D:100(R):VAL:HG21	2.29	0.63
2:B:51:VAL:HG23	2:B:57:THR:HG22	1.81	0.62
1:C:5:LEU:HB3	1:C:99:GLY:HA2	1.81	0.62
6:C:307:PGE:O1	6:C:307:PGE:H3	1.98	0.62
2:B:100(J):TRP:HZ3	2:B:100(L):THR:HG23	1.64	0.62
2:B:1:GLN:CG	1:C:57:GLY:CA	2.78	0.62
1:C:13:VAL:HG11	1:C:78:VAL:HG21	1.81	0.61
1:C:42:GLN:HE21	5:C:304:P6G:C3	2.09	0.61
1:C:13:VAL:HG13	1:C:17:GLU:HG2	1.82	0.61
1:A:209:PRO:O	1:A:210:THR:HG23	2.01	0.61
2:B:119:VAL:HG23	2:B:207:LYS:HG3	1.82	0.61
1:A:53:ASP:OD1	3:A:301:PG4:H61	2.01	0.60
1:C:13:VAL:HG12	1:C:78:VAL:HG21	1.84	0.60
1:A:69:THR:O	1:A:70:THR:HG22	2.01	0.60
1:A:70:THR:HG23	1:A:70:THR:O	2.01	0.60
3:A:301:PG4:H62	2:D:99:ARG:N	2.15	0.59
2:B:11:LEU:HB2	2:B:145:PRO:HG3	1.83	0.59
1:C:31:ARG:HH12	1:C:69:THR:HB	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:197:ASN:OD1	2:D:204:LYS:HE2	2.03	0.58
1:C:57:GLY:N	3:C:306:PG4:H12	2.18	0.58
2:D:2:VAL:HG21	2:D:100(R):VAL:HG21	1.86	0.58
1:C:5:LEU:HD11	1:C:90:MET:CB	2.34	0.58
1:C:42:GLN:NE2	5:C:304:PG6:H31	2.09	0.57
1:A:53:ASP:OD1	2:D:99:ARG:HD3	2.04	0.57
2:D:149[B]:THR:OG1	2:D:197:ASN:HB3	2.05	0.57
1:A:27:SER:HB2	1:A:90:MET:SD	2.45	0.57
2:B:125:SER:O	2:B:128:SER:N	2.38	0.56
1:C:210:THR:C	1:C:211:GLU:HG3	2.24	0.56
2:D:66:ARG:NH2	7:D:303:HOH:O	2.38	0.56
1:A:125:GLU:OE2	1:A:132:THR:HG23	2.06	0.55
1:C:26:ARG:HD2	1:C:68:GLY:O	2.04	0.55
2:D:182:VAL:HG11	2:D:192:TYR:OH	2.06	0.55
1:C:141:TYR:CG	1:C:142:PRO:HA	2.43	0.54
1:A:167:LYS:HE2	1:A:171:ASN:HA	1.90	0.54
3:A:301:PG4:H62	2:D:98:GLY:CA	2.37	0.54
1:C:121:PRO:HD3	1:C:133[B]:LEU:HD23	1.90	0.54
2:D:6:GLU:HG3	2:D:92:CYS:SG	2.48	0.54
1:A:15:PRO:CD	1:A:107:LEU:O	2.50	0.53
2:D:198:HIS:CD2	2:D:200:PRO:HD2	2.43	0.53
2:B:1:GLN:NE2	1:C:57:GLY:C	2.41	0.53
2:D:75:LYS:HB2	2:D:77:GLN:HG2	1.89	0.53
2:D:3:GLN:C	2:D:4:LEU:HD23	2.29	0.53
2:B:2:VAL:HG13	7:B:425:HOH:O	2.09	0.52
2:D:125:SER:O	2:D:126:SER:HB3	2.10	0.51
2:D:24:VAL:HG22	2:D:76:ASN:ND2	2.26	0.51
2:B:152:TRP:HB3	2:B:157:LEU:HD23	1.91	0.51
2:B:211:PRO:O	2:B:212:LYS:HB2	2.10	0.51
1:A:56:SER:O	3:C:306:PG4:H72	2.11	0.51
1:A:13:VAL:CG1	1:A:78:VAL:HG21	2.40	0.50
2:B:40:SER:HB2	2:B:43:LYS:HG3	1.93	0.50
2:B:2:VAL:HG12	2:B:27:ALA:CB	2.39	0.50
3:A:301:PG4:C6	2:D:99:ARG:H	2.23	0.49
1:A:53:ASP:HA	3:A:301:PG4:H42	1.94	0.49
1:C:56:SER:OG	3:C:306:PG4:H32	2.12	0.49
1:A:98:PHE:HE1	2:B:47:TRP:HB2	1.78	0.48
1:C:69:THR:HG22	1:C:70:THR:N	2.28	0.48
1:C:47:VAL:HG12	1:C:48:ILE:HG12	1.93	0.48
1:A:209:PRO:O	1:A:210:THR:CG2	2.61	0.48
1:C:55:PRO:HB2	3:C:305:PG4:H42	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:204:LYS:HB2	2:D:204:LYS:HE3	1.61	0.47
2:D:144:PHE:HA	2:D:145:PRO:HA	1.67	0.47
1:A:23:CYS:SG	1:A:24:GLY:N	2.88	0.46
1:C:103:LYS:HG3	4:C:301:GOL:H32	1.97	0.46
1:A:27:SER:HB3	1:A:69:THR:N	2.31	0.46
1:A:150:LYS:HE2	1:A:195:GLN:OE1	2.15	0.46
1:C:109:GLN:HB2	1:C:141:TYR:CE1	2.50	0.46
5:C:304:P6G:H62	5:C:304:P6G:H92	1.44	0.45
1:C:169:SER:HA	5:C:304:P6G:H61	1.97	0.45
1:C:59:PRO:CB	4:C:302:GOL:H32	2.46	0.45
1:C:125:GLU:OE2	1:C:132:THR:HG23	2.17	0.45
1:A:8:PRO:O	1:A:102:THR:HA	2.17	0.45
2:B:29:ILE:HA	2:B:29:ILE:HD12	1.76	0.45
1:C:186:TRP:O	1:C:209:PRO:HG2	2.17	0.44
1:A:13:VAL:HG12	1:A:78:VAL:HG21	1.98	0.44
1:A:6:THR:CB	1:A:24:GLY:HA3	2.47	0.44
1:A:6:THR:HB	1:A:24:GLY:HA3	1.99	0.44
2:B:26:GLY:O	1:C:60:GLU:HG3	2.16	0.44
1:C:42:GLN:NE2	5:C:304:P6G:H62	2.32	0.44
1:C:54:ARG:NE	1:C:62:PHE:O	2.47	0.44
1:C:26:ARG:O	1:C:27:SER:HB3	2.18	0.44
1:A:14:ALA:O	1:A:17:GLU:HG2	2.17	0.44
2:B:68:ASN:HB3	2:B:81:SER:OG	2.18	0.43
1:C:210:THR:C	1:C:211:GLU:CG	2.85	0.43
2:D:11:LEU:HD22	2:D:114:THR:HG22	2.00	0.43
2:B:204:LYS:HE3	2:B:204:LYS:HB2	1.80	0.43
1:C:121:PRO:HD3	1:C:133[B]:LEU:CD2	2.49	0.43
1:C:5:LEU:HB3	1:C:99:GLY:CA	2.47	0.43
2:D:182:VAL:CG1	2:D:192:TYR:OH	2.66	0.43
3:A:301:PG4:H71	2:D:98:GLY:HA3	2.01	0.43
2:B:100(J):TRP:HZ3	2:B:100(L):THR:CG2	2.32	0.42
1:C:150:LYS:HD3	1:C:155:PRO:HA	2.01	0.42
1:C:56:SER:HA	3:C:306:PG4:H32	2.01	0.42
1:A:17:GLU:O	1:A:78:VAL:HG22	2.19	0.42
2:D:4:LEU:N	2:D:4:LEU:HD23	2.34	0.42
2:B:29:ILE:HD11	2:B:78:VAL:HG23	2.02	0.42
2:D:18:LEU:O	2:D:81:SER:HA	2.20	0.42
2:D:69:LEU:CD2	2:D:80:LEU:HD13	2.49	0.42
1:A:55:PRO:HD2	1:A:58:ILE:HG13	2.01	0.42
2:B:41:PRO:CG	5:B:302:P6G:H152	2.49	0.42
1:A:56:SER:O	3:C:305:PG4:H72	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:ILE:HD12	5:B:302:P6G:H21	1.99	0.42
2:D:144:PHE:O	2:D:198:HIS:CE1	2.73	0.42
2:D:14:PRO:O	2:D:15:SER:HB2	2.20	0.42
2:D:29:ILE:HD11	2:D:73:THR:HA	2.02	0.42
1:C:154:SER:HA	1:C:155:PRO:HD3	1.88	0.41
1:C:55:PRO:HB3	3:C:305:PG4:H62	2.03	0.41
2:D:182:VAL:HG11	2:D:192:TYR:CZ	2.55	0.41
1:A:34:GLN:HG2	2:B:100(O):TYR:HB3	2.03	0.41
1:A:7:GLN:OE1	1:A:101:GLY:CA	2.67	0.41
2:B:14:PRO:O	2:B:15:SER:HB2	2.21	0.41
1:C:84:ALA:HA	4:C:301:GOL:H12	2.02	0.41
1:A:28:LEU:HD12	1:A:28:LEU:HA	1.96	0.41
2:B:12:VAL:HG13	2:B:16:GLU:OE1	2.20	0.41
1:A:7:GLN:HG3	1:A:101:GLY:CA	2.50	0.41
1:C:167:LYS:HE2	1:C:171:ASN:HA	2.02	0.41
3:C:305:PG4:O1	2:D:100(Q):ASP:O	2.33	0.40
2:B:59:TYR:HE1	2:B:69:LEU:HG	1.86	0.40
1:C:17:GLU:O	1:C:78:VAL:HG22	2.20	0.40
1:C:86:TYR:O	1:C:101:GLY:HA2	2.21	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	204/218 (94%)	198 (97%)	6 (3%)	0	100	100
1	C	213/218 (98%)	210 (99%)	2 (1%)	1 (0%)	29	26
2	B	231/236 (98%)	228 (99%)	3 (1%)	0	100	100
2	D	229/236 (97%)	224 (98%)	5 (2%)	0	100	100
All	All	877/908 (97%)	860 (98%)	16 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	27	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	173/183 (94%)	169 (98%)	4 (2%)	50	55
1	C	180/183 (98%)	177 (98%)	3 (2%)	60	67
2	B	200/204 (98%)	198 (99%)	2 (1%)	76	82
2	D	201/204 (98%)	194 (96%)	7 (4%)	36	38
All	All	754/774 (97%)	738 (98%)	16 (2%)	53	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	7	GLN
1	A	9	SER
1	A	205	LYS
2	B	64	LYS
2	B	149	THR
1	C	5	LEU
1	C	13	VAL
1	C	211	GLU
2	D	1	GLN
2	D	43	LYS
2	D	51	VAL
2	D	94	ARG
2	D	141	LYS
2	D	162	HIS
2	D	203	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1	GLN
1	C	42	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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	PG4	C	305	-	12,12,12	0.86	0	11,11,11	0.44	0
4	GOL	C	303	-	5,5,5	0.24	0	5,5,5	0.30	0
3	PG4	A	301	-	12,12,12	0.83	0	11,11,11	0.73	0
4	GOL	B	301	-	5,5,5	0.38	0	5,5,5	0.63	0
4	GOL	C	301	-	5,5,5	0.21	0	5,5,5	0.25	0
4	GOL	C	302	-	5,5,5	0.18	0	5,5,5	0.49	0
6	PGE	C	307	-	9,9,9	0.28	0	8,8,8	0.60	0
5	P6G	C	304	-	18,18,18	0.79	0	17,17,17	0.41	0
5	P6G	B	302	-	18,18,18	0.46	0	17,17,17	0.25	0
3	PG4	C	306	-	12,12,12	0.40	0	11,11,11	0.22	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	PG4	C	305	-	-	6/10/10/10	-
4	GOL	C	303	-	-	3/4/4/4	-
3	PG4	A	301	-	-	6/10/10/10	-
4	GOL	B	301	-	-	2/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-
4	GOL	C	302	-	-	0/4/4/4	-
6	PGE	C	307	-	-	4/7/7/7	-
5	P6G	C	304	-	-	7/16/16/16	-
5	P6G	B	302	-	-	11/16/16/16	-
3	PG4	C	306	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	303	GOL	O1-C1-C2-C3
4	B	301	GOL	C1-C2-C3-O3
4	C	301	GOL	C1-C2-C3-O3
5	C	304	P6G	C9-C8-O7-C6
3	C	305	PG4	C6-C5-O3-C4
3	C	306	PG4	O2-C3-C4-O3
3	C	306	PG4	O3-C5-C6-O4
5	C	304	P6G	O7-C8-C9-O10
3	C	305	PG4	C5-C6-O4-C7
3	C	305	PG4	O3-C5-C6-O4
3	C	305	PG4	O4-C7-C8-O5
5	B	302	P6G	O1-C2-C3-O4
5	C	304	P6G	O10-C11-C12-O13
3	A	301	PG4	O2-C3-C4-O3
4	B	301	GOL	O2-C2-C3-O3
4	C	301	GOL	O2-C2-C3-O3
5	B	302	P6G	O4-C5-C6-O7
5	C	304	P6G	O1-C2-C3-O4
6	C	307	PGE	C1-C2-O2-C3
5	C	304	P6G	O4-C5-C6-O7

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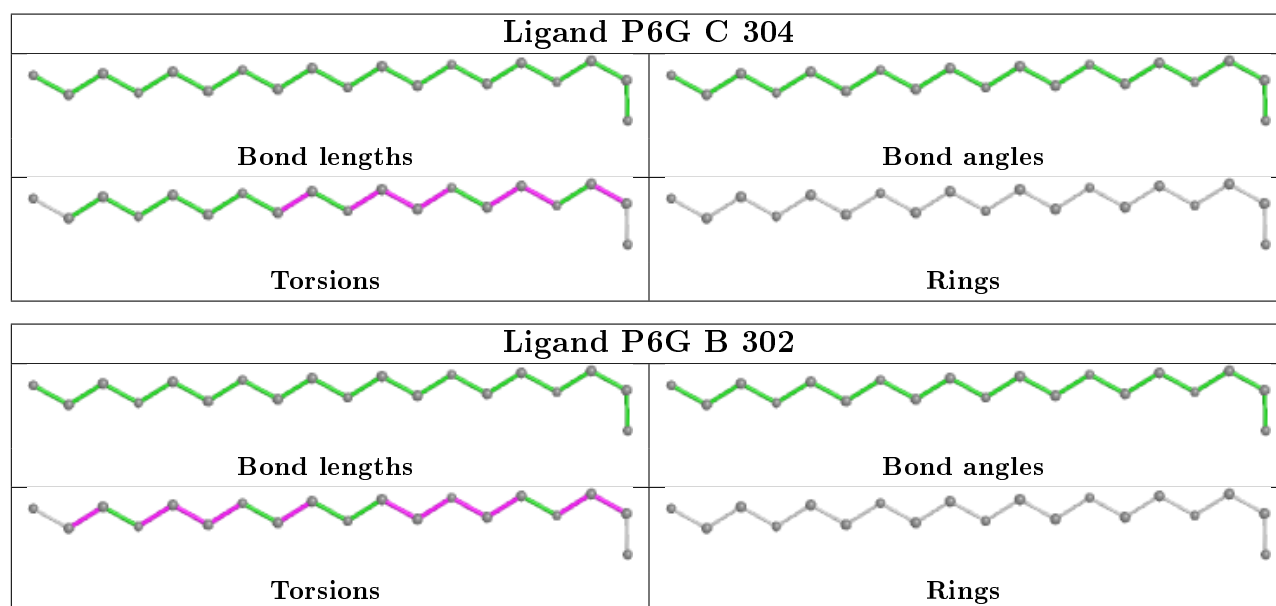
Mol	Chain	Res	Type	Atoms
6	C	307	PGE	O2-C3-C4-O3
3	A	301	PG4	O4-C7-C8-O5
4	C	303	GOL	O1-C1-C2-O2
6	C	307	PGE	O3-C5-C6-O4
5	B	302	P6G	C14-C15-O16-C17
3	C	306	PG4	C3-C4-O3-C5
5	B	302	P6G	C9-C8-O7-C6
3	C	305	PG4	C8-C7-O4-C6
3	C	306	PG4	O4-C7-C8-O5
3	C	306	PG4	C5-C6-O4-C7
3	A	301	PG4	C8-C7-O4-C6
5	B	302	P6G	C15-C14-O13-C12
5	B	302	P6G	O10-C11-C12-O13
3	C	306	PG4	O1-C1-C2-O2
5	B	302	P6G	C5-C6-O7-C8
3	A	301	PG4	C3-C4-O3-C5
3	A	301	PG4	C1-C2-O2-C3
5	C	304	P6G	C8-C9-O10-C11
6	C	307	PGE	C3-C4-O3-C5
4	C	303	GOL	O2-C2-C3-O3
5	C	304	P6G	C6-C5-O4-C3
3	C	305	PG4	O2-C3-C4-O3
5	B	302	P6G	O16-C17-C18-O19
5	B	302	P6G	O13-C14-C15-O16
3	A	301	PG4	O3-C5-C6-O4
5	B	302	P6G	O7-C8-C9-O10
5	B	302	P6G	C2-C3-O4-C5

There are no ring outliers.

9 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	305	PG4	7	0
4	C	303	GOL	1	0
3	A	301	PG4	11	0
4	C	301	GOL	2	0
4	C	302	GOL	2	0
6	C	307	PGE	1	0
5	C	304	P6G	7	0
5	B	302	P6G	4	0
3	C	306	PG4	5	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	207/218 (94%)	0.47	22 (10%) 6 7	24, 37, 70, 96	1 (0%)
1	C	213/218 (97%)	0.32	10 (4%) 31 37	21, 33, 57, 84	2 (0%)
2	B	233/236 (98%)	0.29	9 (3%) 39 45	24, 37, 66, 84	0
2	D	232/236 (98%)	0.29	12 (5%) 27 32	21, 35, 57, 83	4 (1%)
All	All	885/908 (97%)	0.34	53 (5%) 21 27	21, 36, 65, 96	7 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	100(G)	PHE	6.8
2	B	100(F)	ALA	6.3
1	A	107	LEU	6.3
2	D	87	SER	6.3
1	C	210	THR	5.9
1	A	6	THR	5.9
1	A	210	THR	5.4
1	A	72	THR	5.4
1	C	5	LEU	5.3
2	B	100(H)	ARG	4.7
2	D	213	SER	4.5
2	D	130	SER	4.2
1	C	157	LYS	4.1
1	A	157	LYS	4.0
2	D	42	GLY	4.0
1	A	69	THR	3.6
1	A	95	SER	3.6
1	A	70	THR	3.5
1	C	25	GLY	3.5
1	A	9	SER	3.4
1	A	26	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	54	SER	3.3
1	A	156	VAL	3.3
1	A	184	GLU	3.2
2	B	127	LYS	3.2
2	B	1	GLN	3.2
1	A	24	GLY	3.1
1	A	95(A)	ALA	3.1
1	C	26	ARG	3.1
2	D	83	THR	3.0
2	D	55	GLY	2.9
1	A	7	GLN	2.9
2	B	55	GLY	2.9
1	A	189	HIS	2.8
1	A	8	PRO	2.7
1	A	28	LEU	2.6
1	C	8	PRO	2.6
2	D	30	SER	2.6
2	B	100(E)	VAL	2.5
1	C	78	VAL	2.5
1	C	211	GLU	2.5
2	D	129	THR	2.4
2	D	103	GLN	2.4
2	D	53	ASP	2.3
1	A	27	SER	2.3
1	C	20	ARG	2.3
2	B	53	ASP	2.2
1	A	190	LYS	2.2
2	D	100(H)	ARG	2.1
2	D	57	THR	2.1
1	A	67	ASP	2.0
1	A	129	ASN	2.0
1	C	184	GLU	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 carbohydrates in this entry.



## 6.4 Ligands ⓘ

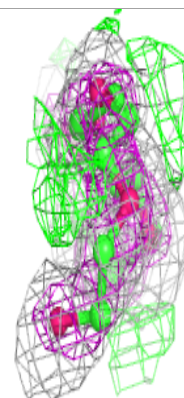
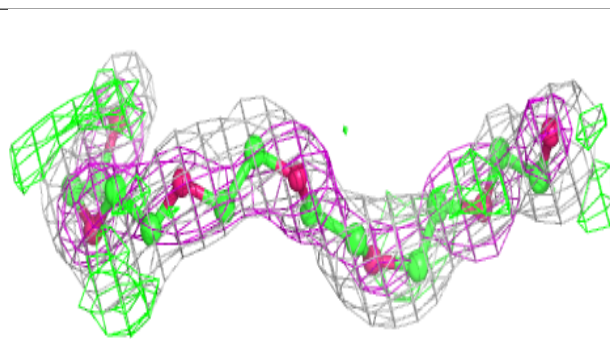
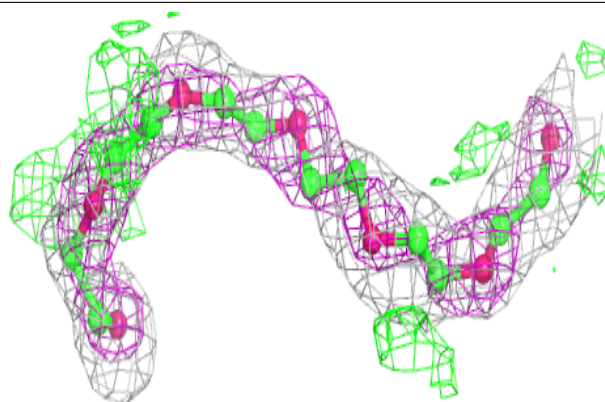
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

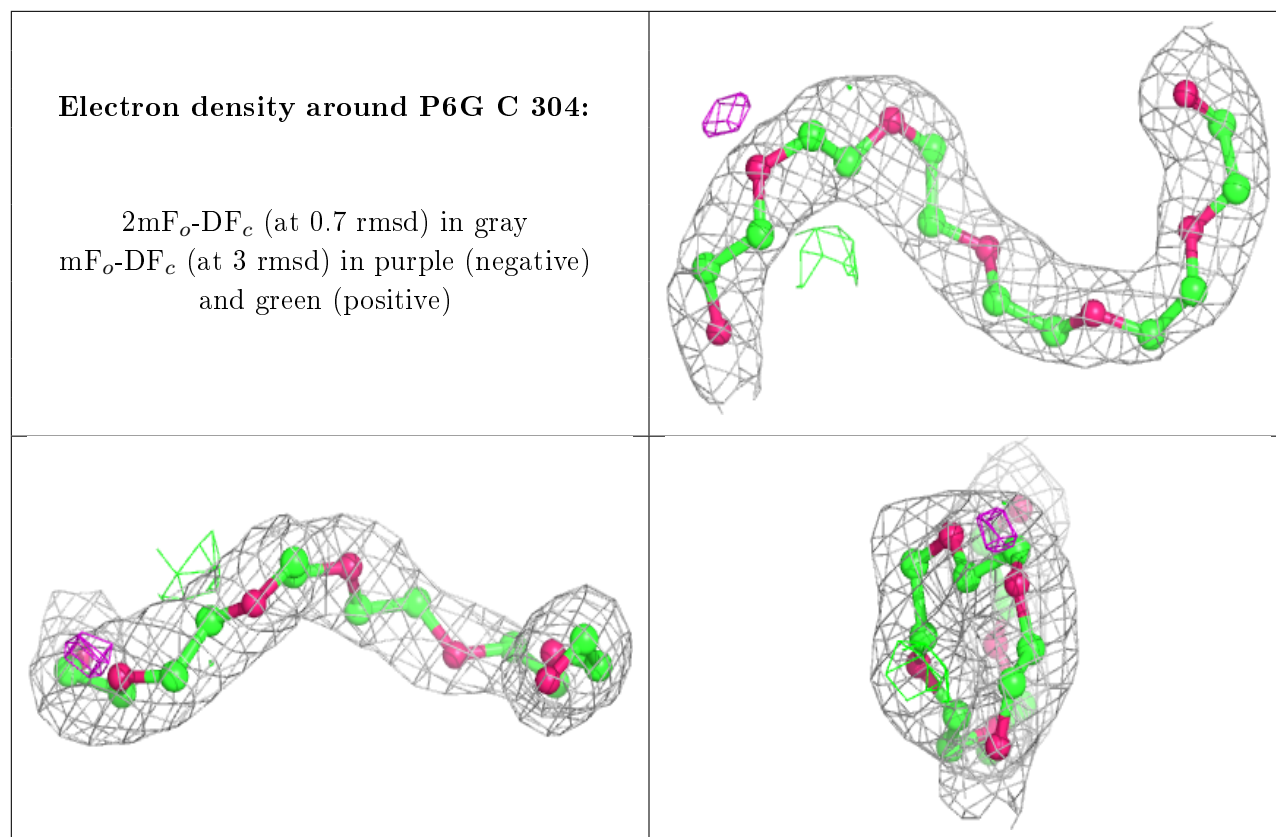
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PG4	C	306	13/13	0.73	0.16	43,50,56,63	0
6	PGE	C	307	10/10	0.75	0.26	20,20,20,20	0
3	PG4	C	305	13/13	0.75	0.34	28,44,57,62	0
5	P6G	B	302	19/19	0.76	0.31	20,20,20,20	0
4	GOL	C	301	6/6	0.82	0.21	37,43,56,58	0
3	PG4	A	301	13/13	0.83	0.28	36,42,53,56	0
4	GOL	C	303	6/6	0.84	0.22	20,20,20,20	0
4	GOL	B	301	6/6	0.86	0.23	38,42,49,63	0
5	P6G	C	304	19/19	0.90	0.15	29,41,47,55	0
4	GOL	C	302	6/6	0.93	0.23	44,52,55,58	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 P6G B 302:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.