



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 06:11 PM EDT

PDB ID : 9C9D / pdb\_00009c9d  
Title : Protein receptor  
Authors : MacLachlan, B.; Awad, W.; Vivian, J.; Rossjohn, J.  
Deposited on : 2024-06-13  
Resolution : 2.90 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 Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

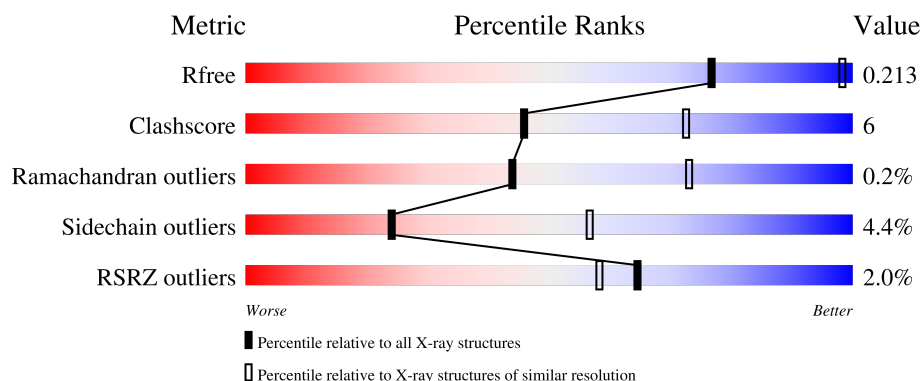
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	271	<div> <div>81%</div> <div>17%</div> <div>..</div> </div>
2	B	100	<div> <div>88%</div> <div>10%</div> <div>..</div> </div>
3	D	204	<div> <div>88%</div> <div>9%</div> <div>..</div> </div>
4	E	246	<div> <div>81%</div> <div>16%</div> <div>..</div> </div>
5	F	211	<div> <div>71%</div> <div>17%</div> <div>• 10%</div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8189 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	2	0
			2203	1410	380	402	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			813	519	138	153	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called T Cell Receptor Alpha Variable 1-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	200	Total	C	N	O	S	0	0	0
			1550	979	248	314	9			

- Molecule 4 is a protein called T cell receptor beta variable 6-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	244	Total	C	N	O	S	0	2	0
			1928	1211	339	369	9			

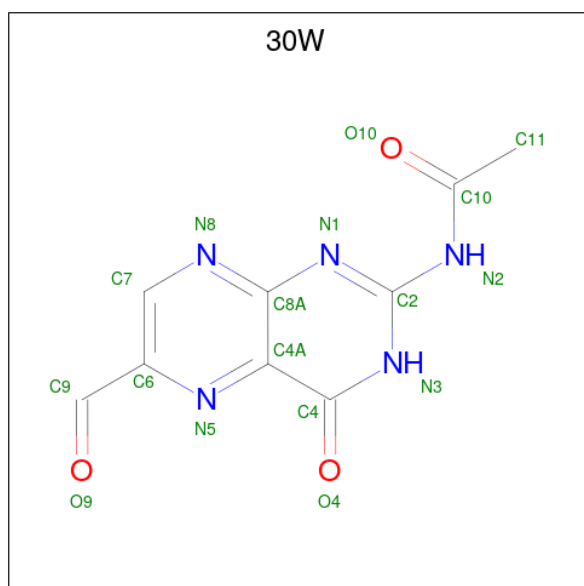
- Molecule 5 is a protein called Leukocyte immunoglobulin-like receptor subfamily B member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	189	Total	C	N	O	S	0	0	0
			1452	923	250	272	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	MET	-	initiating methionine	UNP Q8N423
F	198	GLY	-	expression tag	UNP Q8N423
F	199	SER	-	expression tag	UNP Q8N423
F	200	GLY	-	expression tag	UNP Q8N423
F	201	SER	-	expression tag	UNP Q8N423
F	202	GLY	-	expression tag	UNP Q8N423
F	203	HIS	-	expression tag	UNP Q8N423
F	204	HIS	-	expression tag	UNP Q8N423
F	205	HIS	-	expression tag	UNP Q8N423
F	206	HIS	-	expression tag	UNP Q8N423
F	207	HIS	-	expression tag	UNP Q8N423
F	208	HIS	-	expression tag	UNP Q8N423

- Molecule 6 is N-(6-formyl-4-oxo-3,4-dihydropteridin-2-yl)acetamide (CCD ID: 30W) (formula: C<sub>9</sub>H<sub>7</sub>N<sub>5</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



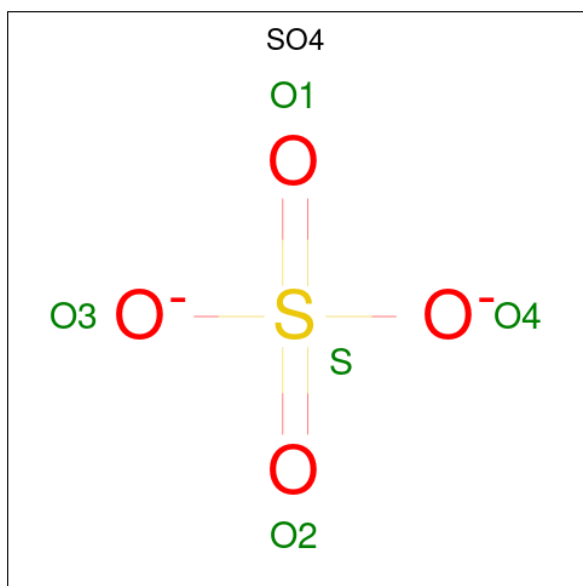
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			16	9	5	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



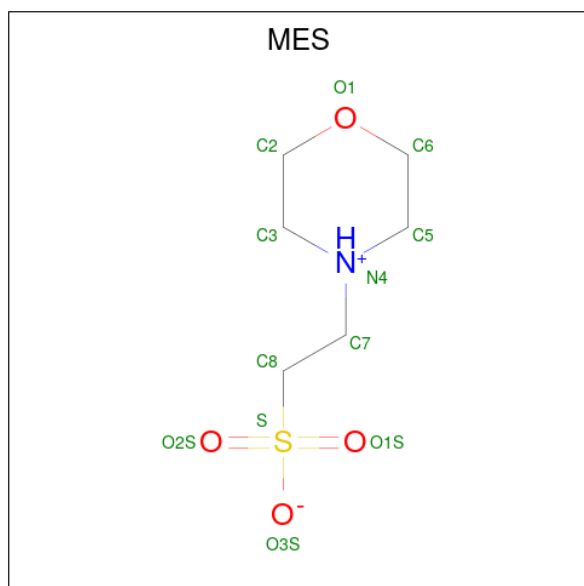
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula:  $Cl$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	E	1	Total	Cl	0	0
			1	1		

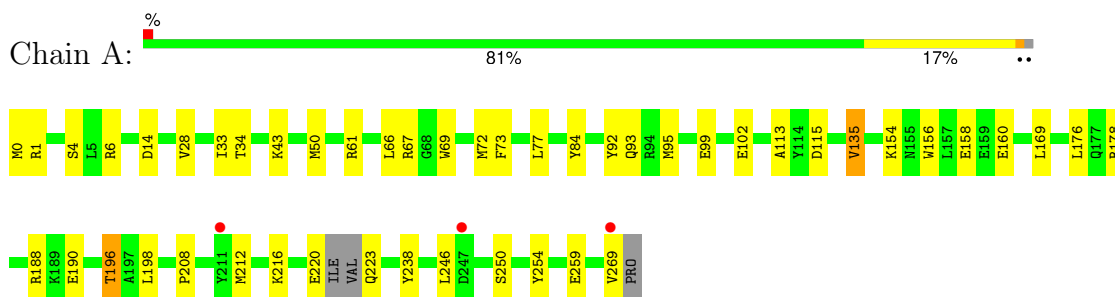
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	62	Total	O	0	0
			62	62		
11	B	15	Total	O	0	0
			15	15		
11	D	33	Total	O	0	0
			33	33		
11	E	24	Total	O	0	0
			24	24		
11	F	22	Total	O	0	0
			22	22		

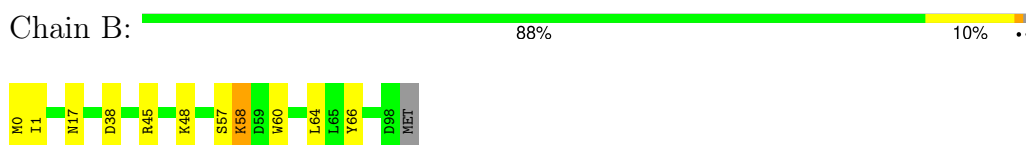
### 3 Residue-property plots

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.

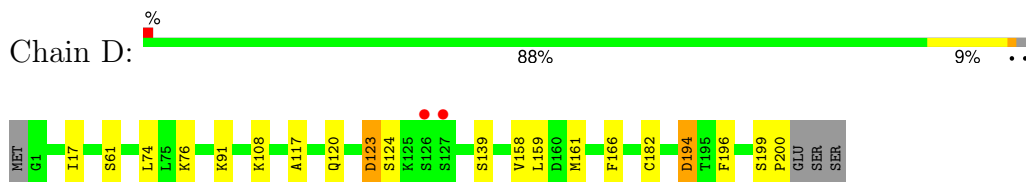
- Molecule 1: Major histocompatibility complex class I-related gene protein



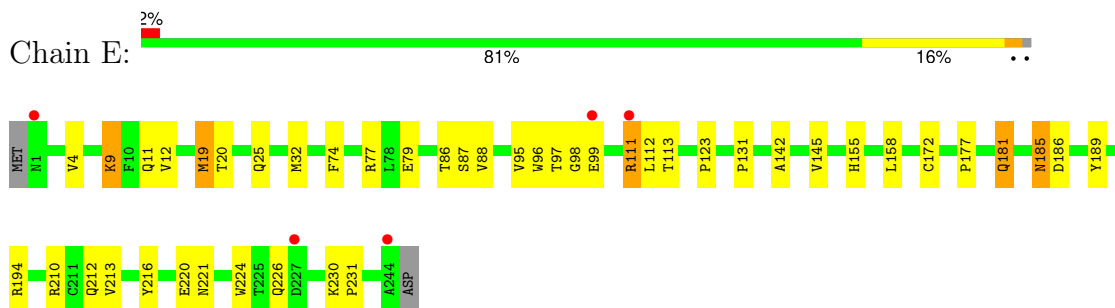
- Molecule 2: Beta-2-microglobulin



- Molecule 3: T Cell Receptor Alpha Variable 1-2

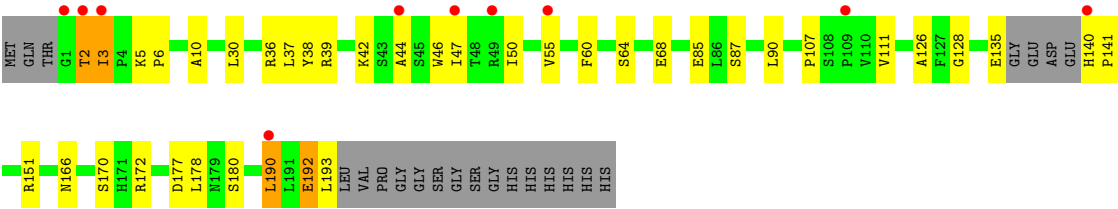


- Molecule 4: T cell receptor beta variable 6-1



- Molecule 5: Leukocyte immunoglobulin-like receptor subfamily B member 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.29Å 115.53Å 92.40Å 90.00° 114.60° 90.00°	Depositor
Resolution (Å)	43.78 – 2.90 43.78 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.78-2.90) 99.7 (43.78-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.190 , 0.215 0.188 , 0.213	Depositor DCC
$R_{free}$ test set	1862 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.5	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MES, GOL, SO4, 3OW

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	0.08	0/2273	0.24	0/3092
2	B	0.08	0/836	0.25	0/1135
3	D	0.08	0/1585	0.26	0/2152
4	E	0.08	0/1979	0.26	0/2694
5	F	0.10	0/1497	0.31	0/2048
All	All	0.09	0/8170	0.27	0/11121

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 [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	2203	0	2062	26	0
2	B	813	0	766	9	0
3	D	1550	0	1449	11	0
4	E	1928	0	1809	31	0
5	F	1452	0	1374	19	0
6	A	16	0	6	0	0
7	A	12	0	16	1	0
7	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	10	0	0	0	0
8	D	15	0	0	0	0
8	E	10	0	0	0	0
8	F	5	0	0	0	0
9	B	12	0	12	2	0
10	E	1	0	0	1	0
11	A	62	0	0	1	0
11	B	15	0	0	0	0
11	D	33	0	0	0	0
11	E	24	0	0	3	0
11	F	22	0	0	0	0
All	All	8189	0	7502	88	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 6.

All (88) 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:58:LYS:H	9:B:102:MES:H51	1.44	0.81
1:A:67:ARG:HH12	7:A:305:GOL:H2	1.53	0.73
1:A:28:VAL:HG23	1:A:33:ILE:HD13	1.75	0.68
1:A:69:TRP:HE1	4:E:98:GLY:HA3	1.60	0.67
1:A:6:ARG:HH21	2:B:58:LYS:HG3	1.58	0.66
2:B:38:ASP:OD1	2:B:45:ARG:NH1	2.28	0.66
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.78	0.65
2:B:1:ILE:HD11	5:F:126:ALA:HB2	1.79	0.64
1:A:190:GLU:HG3	1:A:196:THR:HG23	1.80	0.62
4:E:210:ARG:NH1	10:E:301:CL:CL	2.69	0.61
4:E:221:ASN:ND2	11:E:403:HOH:O	2.33	0.61
5:F:135:GLU:OE2	5:F:172:ARG:HD2	2.01	0.60
5:F:190:LEU:H	5:F:190:LEU:HD23	1.67	0.60
4:E:210:ARG:NH2	4:E:212:GLN:OE1	2.32	0.59
3:D:194:ASP:N	3:D:194:ASP:OD1	2.34	0.58
4:E:25:GLN:HE21	4:E:32:MET:HE2	1.69	0.56
1:A:188:ARG:HB3	1:A:198:LEU:HD23	1.87	0.56
1:A:93:GLN:HB2	1:A:113:ALA:HB3	1.87	0.56
5:F:2:THR:OG1	5:F:3:ILE:N	2.38	0.56
4:E:4:VAL:HG22	4:E:25:GLN:HB3	1.88	0.56
5:F:128:GLY:HA3	5:F:178:LEU:HG	1.88	0.55
3:D:61:SER:HB2	3:D:74:LEU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:185:ASN:OD1	4:E:185:ASN:N	2.37	0.55
5:F:111:VAL:HG21	5:F:193:LEU:HD23	1.89	0.54
3:D:91:LYS:NZ	11:E:401:HOH:O	2.39	0.54
1:A:33:ILE:HB	1:A:50:MET:HE2	1.91	0.53
4:E:158:LEU:HG	4:E:213:VAL:HG12	1.91	0.53
4:E:88:VAL:HG22	4:E:111[B]:ARG:HG3	1.91	0.52
4:E:155:HIS:HB3	4:E:216:TYR:HB2	1.92	0.52
4:E:131:PRO:HG2	4:E:142:ALA:HB1	1.91	0.52
1:A:34:THR:HB	1:A:43:LYS:HE3	1.92	0.51
2:B:57:SER:HA	9:B:102:MES:H81	1.92	0.51
4:E:86:THR:HG23	4:E:113:THR:HA	1.92	0.51
4:E:97:THR:O	11:E:401:HOH:O	2.18	0.51
4:E:11:GLN:HG2	4:E:19:MET:SD	2.50	0.51
1:A:154:LYS:NZ	1:A:158:GLU:OE2	2.45	0.50
3:D:199:SER:HB2	3:D:200:PRO:HD3	1.94	0.50
4:E:123:PRO:HD3	4:E:231:PRO:HB3	1.94	0.50
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.47	0.49
4:E:88:VAL:HG22	4:E:111[A]:ARG:HG3	1.94	0.49
4:E:95:VAL:HG12	4:E:96:TRP:CD1	2.47	0.49
5:F:5:LYS:HE2	5:F:85:GLU:OE2	2.12	0.49
4:E:145:VAL:HG22	4:E:194[B]:ARG:HG2	1.95	0.49
5:F:39:ARG:HH21	5:F:42:LYS:HB3	1.78	0.48
4:E:224:TRP:CE2	4:E:226:GLN:HB2	2.47	0.48
3:D:17:ILE:HG12	3:D:76:LYS:HA	1.96	0.48
3:D:108:LYS:HD2	3:D:139:SER:HB3	1.97	0.47
5:F:10:ALA:HB2	5:F:90:LEU:HD21	1.97	0.46
1:A:1:ARG:NH2	1:A:178:ARG:O	2.41	0.46
1:A:156:TRP:HA	1:A:160:GLU:HB2	1.98	0.45
5:F:177:ASP:OD1	5:F:178:LEU:N	2.49	0.45
4:E:186:ASP:OD1	4:E:186:ASP:N	2.50	0.44
1:A:69:TRP:NE1	4:E:98:GLY:HA3	2.28	0.43
1:A:95:MET:HE2	1:A:95:MET:HB3	1.88	0.43
3:D:117:ALA:HB2	3:D:196:PHE:HB3	2.01	0.43
3:D:123:ASP:OD1	3:D:123:ASP:N	2.35	0.43
4:E:19:MET:HB3	4:E:19:MET:HE2	1.61	0.43
4:E:177:PRO:HB2	4:E:189:TYR:HB3	2.01	0.43
5:F:6:PRO:HG2	5:F:87:SER:HB3	2.01	0.43
5:F:44:ALA:HB1	5:F:46:TRP:CD1	2.53	0.43
1:A:0:MET:O	1:A:102:GLU:HG3	2.19	0.43
5:F:68:GLU:OE1	5:F:68:GLU:N	2.41	0.43
1:A:115:ASP:HB3	2:B:0:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:120:GLN:HB2	3:D:182:CYS:SG	2.58	0.42
4:E:9:LYS:CD	4:E:9:LYS:H	2.33	0.42
1:A:72:MET:HG3	4:E:96:TRP:CE3	2.54	0.42
1:A:208:PRO:HB3	1:A:238:TYR:CG	2.53	0.42
3:D:161:MET:HG3	3:D:166:PHE:HD2	1.85	0.42
3:D:159:LEU:HB3	4:E:172:CYS:HB2	2.02	0.42
4:E:32:MET:SD	4:E:74:PHE:HB2	2.59	0.42
1:A:216:LYS:HB2	1:A:254:TYR:CE2	2.55	0.42
5:F:50:ILE:HG22	5:F:55:VAL:HG23	2.02	0.42
1:A:4:SER:HB3	1:A:99:GLU:HG2	2.01	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.89	0.41
5:F:44:ALA:HB3	5:F:47:ILE:HD12	2.01	0.41
2:B:17:ASN:OD1	2:B:17:ASN:N	2.53	0.41
5:F:37:LEU:HD22	5:F:60:PHE:CD2	2.55	0.41
5:F:140:HIS:HB3	5:F:141:PRO:HD3	2.02	0.41
1:A:169:LEU:HD23	1:A:176:LEU:HD13	2.03	0.41
4:E:19:MET:HG2	4:E:20:THR:N	2.35	0.41
2:B:64:LEU:HD13	2:B:66:TYR:HE1	1.86	0.41
4:E:87:SER:OG	4:E:88:VAL:N	2.54	0.41
5:F:36:ARG:HD3	5:F:38:TYR:OH	2.20	0.41
5:F:170:SER:OG	5:F:192:GLU:OE2	2.34	0.41
1:A:84:TYR:CZ	1:A:135:VAL:HG11	2.56	0.40
1:A:93:GLN:NE2	11:A:407:HOH:O	2.53	0.40
4:E:230:LYS:HA	4:E:231:PRO:HD3	1.87	0.40
4:E:181:GLN:HE21	4:E:181:GLN:HB3	1.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	266/271 (98%)	260 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
3	D	198/204 (97%)	191 (96%)	7 (4%)	0	100	100
4	E	244/246 (99%)	240 (98%)	4 (2%)	0	100	100
5	F	185/211 (88%)	182 (98%)	1 (0%)	2 (1%)	12	37
All	All	990/1032 (96%)	968 (98%)	20 (2%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	2	THR
5	F	107	PRO

### 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	230/241 (95%)	217 (94%)	13 (6%)	17	47
2	B	90/95 (95%)	88 (98%)	2 (2%)	47	78
3	D	171/181 (94%)	167 (98%)	4 (2%)	45	77
4	E	205/212 (97%)	193 (94%)	12 (6%)	16	45
5	F	157/183 (86%)	149 (95%)	8 (5%)	20	51
All	All	853/912 (94%)	814 (95%)	39 (5%)	24	55

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	61[A]	ARG
1	A	61[B]	ARG
1	A	66	LEU
1	A	73	PHE
1	A	135	VAL

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Mol	Chain	Res	Type
1	A	196	THR
1	A	212	MET
1	A	220	GLU
1	A	223	GLN
1	A	250	SER
1	A	259	GLU
1	A	269	VAL
2	B	48	LYS
2	B	58	LYS
3	D	123	ASP
3	D	124	SER
3	D	158	VAL
3	D	194	ASP
4	E	9	LYS
4	E	12	VAL
4	E	19	MET
4	E	77	ARG
4	E	79	GLU
4	E	99	GLU
4	E	111[A]	ARG
4	E	111[B]	ARG
4	E	112	LEU
4	E	181	GLN
4	E	185	ASN
4	E	220	GLU
5	F	3	ILE
5	F	30	LEU
5	F	64	SER
5	F	151	ARG
5	F	166	ASN
5	F	180	SER
5	F	190	LEU
5	F	192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
3	D	94	ASN
3	D	96	GLN
4	E	17	GLN
4	E	28	ASN

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Mol	Chain	Res	Type
4	E	140	GLN
4	E	181	GLN
4	E	226	GLN
5	F	18	GLN
5	F	27	GLN
5	F	59	GLN
5	F	106	GLN
5	F	142	GLN
5	F	147	GLN
5	F	166	ASN

### 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 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\# Z  > 2$
8	SO4	F	301	-	4,4,4	0.24	0	6,6,6	0.06	0
8	SO4	D	303	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	E	302	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	A	303	-	4,4,4	0.23	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	30W	A	301	1	16,17,18	0.58	1 (6%)	18,24,25	1.02	1 (5%)
8	SO4	A	304	-	4,4,4	0.23	0	6,6,6	0.07	0
7	GOL	A	305	-	5,5,5	0.93	0	5,5,5	1.08	0
8	SO4	E	303	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	D	301	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	D	302	-	4,4,4	0.23	0	6,6,6	0.09	0
7	GOL	A	302	-	5,5,5	0.95	0	5,5,5	1.04	0
9	MES	B	102	-	12,12,12	2.32	1 (8%)	15,16,16	2.35	4 (26%)
7	GOL	B	101	-	5,5,5	0.94	0	5,5,5	1.07	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
6	30W	A	301	1	-	0/4/4/6	0/2/2/2
7	GOL	A	305	-	-	2/4/4/4	-
7	GOL	A	302	-	-	3/4/4/4	-
9	MES	B	102	-	-	2/6/14/14	0/1/1/1
7	GOL	B	101	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	102	MES	C8-S	-7.73	1.66	1.77
6	A	301	30W	C4A-C8A	2.12	1.44	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	102	MES	C5-N4-C3	5.06	119.74	108.84
9	B	102	MES	C2-C3-N4	-4.02	104.01	110.12
6	A	301	30W	C4A-C8A-N1	-3.58	118.17	123.19
9	B	102	MES	C7-N4-C5	3.19	119.75	111.24
9	B	102	MES	C7-N4-C3	2.85	118.84	111.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

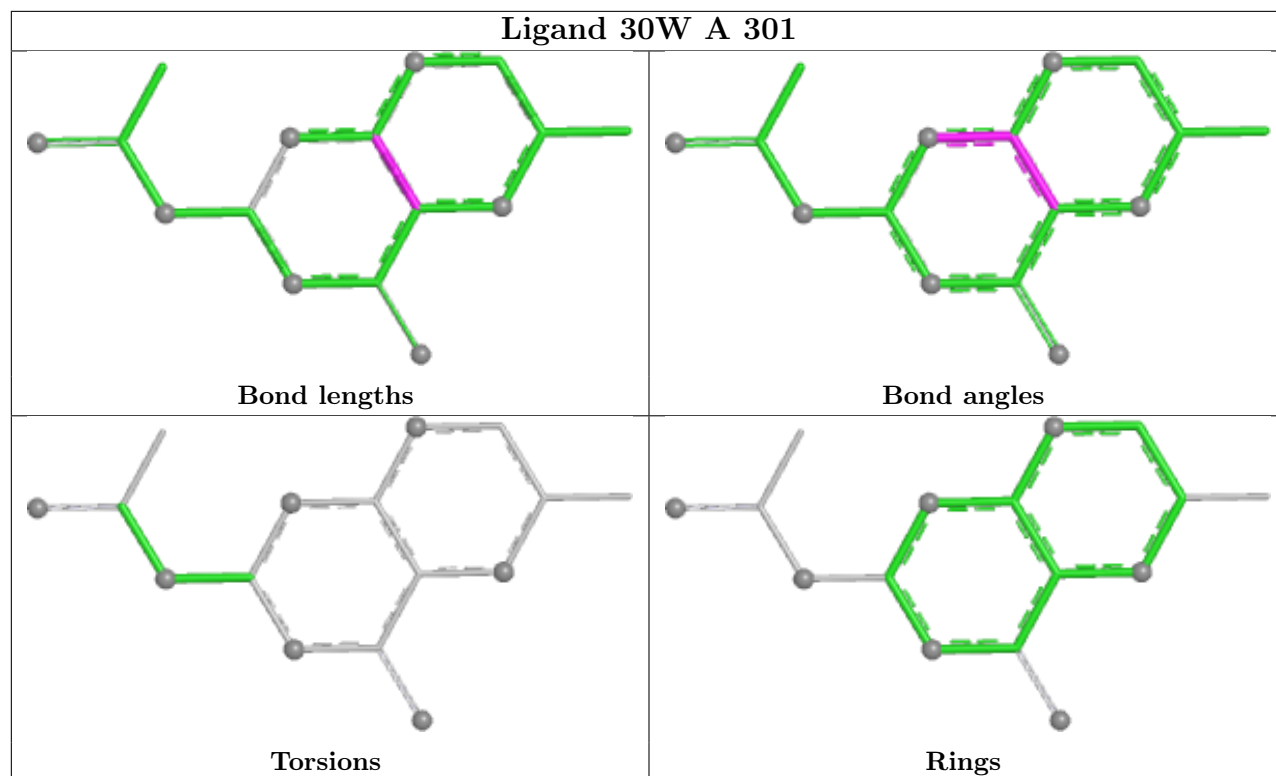
Mol	Chain	Res	Type	Atoms
7	A	305	GOL	O2-C2-C3-O3
7	A	302	GOL	O1-C1-C2-C3
7	A	305	GOL	C1-C2-C3-O3
9	B	102	MES	C8-C7-N4-C3
7	A	302	GOL	O1-C1-C2-O2
9	B	102	MES	C7-C8-S-O1S
7	A	302	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	305	GOL	1	0
9	B	102	MES	2	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	268/271 (98%)	-0.26	3 (1%) 77 72	28, 56, 99, 142	3 (1%)
2	B	99/100 (99%)	-0.35	0 100 100	43, 64, 98, 117	1 (1%)
3	D	200/204 (98%)	-0.04	2 (1%) 79 74	39, 64, 126, 147	2 (1%)
4	E	244/246 (99%)	-0.04	5 (2%) 64 58	30, 74, 97, 117	6 (2%)
5	F	189/211 (89%)	0.13	10 (5%) 33 28	44, 73, 143, 161	5 (2%)
All	All	1000/1032 (96%)	-0.10	20 (2%) 64 58	28, 66, 117, 161	17 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	111[A]	ARG	3.4
5	F	109	PRO	3.0
3	D	126	SER	2.8
4	E	99	GLU	2.8
3	D	127	SER	2.5
4	E	227	ASP	2.5
5	F	3	ILE	2.5
5	F	49	ARG	2.4
5	F	190	LEU	2.4
5	F	1	GLY	2.3
1	A	269	VAL	2.3
5	F	47	ILE	2.3
4	E	244	ALA	2.3
5	F	44	ALA	2.3
5	F	55	VAL	2.2
1	A	247	ASP	2.2
5	F	140	HIS	2.1
1	A	211	TYR	2.1
5	F	2	THR	2.0
4	E	1	ASN	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](#)

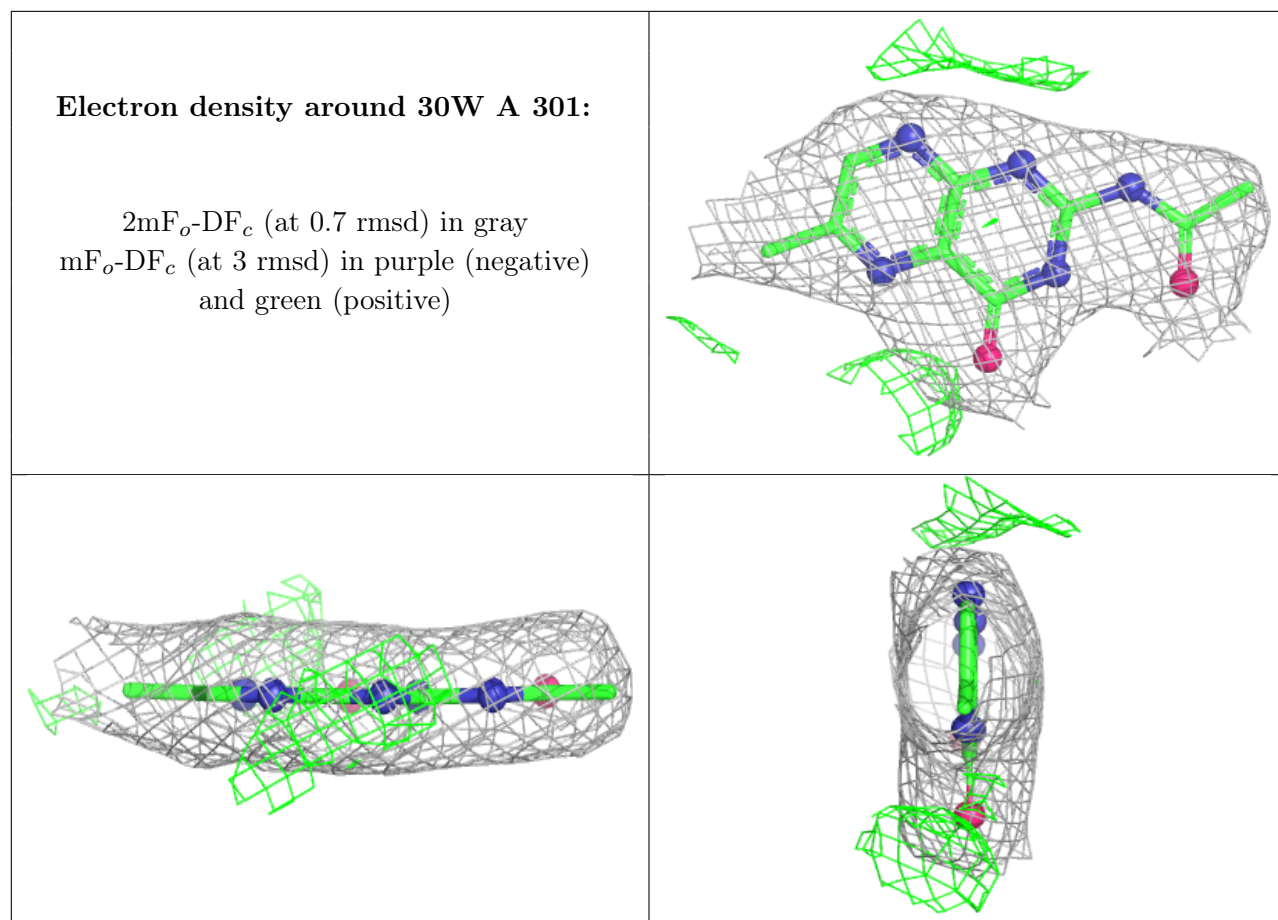
There are no oligosaccharides in this entry.

## 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( $\text{\AA}^2$ )	Q<0.9
8	SO4	A	303	5/5	0.78	0.14	106,109,136,150	0
7	GOL	A	305	6/6	0.81	0.14	53,58,69,70	1
8	SO4	F	301	5/5	0.81	0.18	82,91,107,113	5
8	SO4	E	303	5/5	0.84	0.18	73,77,94,100	3
7	GOL	B	101	6/6	0.84	0.12	70,77,86,94	1
8	SO4	D	303	5/5	0.86	0.15	64,79,85,104	4
9	MES	B	102	12/12	0.90	0.18	56,70,86,86	4
8	SO4	A	304	5/5	0.91	0.12	72,76,80,81	5
8	SO4	E	302	5/5	0.92	0.09	68,71,75,82	2
8	SO4	D	301	5/5	0.92	0.15	85,94,104,110	0
8	SO4	D	302	5/5	0.94	0.09	51,53,62,63	1
7	GOL	A	302	6/6	0.95	0.14	58,69,76,78	0
6	30W	A	301	16/17	0.97	0.07	46,49,53,57	0
10	CL	E	301	1/1	0.97	0.05	88,88,88,88	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 ⓘ

There are no such residues in this entry.