



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 01:34 PM EDT

PDB ID : 3OS6  
Title : Crystal structure of putative 2,3-dihydroxybenzoate-specific isochorismate synthase, Dhbc from Bacillus anthracis.  
Authors : Domagalski, M.J.; Chruszcz, M.; Skarina, T.; Onopriyenko, O.; Cymborowski, M.; Savchenko, A.; Edwards, A.; Anderson, W.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2010-09-08  
Resolution : 2.40 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 : 2.27  
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) : 2.27

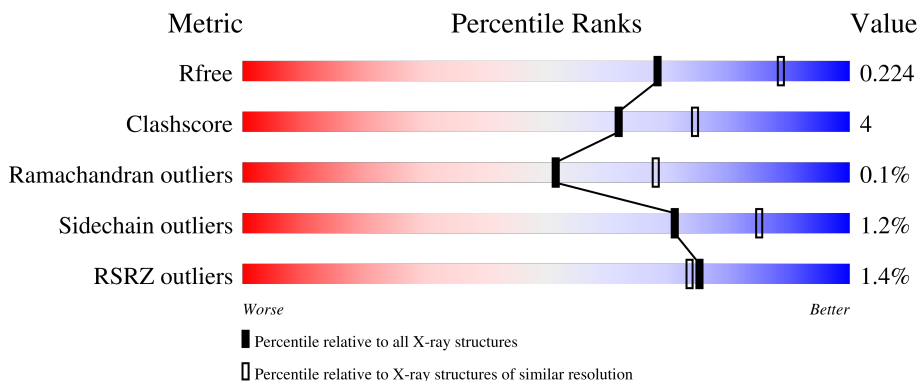
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	399	 3% 83% 10% • 7%
1	B	399	 84% 9% • 6%
1	C	399	 84% 10% • 6%
1	D	399	 2% 82% 11% 7%

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>
2	SO4	B	400	-	-	X	-
2	SO4	C	400	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12607 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 Isochorismate synthase DhbC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	373	2882	1821	498	553	3	7	0	0	0
1	B	374	2938	1853	508	567	3	7	0	4	0
1	C	375	2938	1854	506	567	3	8	0	5	0
1	D	373	2872	1816	496	550	3	7	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	LEU	PHE	cloning artifact	UNP Q81QQ0
B	24	LEU	PHE	cloning artifact	UNP Q81QQ0
C	24	LEU	PHE	cloning artifact	UNP Q81QQ0
D	24	LEU	PHE	cloning artifact	UNP Q81QQ0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



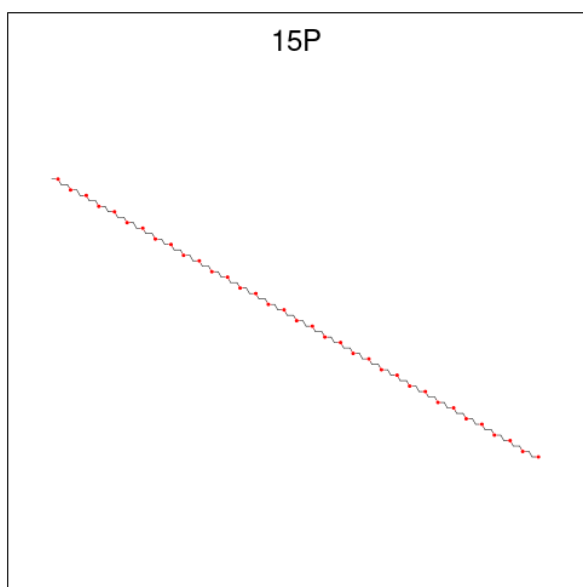
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: C<sub>69</sub>H<sub>140</sub>O<sub>35</sub>).



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

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



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

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

- Molecule 5 is water.

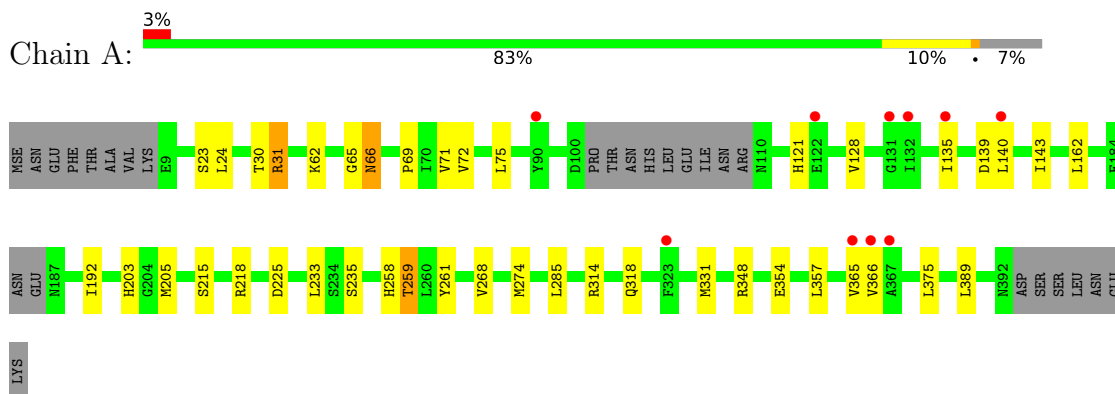
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	147	Total	O	0	0
			147	147		
5	B	249	Total	O	0	0
			249	249		
5	C	228	Total	O	0	0
			228	228		
5	D	139	Total	O	0	0
			139	139		



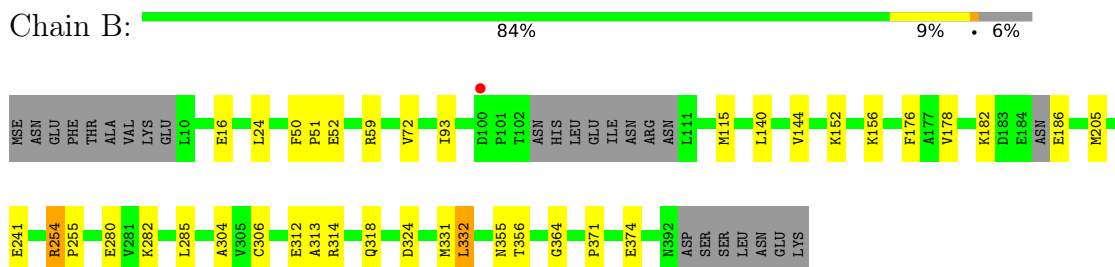
### 3 Residue-property plots [i](#)

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.

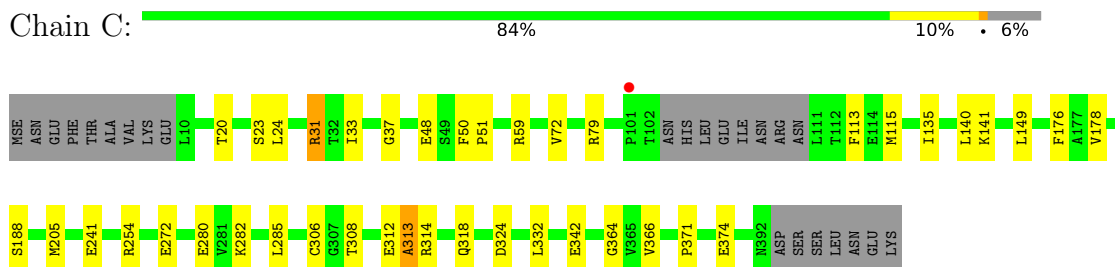
- Molecule 1: Isochorismate synthase Dhbc



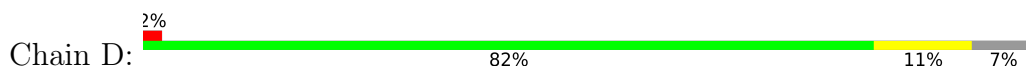
- Molecule 1: Isochorismate synthase Dhbc

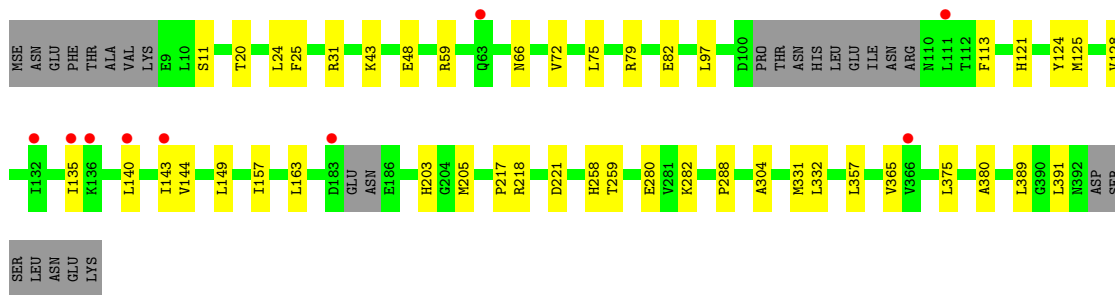


- Molecule 1: Isochorismate synthase Dhbc



- Molecule 1: Isochorismate synthase Dhbc





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.39Å 201.39Å 201.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 48.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.40) 93.8 (48.84-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.6.0070	Depositor
R, $R_{free}$	0.171 , 0.212 0.187 , 0.224	Depositor DCC
$R_{free}$ test set	4978 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.479 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: GOL, SO4, 15P

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	0.78	0/2931	0.80	4/3961 (0.1%)
1	B	0.98	2/2992 (0.1%)	0.88	3/4044 (0.1%)
1	C	1.00	4/2996 (0.1%)	0.87	3/4053 (0.1%)
1	D	0.76	0/2921	0.81	3/3952 (0.1%)
All	All	0.89	6/11840 (0.1%)	0.84	13/16010 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	CYS	CB-SG	9.13	1.97	1.82
1	C	241	GLU	CG-CD	5.80	1.60	1.51
1	C	306	CYS	CB-SG	5.51	1.91	1.82
1	C	313	ALA	CA-CB	-5.09	1.41	1.52
1	B	241	GLU	CG-CD	5.08	1.59	1.51
1	C	342	GLU	CD-OE2	5.07	1.31	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	324[A]	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	324[B]	ASP	CB-CG-OD1	6.36	124.02	118.30
1	D	31	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	31	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	225	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	324[A]	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	324[B]	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	218	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	218	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	254	ARG	NE-CZ-NH1	5.18	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	348	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2882	0	2861	27	0
1	B	2938	0	2911	20	0
1	C	2938	0	2903	29	0
1	D	2872	0	2834	31	0
2	A	40	0	0	1	0
2	B	35	0	0	2	0
2	C	30	0	0	3	0
2	D	35	0	0	0	0
3	A	19	0	25	6	0
3	D	19	0	25	2	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	12	0	16	1	0
4	D	12	0	16	0	0
5	A	147	0	0	0	0
5	B	249	0	0	3	0
5	C	228	0	0	3	0
5	D	139	0	0	1	0
All	All	12607	0	11607	104	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 4.

All (104) 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:D:357:LEU:HD22	1:D:389:LEU:HD11	1.58	0.84
1:D:205:MSE:HE2	1:D:205:MSE:HA	1.60	0.84
1:A:203:HIS:CD2	3:A:408:15P:H25	2.13	0.83
1:D:203:HIS:HB2	3:D:409:15P:H23	1.65	0.78
1:A:258:HIS:ND1	1:A:259:THR:HG23	2.06	0.71
1:A:357:LEU:HD22	1:A:389:LEU:HD11	1.74	0.70
1:A:24:LEU:HD22	1:A:72:VAL:HB	1.72	0.70
1:A:203:HIS:HD2	3:A:408:15P:H25	1.55	0.70
1:D:128:VAL:HG13	1:D:365:VAL:HG21	1.74	0.69
1:C:140:LEU:HD21	1:C:313:ALA:N	2.07	0.69
1:D:258:HIS:ND1	1:D:259:THR:HG23	2.08	0.68
1:B:280:GLU:OE1	1:B:282:LYS:NZ	2.28	0.67
1:D:121:HIS:ND1	1:D:375:LEU:HD21	2.10	0.65
1:B:59:ARG:NH2	2:B:400:SO4:O3	2.30	0.65
1:C:48:GLU:OE2	1:C:79:ARG:NH2	2.30	0.65
1:D:205:MSE:HE1	1:D:288:PRO:HA	1.79	0.64
1:A:128:VAL:HG13	1:A:365:VAL:HG21	1.80	0.64
1:C:115[B]:MSE:SE	1:C:149:LEU:HD11	2.48	0.63
1:B:140:LEU:HD21	1:B:313:ALA:N	2.13	0.63
1:C:59:ARG:NH2	2:C:400:SO4:S	2.73	0.62
1:A:261:TYR:HE2	1:C:115[B]:MSE:HE2	1.65	0.61
1:A:135:ILE:HG23	1:A:140:LEU:O	2.00	0.61
1:A:261:TYR:CE2	1:C:115[B]:MSE:HE2	2.37	0.60
1:C:280:GLU:OE1	1:C:282:LYS:NZ	2.31	0.60
1:D:24:LEU:HD22	1:D:72:VAL:HB	1.84	0.60
1:A:135:ILE:HD11	1:A:143:ILE:HG22	1.82	0.59
1:B:314:ARG:O	1:B:318:GLN:HG2	2.02	0.59
1:C:314:ARG:O	1:C:318:GLN:HG2	2.02	0.59
1:A:205:MSE:HE3	1:A:285:LEU:O	2.04	0.58
1:A:30:THR:HG21	3:A:408:15P:C2	2.34	0.58
1:D:124:TYR:O	1:D:128:VAL:HG23	2.03	0.58
1:C:31:ARG:HD2	1:C:33:ILE:HD11	1.86	0.57
1:D:75:LEU:HD22	1:D:331:MSE:HE2	1.88	0.56
1:D:135:ILE:HD11	1:D:143:ILE:HG22	1.90	0.54
1:A:233:LEU:HD13	1:A:268:VAL:HG23	1.90	0.53
1:C:205:MSE:HE2	1:C:285:LEU:O	2.10	0.52
1:B:144:VAL:HG21	1:B:304:ALA:O	2.10	0.52
1:B:93:ILE:HD13	5:B:547:HOH:O	2.08	0.51
1:D:113:PHE:CD2	1:D:391:LEU:HD21	2.46	0.50
1:A:31:ARG:NH2	3:A:408:15P:H29	2.27	0.49
1:D:11:SER:HB2	1:D:97:LEU:HD23	1.95	0.49
1:B:140:LEU:HD21	1:B:312:GLU:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:PHE:CD1	1:B:332:LEU:HD21	2.48	0.49
1:B:24:LEU:HD22	1:B:72:VAL:HB	1.95	0.48
1:C:140:LEU:HD21	1:C:312:GLU:C	2.33	0.48
1:C:59:ARG:NH2	2:C:400:SO4:O3	2.46	0.48
1:C:364:GLY:O	1:C:374:GLU:OE2	2.31	0.48
1:D:357:LEU:CD2	1:D:389:LEU:HD11	2.37	0.48
1:C:24:LEU:HD22	1:C:72:VAL:HB	1.95	0.47
1:A:75:LEU:HD22	1:A:331:MSE:HE2	1.95	0.47
1:B:24:LEU:CD1	1:B:178:VAL:HG22	2.45	0.47
1:C:308:THR:HG23	5:C:647:HOH:O	2.14	0.47
1:C:176:PHE:CD1	1:C:332:LEU:HD21	2.50	0.47
1:B:59:ARG:NH2	2:B:400:SO4:S	2.89	0.46
1:A:30:THR:HG21	3:A:408:15P:H12	1.97	0.46
1:C:50:PHE:N	1:C:51:PRO:CD	2.79	0.46
1:C:176:PHE:CE1	1:C:332:LEU:HD21	2.51	0.46
1:B:205:MSE:HE2	1:B:285:LEU:O	2.15	0.46
1:D:25:PHE:CD2	1:D:163:LEU:HD21	2.51	0.46
1:D:125:MSE:HE2	1:D:375:LEU:HD22	1.98	0.45
1:A:314:ARG:O	1:A:318:GLN:HG2	2.17	0.45
1:D:121:HIS:ND1	1:D:375:LEU:HD11	2.32	0.45
1:A:215:SER:OG	2:A:404:SO4:O3	2.29	0.45
1:C:115[B]:MSE:SE	1:C:149:LEU:HD21	2.67	0.45
1:D:205:MSE:HE2	1:D:205:MSE:CA	2.36	0.45
1:C:20:THR:HG21	1:C:188:SER:OG	2.17	0.45
1:D:157:ILE:CD1	1:D:357:LEU:HD11	2.47	0.45
1:D:217:PRO:HB3	1:D:380:ALA:HB1	1.99	0.45
1:A:121:HIS:ND1	1:A:375:LEU:HD21	2.33	0.44
1:C:59:ARG:NH1	5:C:514:HOH:O	2.50	0.44
1:D:135:ILE:HG23	1:D:140:LEU:O	2.18	0.44
1:C:272:GLU:HG2	4:C:407:GOL:H32	1.99	0.44
1:D:43:LYS:HZ3	1:D:82:GLU:HB3	1.83	0.43
1:D:144:VAL:HG21	1:D:304:ALA:O	2.18	0.43
1:B:52:GLU:HG3	5:B:416:HOH:O	2.18	0.43
1:D:332:LEU:HD12	1:D:332:LEU:C	2.39	0.43
1:A:66:ASN:O	1:A:69:PRO:HD3	2.17	0.43
1:B:364:GLY:O	1:B:374:GLU:OE2	2.37	0.43
1:B:254:ARG:HB3	1:B:255:PRO:HD3	2.00	0.43
1:D:59:ARG:NH1	5:D:457:HOH:O	2.33	0.43
1:A:233:LEU:HD13	1:A:268:VAL:CG2	2.49	0.43
1:D:48:GLU:OE2	1:D:79:ARG:NH2	2.52	0.43
1:C:141:LYS:O	5:C:728:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLU:HG2	5:B:761:HOH:O	2.19	0.42
1:B:50:PHE:N	1:B:51:PRO:CD	2.83	0.42
1:C:135:ILE:HG23	1:C:140:LEU:O	2.20	0.42
1:A:31:ARG:NH2	3:A:408:15P:H24	2.35	0.42
1:A:62:LYS:O	1:A:65:GLY:N	2.45	0.42
1:C:59:ARG:NH2	2:C:400:SO4:O4	2.53	0.42
1:C:23:SER:OG	1:C:37:GLY:O	2.35	0.42
1:D:143:ILE:HG23	1:D:143:ILE:O	2.20	0.42
1:A:215:SER:HB2	1:A:274:MSE:HE3	2.02	0.42
1:A:357:LEU:CD2	1:A:389:LEU:HD11	2.47	0.42
1:C:24:LEU:CD1	1:C:178:VAL:HG22	2.49	0.41
1:D:157:ILE:CD1	1:D:357:LEU:CD1	2.98	0.41
1:D:221:ASP:C	1:D:221:ASP:OD1	2.59	0.41
1:B:156:LYS:HA	1:B:355[A]:ASN:OD1	2.20	0.41
1:D:203:HIS:ND1	3:D:409:15P:H25	2.36	0.41
1:D:280:GLU:OE1	1:D:282:LYS:NZ	2.53	0.41
1:B:152:LYS:HG2	1:B:356:THR:HG22	2.01	0.41
1:C:135:ILE:HD13	1:C:366:VAL:HA	2.03	0.41
1:A:162:LEU:HD23	1:A:192:ILE:HD13	2.02	0.41
1:B:182:LYS:HB2	1:B:186:GLU:HG3	2.04	0.40
1:A:259:THR:HA	1:C:113:PHE:O	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	367/399 (92%)	357 (97%)	9 (2%)	1 (0%)	41	55
1	B	372/399 (93%)	361 (97%)	11 (3%)	0	100	100
1	C	376/399 (94%)	366 (97%)	10 (3%)	0	100	100
1	D	368/399 (92%)	359 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1483/1596 (93%)	1443 (97%)	39 (3%)	1 (0%)	51 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	GLU

### 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	312/341 (92%)	305 (98%)	7 (2%)	52 71
1	B	321/341 (94%)	317 (99%)	4 (1%)	71 85
1	C	320/341 (94%)	318 (99%)	2 (1%)	86 94
1	D	308/341 (90%)	306 (99%)	2 (1%)	86 94
All	All	1261/1364 (92%)	1246 (99%)	15 (1%)	71 85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	66	ASN
1	A	71	VAL
1	A	139	ASP
1	A	235	SER
1	A	259	THR
1	A	366	VAL
1	B	115	MSE
1	B	331	MSE
1	B	332	LEU
1	B	371	PRO
1	C	31	ARG
1	C	371	PRO
1	D	20	THR

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Mol	Chain	Res	Type
1	D	66	ASN

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

Mol	Chain	Res	Type
1	A	203	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

36 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	$\# Z  > 2$
2	SO4	A	405	-	4,4,4	0.36	0	6,6,6	0.45	0
2	SO4	C	401	-	4,4,4	0.20	0	6,6,6	0.50	0
2	SO4	B	404	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	D	402	-	4,4,4	0.18	0	6,6,6	0.49	0
2	SO4	B	405	-	4,4,4	0.26	0	6,6,6	1.05	0
2	SO4	C	403	-	4,4,4	0.25	0	6,6,6	0.70	0
3	15P	A	408	-	18,18,103	0.39	0	17,17,102	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	401	-	4,4,4	0.20	0	6,6,6	0.64	0
2	SO4	C	404	-	4,4,4	0.16	0	6,6,6	0.27	0
4	GOL	A	409	-	5,5,5	0.38	0	5,5,5	0.57	0
4	GOL	D	407	-	5,5,5	0.57	0	5,5,5	0.47	0
2	SO4	B	400	-	4,4,4	0.30	0	6,6,6	0.20	0
2	SO4	B	403	-	4,4,4	0.21	0	6,6,6	0.78	0
2	SO4	D	400	-	4,4,4	0.25	0	6,6,6	0.54	0
4	GOL	B	407	-	5,5,5	0.57	0	5,5,5	0.68	0
2	SO4	A	407	-	4,4,4	1.55	1 (25%)	6,6,6	0.51	0
2	SO4	D	403	-	4,4,4	0.20	0	6,6,6	0.46	0
2	SO4	B	406	-	4,4,4	0.41	0	6,6,6	0.65	0
4	GOL	C	406	-	5,5,5	0.37	0	5,5,5	0.78	0
2	SO4	B	402	-	4,4,4	0.17	0	6,6,6	0.27	0
2	SO4	D	406	-	4,4,4	0.04	0	6,6,6	0.45	0
2	SO4	A	403	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	A	400	-	4,4,4	0.12	0	6,6,6	0.22	0
3	15P	D	409	-	18,18,103	0.66	0	17,17,102	0.97	0
2	SO4	A	402	-	4,4,4	0.25	0	6,6,6	0.43	0
2	SO4	D	401	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	A	406	-	4,4,4	0.37	0	6,6,6	0.53	0
4	GOL	D	408	-	5,5,5	0.44	0	5,5,5	0.44	0
2	SO4	D	404	-	4,4,4	0.27	0	6,6,6	0.39	0
2	SO4	D	405	-	4,4,4	0.38	0	6,6,6	0.57	0
2	SO4	C	405	-	4,4,4	0.44	0	6,6,6	0.65	0
4	GOL	C	407	-	5,5,5	0.37	0	5,5,5	1.12	0
2	SO4	A	401	-	4,4,4	0.15	0	6,6,6	0.49	0
2	SO4	C	402	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	A	404	-	4,4,4	0.20	0	6,6,6	0.53	0
2	SO4	C	400	-	4,4,4	0.24	0	6,6,6	0.47	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
4	GOL	C	406	-	-	2/4/4/4	-
4	GOL	C	407	-	-	1/4/4/4	-
3	15P	A	408	-	-	12/16/16/101	-
4	GOL	D	408	-	-	2/4/4/4	-
4	GOL	A	409	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	407	-	-	4/4/4/4	-
4	GOL	B	407	-	-	2/4/4/4	-
3	15P	D	409	-	-	12/16/16/101	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	407	SO4	O1-S	2.00	1.56	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	409	GOL	C1-C2-C3-O3
4	C	406	GOL	O1-C1-C2-C3
4	D	407	GOL	O1-C1-C2-O2
4	D	407	GOL	C1-C2-C3-O3
4	D	407	GOL	O2-C2-C3-O3
4	D	408	GOL	C1-C2-C3-O3
3	A	408	15P	O1-C3-C4-O2
3	A	408	15P	O5-C10-C9-O4
3	A	408	15P	O2-C5-C6-O3
3	D	409	15P	O5-C10-C9-O4
3	D	409	15P	C12-C11-O5-C10
4	B	407	GOL	O2-C2-C3-O3
4	C	406	GOL	O1-C1-C2-O2
4	D	408	GOL	O2-C2-C3-O3
3	D	409	15P	OXT-C1-C2-O1
3	D	409	15P	O2-C5-C6-O3
4	B	407	GOL	C1-C2-C3-O3
4	D	407	GOL	O1-C1-C2-C3
3	A	408	15P	O5-C11-C12-O6
3	D	409	15P	O5-C11-C12-O6
4	A	409	GOL	O2-C2-C3-O3
3	D	409	15P	O1-C3-C4-O2
3	D	409	15P	C4-C3-O1-C2
3	A	408	15P	C8-C7-O3-C6
3	D	409	15P	C9-C10-O5-C11
3	A	408	15P	C9-C10-O5-C11

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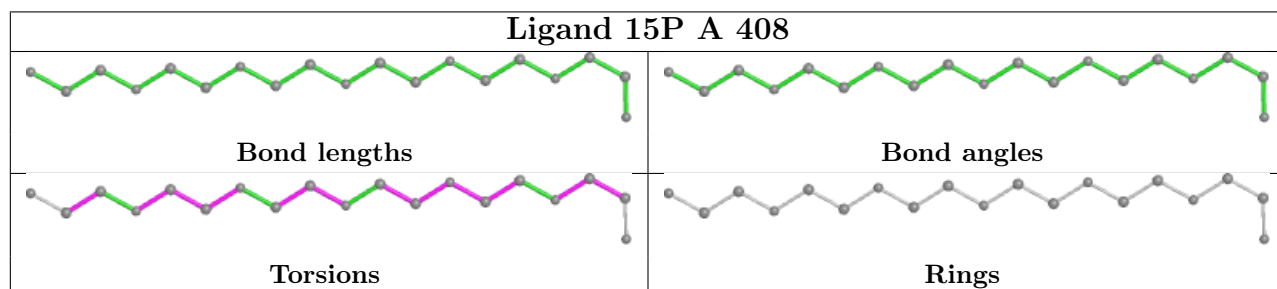
Mol	Chain	Res	Type	Atoms
3	D	409	15P	C6-C5-O2-C4
3	A	408	15P	C10-C9-O4-C8
3	D	409	15P	C8-C7-O3-C6
3	A	408	15P	C3-C4-O2-C5
3	A	408	15P	OXT-C1-C2-O1
3	A	408	15P	C1-C2-O1-C3
3	D	409	15P	C5-C6-O3-C7
3	A	408	15P	C6-C5-O2-C4
3	D	409	15P	O3-C7-C8-O4
4	C	407	GOL	O1-C1-C2-O2
3	A	408	15P	O3-C7-C8-O4

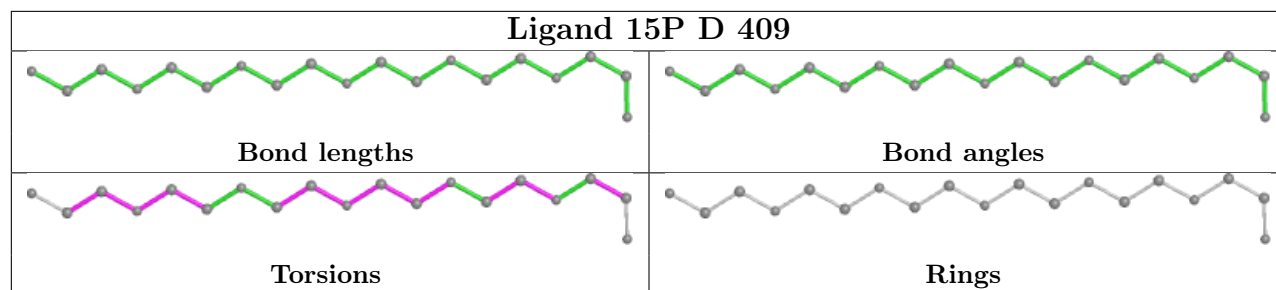
There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	408	15P	6	0
2	B	400	SO4	2	0
3	D	409	15P	2	0
4	C	407	GOL	1	0
2	A	404	SO4	1	0
2	C	400	SO4	3	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	366/399 (91%)	0.07	10 (2%) 54 52	19, 46, 106, 129	0
1	B	367/399 (91%)	-0.21	1 (0%) 94 93	12, 31, 74, 125	0
1	C	368/399 (92%)	-0.21	1 (0%) 94 93	12, 31, 75, 131	1 (0%)
1	D	366/399 (91%)	0.05	9 (2%) 57 55	19, 45, 103, 131	3 (0%)
All	All	1467/1596 (91%)	-0.08	21 (1%) 75 73	12, 39, 93, 131	4 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	111	LEU	5.1
1	A	132	ILE	3.2
1	A	140	LEU	2.8
1	C	101	PRO	2.8
1	D	140	LEU	2.5
1	D	135	ILE	2.5
1	D	183	ASP	2.5
1	A	323	PHE	2.4
1	D	143	ILE	2.4
1	A	131	GLY	2.3
1	A	366	VAL	2.3
1	D	132	ILE	2.3
1	D	63	GLN	2.3
1	D	136	LYS	2.2
1	A	90	TYR	2.2
1	B	100	ASP	2.2
1	A	365	VAL	2.1
1	D	366	VAL	2.1
1	A	122	GLU	2.1
1	A	367	ALA	2.0
1	A	135	ILE	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
2	SO4	D	406	5/5	0.81	0.31	49,51,66,67	5
4	GOL	C	407	6/6	0.82	0.20	55,60,63,64	0
4	GOL	A	409	6/6	0.83	0.21	60,68,69,78	0
2	SO4	D	403	5/5	0.84	0.49	75,81,113,117	0
2	SO4	B	406	5/5	0.86	0.16	62,66,109,110	0
4	GOL	B	407	6/6	0.88	0.11	53,59,63,64	0
2	SO4	D	402	5/5	0.88	0.15	64,73,100,102	0
4	GOL	D	408	6/6	0.88	0.12	77,82,86,89	0
2	SO4	C	404	5/5	0.89	0.15	91,93,105,121	0
2	SO4	B	402	5/5	0.90	0.29	81,98,107,108	0
2	SO4	A	400	5/5	0.90	0.25	104,106,122,128	0
2	SO4	D	404	5/5	0.90	0.24	70,74,125,133	0
2	SO4	A	406	5/5	0.90	0.35	30,35,51,59	5
2	SO4	C	402	5/5	0.91	0.22	96,102,110,116	0
2	SO4	A	402	5/5	0.91	0.23	65,78,94,95	0
2	SO4	C	405	5/5	0.92	0.27	35,39,42,42	5
3	15P	A	408	19/104	0.92	0.15	40,55,62,65	0
2	SO4	A	407	5/5	0.92	0.36	39,39,48,52	0
2	SO4	D	405	5/5	0.93	0.21	60,69,87,95	0
2	SO4	B	401	5/5	0.93	0.26	70,74,87,103	0
4	GOL	C	406	6/6	0.93	0.12	51,57,60,61	0
2	SO4	C	400	5/5	0.93	0.23	59,62,93,97	0
3	15P	D	409	19/104	0.93	0.14	35,53,74,76	0
2	SO4	B	400	5/5	0.94	0.22	65,83,89,102	0
2	SO4	C	401	5/5	0.94	0.35	76,85,93,107	0
2	SO4	B	404	5/5	0.94	0.14	46,49,53,54	5
2	SO4	B	405	5/5	0.94	0.21	22,30,43,47	5

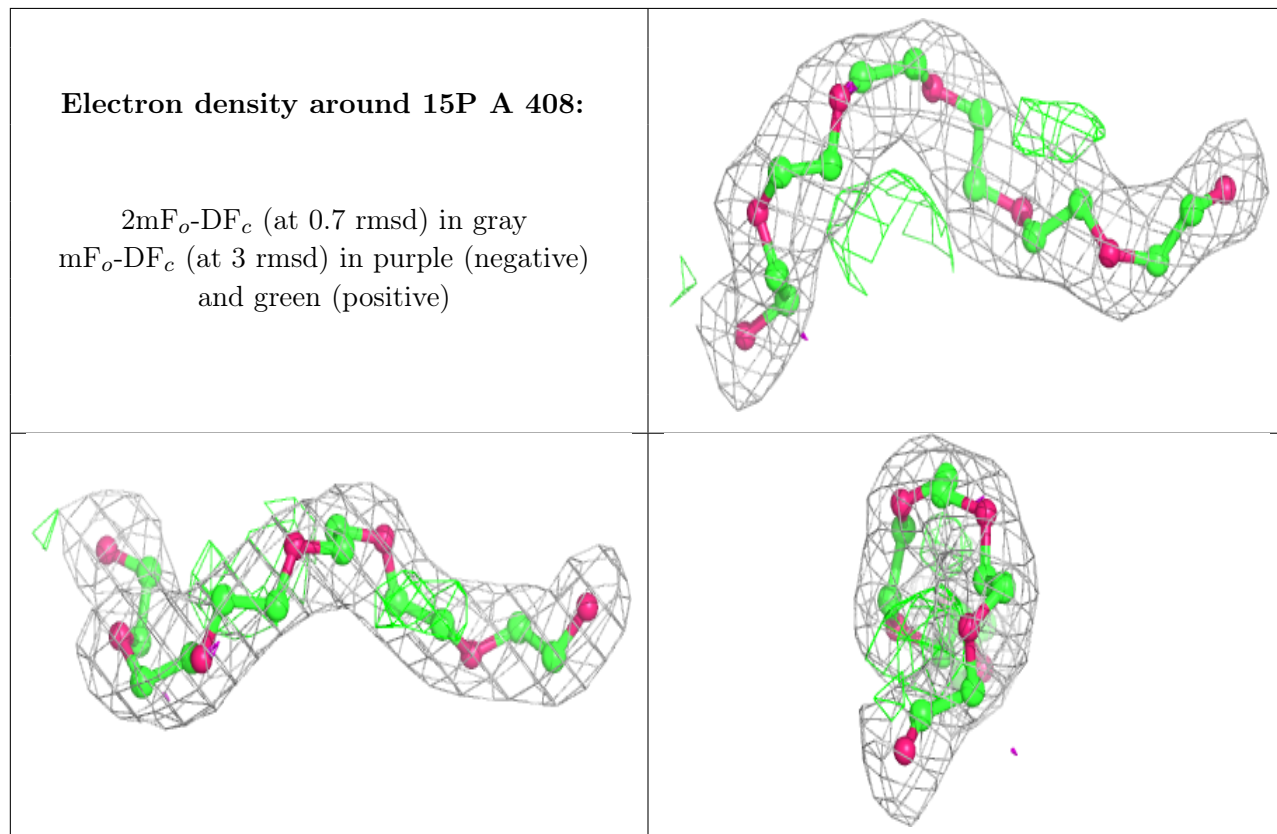
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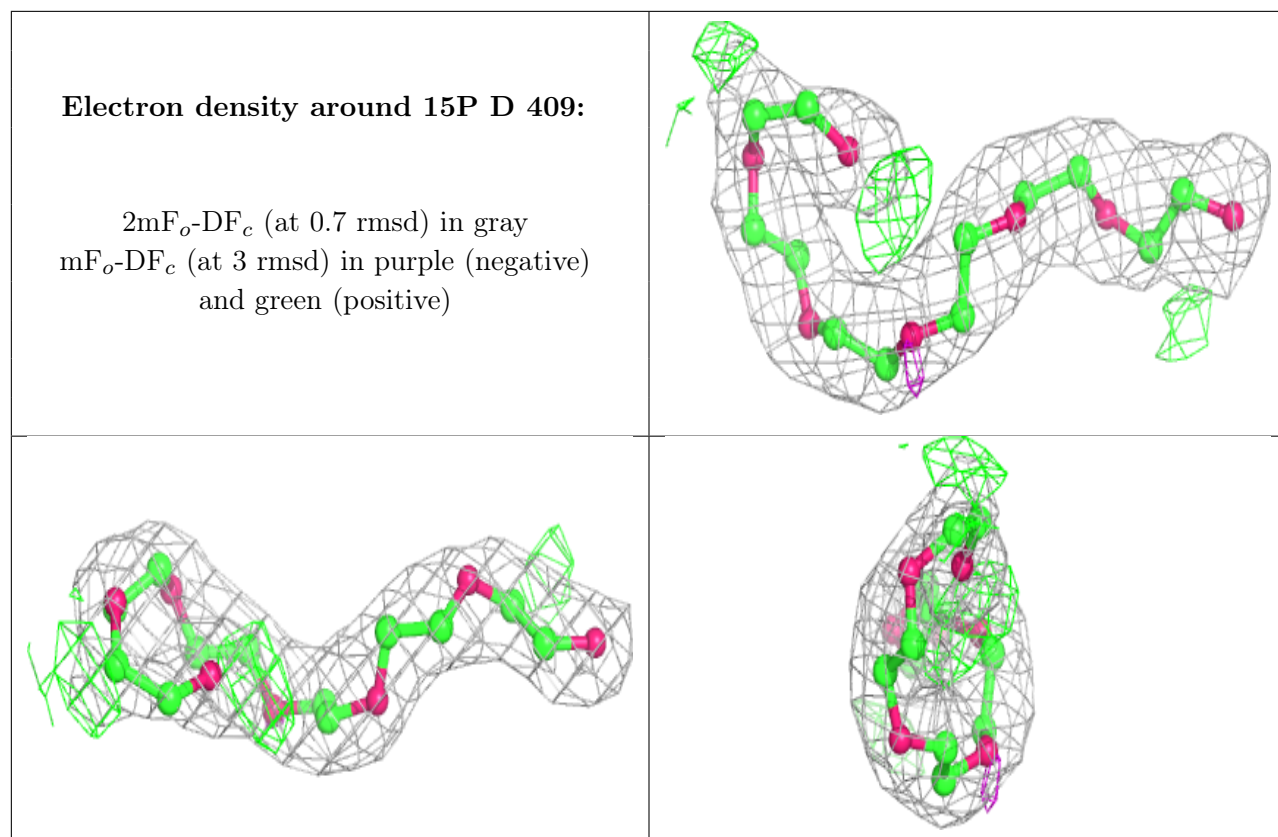


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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	403	5/5	0.94	0.15	83,85,96,101	0
4	GOL	D	407	6/6	0.94	0.24	40,52,55,62	0
2	SO4	D	401	5/5	0.94	0.28	102,103,112,112	0
2	SO4	A	405	5/5	0.95	0.18	27,41,59,62	5
2	SO4	A	401	5/5	0.96	0.14	65,67,92,94	0
2	SO4	A	404	5/5	0.97	0.09	54,58,70,72	0
2	SO4	D	400	5/5	0.98	0.13	51,61,66,68	0
2	SO4	C	403	5/5	0.99	0.13	46,47,52,55	0
2	SO4	B	403	5/5	0.99	0.12	41,45,50,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.