



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2020 – 10:38 PM BST

PDB ID : 6ZEE  
Title : Structure of PP1(7-300) bound to Phactr1 (507-580) at pH8.4  
Authors : Mouilleron, S.; Treisman, R.; Fedoryshchak, R.; Lee, R.; Butler, A.M.; Prechova, M.  
Deposited on : 2020-06-16  
Resolution : 1.90 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.

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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 : 2.14.6  
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) : 2.14.6

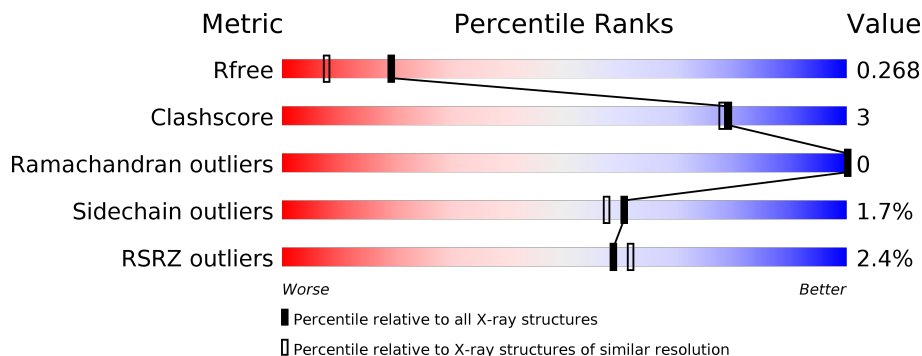
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	299	
1	B	299	
1	I	299	
1	K	299	
1	P	299	
1	Q	299	

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Mol	Chain	Length	Quality of chain
2	C	78	<p>4% 77% 12% 12%</p>
2	D	78	<p>78% 17%</p>
2	U	78	<p>4% 77% 6% 17%</p>
2	V	78	<p>6% 85% 12%</p>
2	W	78	<p>5% 78% 9% 13%</p>
2	X	78	<p>6% 81% 5% 13%</p>

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 35835 atoms, of which 17334 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 Serine/threonine-protein phosphatase PP1-alpha catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	P	294	4632	1502	2293	394	425	18	0	0	0
1	Q	294	4606	1499	2270	386	432	19	0	1	0
1	B	294	4646	1508	2296	393	431	18	0	3	0
1	A	294	4676	1516	2312	394	435	19	0	4	0
1	I	294	4631	1505	2287	390	431	18	0	2	0
1	K	294	4609	1501	2272	384	433	19	0	2	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	2	GLY	-	expression tag	UNP P62136
P	3	HIS	-	expression tag	UNP P62136
P	4	MET	-	expression tag	UNP P62136
P	5	GLY	-	expression tag	UNP P62136
P	6	SER	-	expression tag	UNP P62136
Q	2	GLY	-	expression tag	UNP P62136
Q	3	HIS	-	expression tag	UNP P62136
Q	4	MET	-	expression tag	UNP P62136
Q	5	GLY	-	expression tag	UNP P62136
Q	6	SER	-	expression tag	UNP P62136
B	2	GLY	-	expression tag	UNP P62136
B	3	HIS	-	expression tag	UNP P62136
B	4	MET	-	expression tag	UNP P62136
B	5	GLY	-	expression tag	UNP P62136
B	6	SER	-	expression tag	UNP P62136
A	2	GLY	-	expression tag	UNP P62136

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3	HIS	-	expression tag	UNP P62136
A	4	MET	-	expression tag	UNP P62136
A	5	GLY	-	expression tag	UNP P62136
A	6	SER	-	expression tag	UNP P62136
I	2	GLY	-	expression tag	UNP P62136
I	3	HIS	-	expression tag	UNP P62136
I	4	MET	-	expression tag	UNP P62136
I	5	GLY	-	expression tag	UNP P62136
I	6	SER	-	expression tag	UNP P62136
K	2	GLY	-	expression tag	UNP P62136
K	3	HIS	-	expression tag	UNP P62136
K	4	MET	-	expression tag	UNP P62136
K	5	GLY	-	expression tag	UNP P62136
K	6	SER	-	expression tag	UNP P62136

- Molecule 2 is a protein called Phosphatase and actin regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	W	68	1133	357	562	109	104	1	0	0	0
2	X	68	1101	351	540	105	104	1	0	0	0
2	D	65	1053	336	514	101	101	1	0	0	0
2	C	69	1125	357	553	109	105	1	0	0	0
2	U	65	1060	337	521	102	99	1	0	0	0
2	V	69	1099	353	535	103	107	1	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	503	GLY	-	expression tag	UNP Q4VY12
W	504	PRO	-	expression tag	UNP Q4VY12
W	505	LEU	-	expression tag	UNP Q4VY12
W	506	GLY	-	expression tag	UNP Q4VY12
W	507	SER	-	expression tag	UNP Q4VY12
X	503	GLY	-	expression tag	UNP Q4VY12
X	504	PRO	-	expression tag	UNP Q4VY12
X	505	LEU	-	expression tag	UNP Q4VY12

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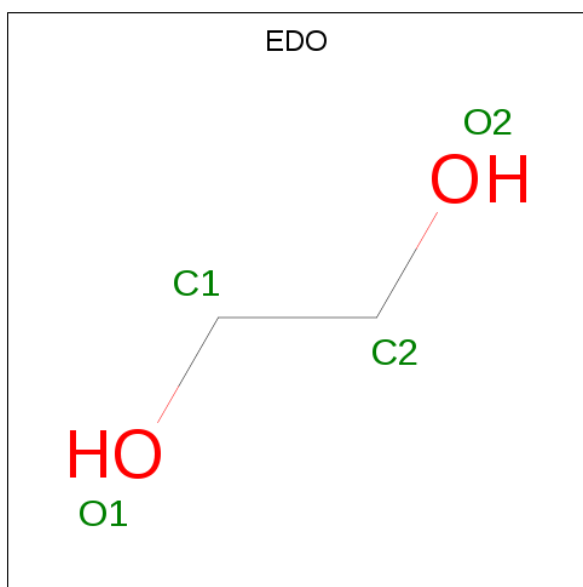
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Chain	Residue	Modelled	Actual	Comment	Reference
X	506	GLY	-	expression tag	UNP Q4VY12
X	507	SER	-	expression tag	UNP Q4VY12
D	503	GLY	-	expression tag	UNP Q4VY12
D	504	PRO	-	expression tag	UNP Q4VY12
D	505	LEU	-	expression tag	UNP Q4VY12
D	506	GLY	-	expression tag	UNP Q4VY12
D	507	SER	-	expression tag	UNP Q4VY12
C	503	GLY	-	expression tag	UNP Q4VY12
C	504	PRO	-	expression tag	UNP Q4VY12
C	505	LEU	-	expression tag	UNP Q4VY12
C	506	GLY	-	expression tag	UNP Q4VY12
C	507	SER	-	expression tag	UNP Q4VY12
U	503	GLY	-	expression tag	UNP Q4VY12
U	504	PRO	-	expression tag	UNP Q4VY12
U	505	LEU	-	expression tag	UNP Q4VY12
U	506	GLY	-	expression tag	UNP Q4VY12
U	507	SER	-	expression tag	UNP Q4VY12
V	503	GLY	-	expression tag	UNP Q4VY12
V	504	PRO	-	expression tag	UNP Q4VY12
V	505	LEU	-	expression tag	UNP Q4VY12
V	506	GLY	-	expression tag	UNP Q4VY12
V	507	SER	-	expression tag	UNP Q4VY12

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	2	Total Mn 2 2	0	0
3	Q	2	Total Mn 2 2	0	0
3	K	2	Total Mn 2 2	0	0
3	B	2	Total Mn 2 2	0	0
3	I	2	Total Mn 2 2	0	0
3	A	2	Total Mn 2 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	P	1	10	2	6	2	0	0
4	P	1	10	2	6	2	0	0
4	P	1	10	2	6	2	0	0
4	P	1	10	2	6	2	0	0
4	P	1	10	2	6	2	0	0
4	P	1	10	2	6	2	0	0
4	P	1	10	2	6	2	0	0
4	P	1	10	2	6	2	0	0
4	Q	1	10	2	6	2	0	0
4	Q	1	10	2	6	2	0	0
4	Q	1	10	2	6	2	0	0
4	Q	1	10	2	6	2	0	0
4	Q	1	10	2	6	2	0	0
4	B	1	10	2	6	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0

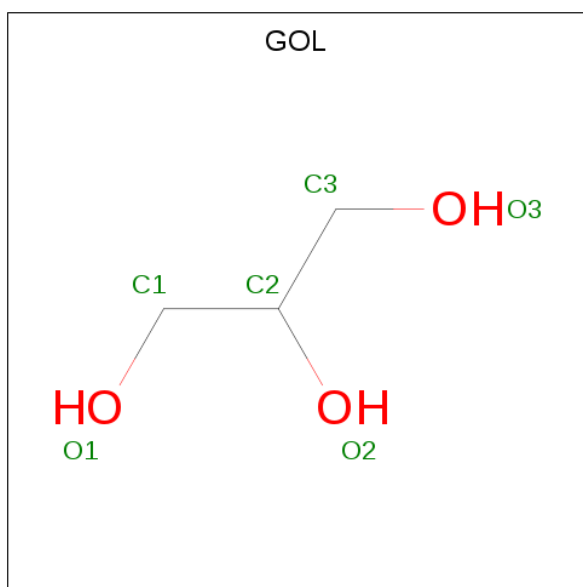
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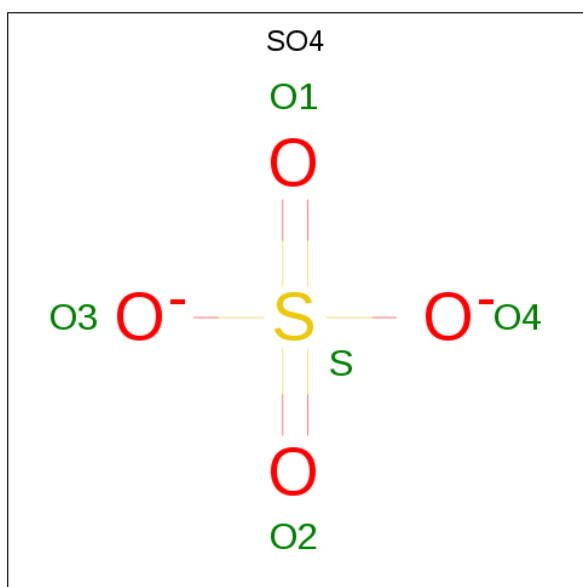
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	I	1	Total	C	H	O	0	0
			10	2	6	2		
4	I	1	Total	C	H	O	0	0
			10	2	6	2		
4	I	1	Total	C	H	O	0	0
			10	2	6	2		
4	I	1	Total	C	H	O	0	0
			10	2	6	2		
4	I	1	Total	C	H	O	0	0
			10	2	6	2		
4	I	1	Total	C	H	O	0	0
			10	2	6	2		
4	I	1	Total	C	H	O	0	0
			10	2	6	2		
4	K	1	Total	C	H	O	0	0
			10	2	6	2		
4	K	1	Total	C	H	O	0	0
			10	2	6	2		
4	K	1	Total	C	H	O	0	0
			10	2	6	2		
4	K	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	U	1	Total	C	H	O	0	0
			10	2	6	2		
4	V	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



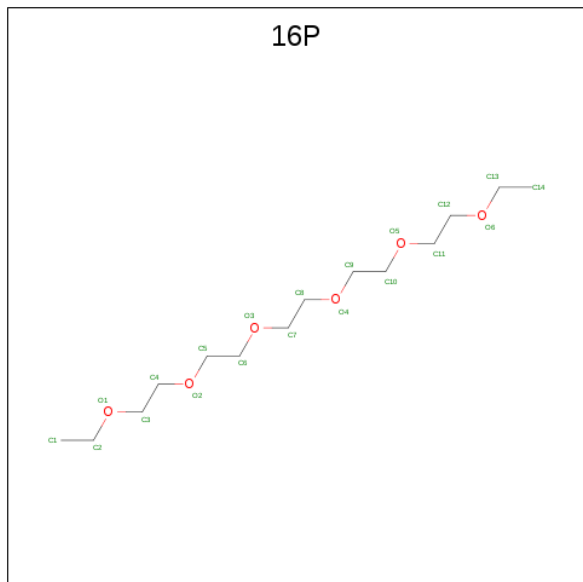
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	P	1	13	3	7	3	0	0
5	K	1	13	3	7	3	0	0
5	K	1	13	3	7	3	0	0
5	X	1	13	3	7	3	0	0
5	D	1	12	3	6	3	0	0
5	C	1	13	3	7	3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	P	1	Total	O	S	0	0
			5	4	1		
6	P	1	Total	O	S	0	0
			5	4	1		
6	Q	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	W	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	U	1	Total	O	S	0	0
			5	4	1		
6	V	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 3,6,9,12,15,18-HEXAOXAICOSANE (three-letter code: 16P) (formula:  $C_{14}H_{30}O_6$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
7	A	1	25	7	14	4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	95	Total	O	0	0
			95	95		
8	Q	58	Total	O	0	0
			58	58		
8	B	125	Total	O	0	0
			125	125		
8	A	135	Total	O	0	0
			135	135		
8	I	86	Total	O	0	0
			86	86		
8	K	92	Total	O	0	0
			92	92		
8	W	17	Total	O	0	0
			17	17		
8	X	24	Total	O	0	0
			24	24		
8	D	33	Total	O	0	0
			33	33		

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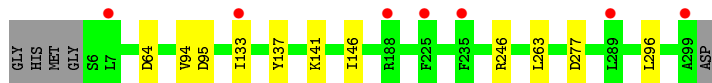
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
8	C	36	Total O 36 36	0	0
8	U	24	Total O 24 24	0	0
8	V	15	Total O 15 15	0	0

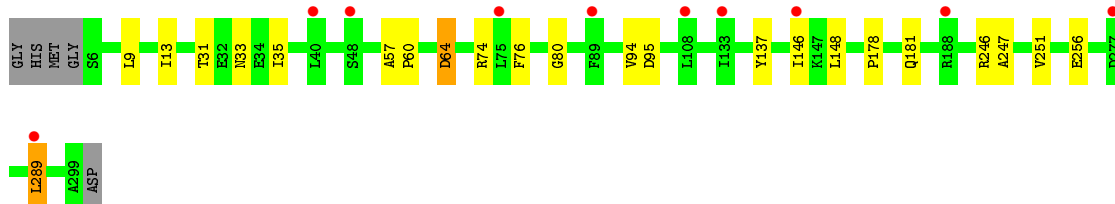
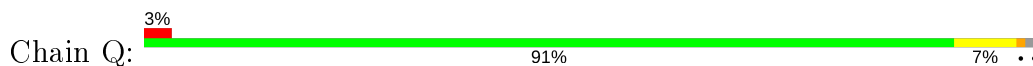
### 3 Residue-property plots [i](#)

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.

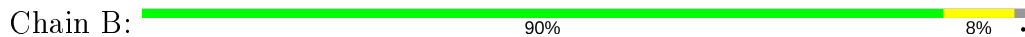
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



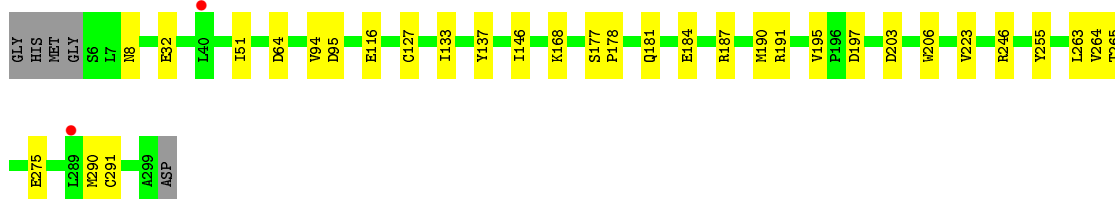
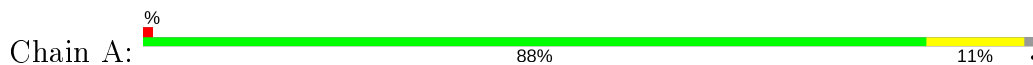
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



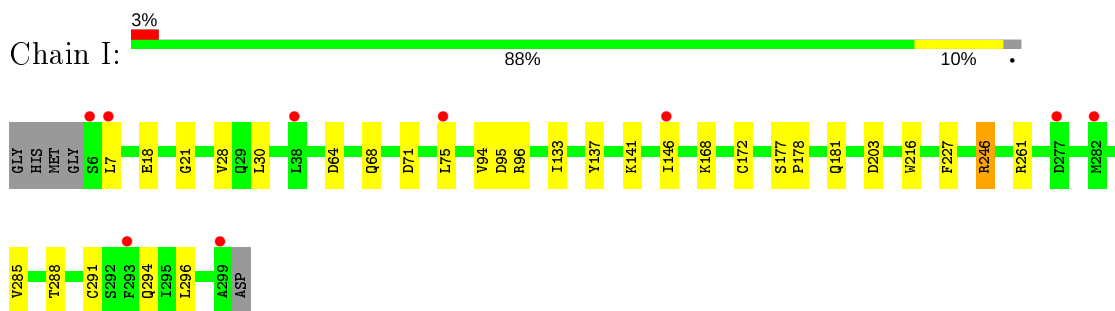
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



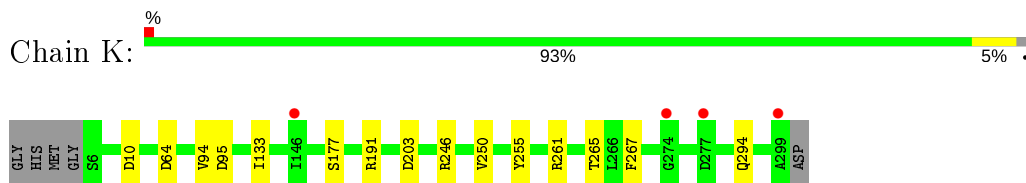
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



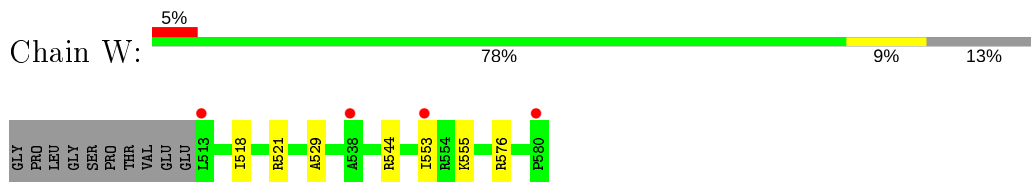
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



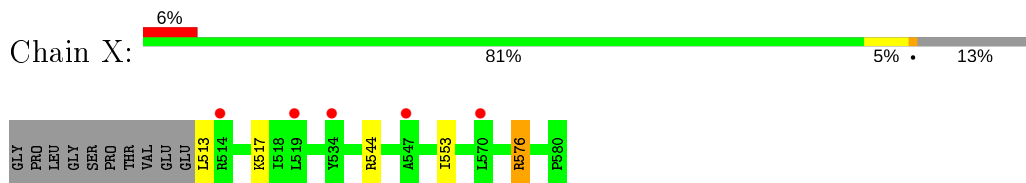
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



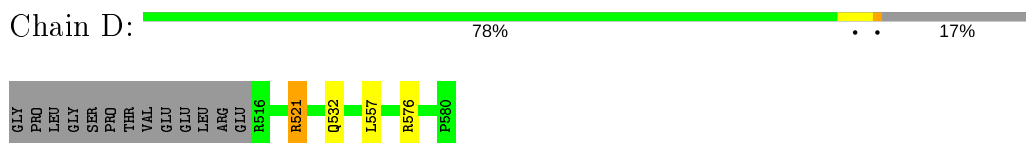
- Molecule 2: Phosphatase and actin regulator



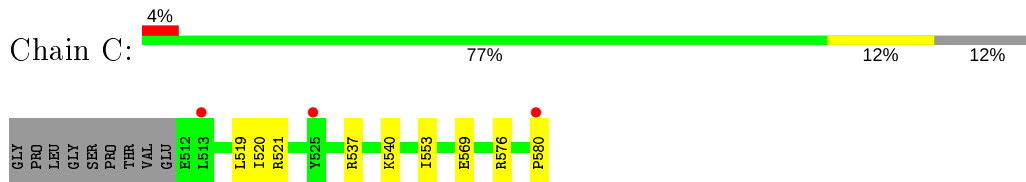
- Molecule 2: Phosphatase and actin regulator



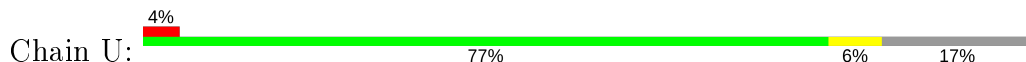
- Molecule 2: Phosphatase and actin regulator

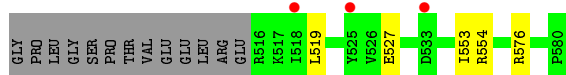


- Molecule 2: Phosphatase and actin regulator

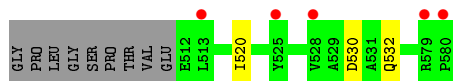
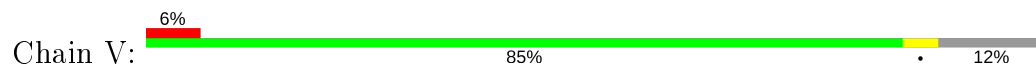


- Molecule 2: Phosphatase and actin regulator





- Molecule 2: Phosphatase and actin regulator





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.69Å 137.69Å 238.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.25 – 1.90 119.25 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (119.25-1.90) 99.5 (119.25-1.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.18_3845, PHENIX 1.18_3845	Depositor
R, $R_{free}$	0.236 , 0.268 0.236 , 0.268	Depositor DCC
$R_{free}$ test set	10131 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtrriage
Anisotropy	0.476	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.417 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	35835	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	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 51.62 % 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 5.4620e-05. 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: GOL, MN, 16P, EDO, 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	0.28	0/2430	0.49	0/3288
1	B	0.28	0/2413	0.47	0/3266
1	I	0.26	0/2404	0.44	0/3254
1	K	0.26	0/2397	0.45	0/3246
1	P	0.27	0/2393	0.46	0/3236
1	Q	0.26	0/2393	0.45	0/3239
2	C	0.25	0/583	0.45	0/784
2	D	0.24	0/550	0.47	0/741
2	U	0.24	0/550	0.43	0/740
2	V	0.23	0/575	0.41	0/775
2	W	0.25	0/582	0.44	0/781
2	X	0.24	0/572	0.42	0/770
All	All	0.26	0/17842	0.45	0/24120

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	2364	2312	2311	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2350	2296	2295	15	1
1	I	2344	2287	2286	22	1
1	K	2337	2272	2271	7	0
1	P	2339	2293	2291	6	0
1	Q	2336	2270	2269	15	0
2	C	572	553	553	6	0
2	D	539	514	514	2	0
2	U	539	521	521	4	0
2	V	564	535	535	3	0
2	W	571	562	562	4	0
2	X	561	540	540	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	I	2	0	0	0	0
3	K	2	0	0	0	0
3	P	2	0	0	0	0
3	Q	2	0	0	0	0
4	A	56	84	84	2	0
4	B	52	78	78	1	0
4	D	4	6	6	0	0
4	I	28	42	42	3	0
4	K	16	24	24	0	0
4	P	32	48	48	0	0
4	Q	20	30	30	0	0
4	U	4	6	6	0	0
4	V	4	6	6	0	0
5	C	6	7	8	0	0
5	D	6	6	8	1	0
5	K	12	14	16	1	0
5	P	6	7	8	0	0
5	X	6	7	8	1	0
6	A	5	0	0	0	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	I	10	0	0	1	0
6	K	5	0	0	0	0
6	P	10	0	0	0	0
6	Q	5	0	0	1	0
6	U	5	0	0	0	0
6	V	5	0	0	0	0
6	W	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	11	14	12	5	0
8	A	135	0	0	2	0
8	B	125	0	0	3	0
8	C	36	0	0	2	0
8	D	33	0	0	1	0
8	I	86	0	0	0	0
8	K	92	0	0	1	0
8	P	95	0	0	0	0
8	Q	58	0	0	1	0
8	U	24	0	0	1	0
8	V	15	0	0	1	0
8	W	17	0	0	0	0
8	X	24	0	0	0	0
All	All	18501	17334	17332	99	1

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 (99) 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:C:569:GLU:OE2	8:C:701:HOH:O	1.95	0.84
1:Q:251:VAL:HG11	1:Q:256:GLU:HB2	1.64	0.78
6:Q:508:SO4:O2	8:Q:601:HOH:O	2.04	0.75
1:B:220:ASP:OD1	8:B:601:HOH:O	2.14	0.65
5:D:601:GOL:O1	8:D:701:HOH:O	2.09	0.65
1:I:18:GLU:OE1	4:I:504:EDO:O1	2.10	0.64
1:I:141:LYS:HD2	1:I:146:ILE:HD11	1.80	0.63
1:Q:251:VAL:HG11	1:Q:256:GLU:CB	2.29	0.62
2:V:532:GLN:NE2	8:V:701:HOH:O	2.31	0.62
2:C:580:PRO:OXT	8:C:702:HOH:O	2.16	0.61
1:K:250[B]:VAL:HG22	1:K:267:PHE:CZ	2.39	0.57
1:B:297:LYS:NZ	8:B:608:HOH:O	2.38	0.57
2:U:554:ARG:NH1	8:U:701:HOH:O	2.31	0.56
1:A:197:ASP:O	4:A:514:EDO:O2	2.21	0.56
1:P:141:LYS:HD2	1:P:146:ILE:HD11	1.88	0.55
1:A:127[B]:CYS:SG	1:A:195:VAL:HG21	2.46	0.55
1:I:71:ASP:O	1:I:75:LEU:HD23	2.07	0.54
1:A:191:ARG:HE	7:A:509:16P:H71	1.73	0.54
1:I:75:LEU:HD22	1:I:296:LEU:CD1	2.39	0.53
1:A:137:TYR:CE1	1:A:146:ILE:HD12	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:HD23	1:A:264:VAL:N	2.23	0.53
1:B:94:VAL:O	1:B:95:ASP:HB2	2.11	0.51
1:K:10:ASP:OD1	8:K:601:HOH:O	2.19	0.50
1:K:133:ILE:HD11	2:X:553:ILE:HG21	1.92	0.50
1:I:285:VAL:HG12	1:I:291:CYS:SG	2.52	0.50
1:B:141:LYS:HD2	1:B:146:ILE:HD11	1.94	0.50
1:Q:178:PRO:O	1:Q:181:GLN:NE2	2.45	0.49
1:Q:74:ARG:NH1	2:V:530:ASP:O	2.46	0.49
1:B:137:TYR:CE2	1:B:146:ILE:HD12	2.48	0.49
1:I:28:VAL:HG12	1:I:30:LEU:HD22	1.95	0.49
1:P:137:TYR:CE2	1:P:146:ILE:HD12	2.48	0.49
1:K:191:ARG:HE	5:K:508:GOL:H32	1.79	0.48
1:Q:31:THR:HG22	1:Q:33:ASN:H	1.78	0.48
1:I:133:ILE:HD11	2:U:553:ILE:HG21	1.94	0.48
1:I:94:VAL:O	1:I:95:ASP:HB2	2.13	0.48
1:I:30:LEU:HD23	4:I:511:EDO:H12	1.96	0.48
1:I:288:THR:O	1:I:288:THR:HG22	2.15	0.47
1:A:184:GLU:OE1	1:A:187:ARG:NE	2.44	0.47
1:Q:35:ILE:CG2	1:Q:148:LEU:HD11	2.44	0.47
1:P:133:ILE:HD11	2:W:553:ILE:HG21	1.96	0.47
1:A:191:ARG:HH21	7:A:509:16P:H62	1.79	0.47
1:I:168:LYS:HE3	2:U:519:LEU:HD12	1.96	0.47
1:Q:76:PHE:O	1:Q:80:GLY:N	2.49	0.46
1:B:288:THR:O	2:D:521:ARG:NH1	2.42	0.46
1:I:261:ARG:NH2	2:W:544:ARG:HE	2.14	0.45
1:A:51:ILE:HG22	7:A:509:16P:H52	1.97	0.45
1:Q:94:VAL:O	1:Q:95:ASP:HB2	2.17	0.45
1:B:181:GLN:NE2	8:B:617:HOH:O	2.47	0.45
1:I:75:LEU:HD22	1:I:296:LEU:HD12	1.98	0.45
1:A:94:VAL:O	1:A:95:ASP:HB2	2.16	0.45
1:A:178:PRO:O	1:A:181:GLN:NE2	2.50	0.44
1:B:76:PHE:O	1:B:80:GLY:N	2.48	0.44
1:P:296:LEU:HD23	2:W:529:ALA:HB3	1.99	0.44
1:A:32:GLU:OE2	8:A:601:HOH:O	2.21	0.44
1:I:68:GLN:NE2	1:I:71:ASP:OD2	2.46	0.44
1:K:177:SER:HB2	1:K:203:ASP:HB2	1.98	0.44
1:Q:9:LEU:O	1:Q:13:ILE:HG22	2.17	0.44
1:Q:137:TYR:CE2	1:Q:146:ILE:HD12	2.53	0.44
1:A:116:GLU:OE2	8:A:602:HOH:O	2.21	0.44
1:A:191:ARG:HE	7:A:509:16P:C7	2.30	0.44
1:A:275:GLU:OE2	2:C:540:LYS:NZ	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:TYR:HA	1:B:265:THR:O	2.17	0.44
1:A:263:LEU:C	1:A:263:LEU:HD23	2.38	0.44
1:A:133:ILE:HD11	2:C:553:ILE:HG21	1.98	0.44
1:A:255:TYR:HA	1:A:265:THR:O	2.19	0.43
1:A:177:SER:HB2	1:A:203:ASP:HB2	2.00	0.43
1:I:294:GLN:HG3	2:U:527:GLU:HB3	1.98	0.43
1:A:137:TYR:CZ	1:A:146:ILE:HD12	2.53	0.43
1:B:74[A]:ARG:NH1	2:D:532:GLN:OE1	2.51	0.43
1:P:94:VAL:O	1:P:95:ASP:HB2	2.19	0.43
1:Q:31:THR:HG22	1:Q:33:ASN:N	2.33	0.43
2:W:518:ILE:O	2:W:521:ARG:NH2	2.50	0.43
1:B:216:TRP:CZ3	1:B:227:PHE:HB3	2.54	0.43
2:X:576:ARG:HE	5:X:601:GOL:H2	1.84	0.42
1:K:94:VAL:O	1:K:95:ASP:HB2	2.18	0.42
1:B:177:SER:HB2	1:B:203:ASP:HB2	2.02	0.42
1:A:291:CYS:SG	2:C:520:ILE:HD11	2.59	0.42
1:I:177:SER:HB2	1:I:203:ASP:HB2	2.01	0.42
1:Q:289:LEU:HD12	2:V:520:ILE:HA	2.01	0.42
1:B:58:PRO:HA	1:B:285:VAL:O	2.20	0.42
1:B:75:LEU:C	1:B:75:LEU:HD23	2.40	0.42
1:I:172:CYS:O	1:I:246:ARG:HA	2.20	0.42
1:B:137:TYR:CZ	1:B:146:ILE:HD12	2.55	0.42
1:I:96[B]:ARG:NH1	6:I:505:SO4:O3	2.47	0.42
1:Q:64:ASP:OD1	1:Q:247:ALA:HB1	2.20	0.41
1:I:137:TYR:CE2	1:I:146:ILE:HD12	2.55	0.41
1:I:178:PRO:O	1:I:181:GLN:NE2	2.53	0.41
1:K:255:TYR:HA	1:K:265:THR:O	2.20	0.41
1:I:216:TRP:CZ3	1:I:227:PHE:HB3	2.56	0.41
1:A:206:TRP:CD2	1:A:223:VAL:HG11	2.56	0.41
1:A:190:MET:HA	7:A:509:16P:H81	2.03	0.40
1:A:223:VAL:HG22	4:A:514:EDO:H21	2.03	0.40
1:P:263:LEU:C	1:P:263:LEU:HD23	2.42	0.40
1:A:8:ASN:N	1:A:8:ASN:OD1	2.51	0.40
1:I:133:ILE:O	4:I:507:EDO:O1	2.39	0.40
1:A:168:LYS:HE3	2:C:519:LEU:HD12	2.03	0.40
1:Q:57:ALA:HB1	1:Q:60:PRO:HA	2.04	0.40
1:Q:64:ASP:OD1	1:Q:64:ASP:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ARG:H	1:I:21:GLY:O[6_444]	1.54	0.06

### 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	296/299 (99%)	282 (95%)	14 (5%)	0	100	100
1	B	295/299 (99%)	283 (96%)	12 (4%)	0	100	100
1	I	294/299 (98%)	277 (94%)	17 (6%)	0	100	100
1	K	294/299 (98%)	279 (95%)	15 (5%)	0	100	100
1	P	292/299 (98%)	277 (95%)	15 (5%)	0	100	100
1	Q	293/299 (98%)	276 (94%)	17 (6%)	0	100	100
2	C	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
2	D	63/78 (81%)	63 (100%)	0	0	100	100
2	U	63/78 (81%)	63 (100%)	0	0	100	100
2	V	67/78 (86%)	67 (100%)	0	0	100	100
2	W	66/78 (85%)	65 (98%)	1 (2%)	0	100	100
2	X	66/78 (85%)	63 (96%)	3 (4%)	0	100	100
All	All	2156/2262 (95%)	2061 (96%)	95 (4%)	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	258/262 (98%)	255 (99%)	3 (1%)	71	70
1	B	255/262 (97%)	253 (99%)	2 (1%)	81	82
1	I	254/262 (97%)	251 (99%)	3 (1%)	71	70
1	K	254/262 (97%)	250 (98%)	4 (2%)	62	60
1	P	252/262 (96%)	249 (99%)	3 (1%)	71	70
1	Q	253/262 (97%)	250 (99%)	3 (1%)	71	70
2	C	58/69 (84%)	55 (95%)	3 (5%)	23	14
2	D	55/69 (80%)	52 (94%)	3 (6%)	21	12
2	U	55/69 (80%)	54 (98%)	1 (2%)	59	55
2	V	57/69 (83%)	57 (100%)	0	100	100
2	W	59/69 (86%)	57 (97%)	2 (3%)	37	28
2	X	57/69 (83%)	53 (93%)	4 (7%)	15	7
All	All	1867/1986 (94%)	1836 (98%)	31 (2%)	60	57

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	64	ASP
1	P	246	ARG
1	P	277	ASP
1	Q	64	ASP
1	Q	246	ARG
1	Q	289	LEU
1	B	64	ASP
1	B	246	ARG
1	A	64	ASP
1	A	246	ARG
1	A	290	MET
1	I	7	LEU
1	I	64	ASP
1	I	246	ARG
1	K	64	ASP
1	K	246	ARG
1	K	261	ARG
1	K	294	GLN
2	W	555	LYS
2	W	576	ARG
2	X	513	LEU
2	X	517	LYS

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Mol	Chain	Res	Type
2	X	544	ARG
2	X	576	ARG
2	D	521	ARG
2	D	557	LEU
2	D	576	ARG
2	C	521	ARG
2	C	537	ARG
2	C	576	ARG
2	U	576	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 87 ligands modelled in this entry, 12 are monoatomic - leaving 75 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	EDO	A	510	-	3,3,3	0.49	0	2,2,2	0.28	0
5	GOL	C	601	-	5,5,5	0.89	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	503	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	A	508	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	B	506	-	3,3,3	0.47	0	2,2,2	0.33	0
6	SO4	B	516	3	4,4,4	0.17	0	6,6,6	0.16	0
4	EDO	B	515	-	3,3,3	0.46	0	2,2,2	0.28	0
4	EDO	U	601	-	3,3,3	0.46	0	2,2,2	0.29	0
6	SO4	K	509	3	4,4,4	0.11	0	6,6,6	0.12	0
4	EDO	Q	507	-	3,3,3	0.45	0	2,2,2	0.29	0
4	EDO	B	507	-	3,3,3	0.43	0	2,2,2	0.32	0
4	EDO	A	516	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	Q	503	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	A	512	-	3,3,3	0.45	0	2,2,2	0.33	0
6	SO4	W	601	-	4,4,4	0.14	0	6,6,6	0.06	0
4	EDO	B	504	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	A	504	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	B	512	-	3,3,3	0.47	0	2,2,2	0.33	0
6	SO4	U	602	-	4,4,4	0.14	0	6,6,6	0.09	0
4	EDO	I	504	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	P	508	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	A	506	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	511	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	P	504	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	I	510	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	P	503	-	3,3,3	0.43	0	2,2,2	0.51	0
4	EDO	I	511	-	3,3,3	0.44	0	2,2,2	0.41	0
4	EDO	P	510	-	3,3,3	0.47	0	2,2,2	0.27	0
4	EDO	A	505	-	3,3,3	0.43	0	2,2,2	0.40	0
4	EDO	I	508	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	P	505	-	3,3,3	0.48	0	2,2,2	0.30	0
4	EDO	Q	506	-	3,3,3	0.46	0	2,2,2	0.28	0
6	SO4	C	602	-	4,4,4	0.13	0	6,6,6	0.10	0
4	EDO	B	503	-	3,3,3	0.44	0	2,2,2	0.30	0
6	SO4	D	603	-	4,4,4	0.15	0	6,6,6	0.09	0
4	EDO	B	509	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	P	506	-	3,3,3	0.46	0	2,2,2	0.31	0
6	SO4	V	602	-	4,4,4	0.13	0	6,6,6	0.07	0
4	EDO	K	503	-	3,3,3	0.45	0	2,2,2	0.31	0
6	SO4	I	505	3	4,4,4	0.09	0	6,6,6	0.10	0
5	GOL	K	504	-	5,5,5	0.90	0	5,5,5	0.98	0
4	EDO	A	507	-	3,3,3	0.46	0	2,2,2	0.32	0
5	GOL	K	508	-	5,5,5	1.01	0	5,5,5	0.89	0
4	EDO	A	514	-	3,3,3	0.46	0	2,2,2	0.26	0
4	EDO	K	507	-	3,3,3	0.47	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	515	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	D	602	-	3,3,3	0.44	0	2,2,2	0.34	0
6	SO4	A	518	3	4,4,4	0.13	0	6,6,6	0.16	0
4	EDO	K	506	-	3,3,3	0.46	0	2,2,2	0.31	0
6	SO4	I	506	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	K	505	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	A	513	-	3,3,3	0.46	0	2,2,2	0.35	0
5	GOL	P	509	-	5,5,5	0.90	0	5,5,5	0.98	0
4	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	B	513	-	3,3,3	0.45	0	2,2,2	0.31	0
4	EDO	A	517	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	V	601	-	3,3,3	0.46	0	2,2,2	0.35	0
5	GOL	X	601	-	5,5,5	0.93	0	5,5,5	0.95	0
4	EDO	A	511	-	3,3,3	0.46	0	2,2,2	0.34	0
6	SO4	B	517	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	B	510	-	3,3,3	0.47	0	2,2,2	0.29	0
4	EDO	I	507	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	Q	504	-	3,3,3	0.45	0	2,2,2	0.31	0
4	EDO	I	503	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	I	509	-	3,3,3	0.46	0	2,2,2	0.27	0
6	SO4	P	513	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	Q	508	3	4,4,4	0.16	0	6,6,6	0.17	0
7	16P	A	509	-	10,10,19	0.49	0	9,9,18	0.39	0
4	EDO	B	508	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	B	514	-	3,3,3	0.47	0	2,2,2	0.29	0
4	EDO	P	511	-	3,3,3	0.47	0	2,2,2	0.36	0
6	SO4	P	512	3	4,4,4	0.15	0	6,6,6	0.19	0
4	EDO	P	507	-	3,3,3	0.48	0	2,2,2	0.22	0
5	GOL	D	601	-	5,5,5	0.89	0	5,5,5	0.98	0
4	EDO	Q	505	-	3,3,3	0.45	0	2,2,2	0.32	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	EDO	A	510	-	-	1/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	A	508	-	-	0/1/1/1	-
4	EDO	B	506	-	-	0/1/1/1	-
4	EDO	B	515	-	-	1/1/1/1	-
4	EDO	U	601	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	Q	507	-	-	0/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	A	516	-	-	0/1/1/1	-
4	EDO	Q	503	-	-	0/1/1/1	-
5	GOL	C	601	-	-	0/4/4/4	-
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	B	512	-	-	0/1/1/1	-
4	EDO	K	505	-	-	1/1/1/1	-
4	EDO	I	504	-	-	0/1/1/1	-
4	EDO	P	508	-	-	1/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	B	511	-	-	0/1/1/1	-
4	EDO	P	504	-	-	0/1/1/1	-
4	EDO	I	510	-	-	0/1/1/1	-
4	EDO	P	503	-	-	0/1/1/1	-
4	EDO	I	511	-	-	0/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	I	508	-	-	1/1/1/1	-
4	EDO	P	505	-	-	1/1/1/1	-
4	EDO	Q	506	-	-	0/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	B	509	-	-	1/1/1/1	-
4	EDO	P	506	-	-	0/1/1/1	-
4	EDO	P	510	-	-	0/1/1/1	-
4	EDO	K	503	-	-	1/1/1/1	-
5	GOL	K	504	-	-	0/4/4/4	-
4	EDO	A	507	-	-	0/1/1/1	-
5	GOL	K	508	-	-	2/4/4/4	-
4	EDO	A	514	-	-	1/1/1/1	-
4	EDO	K	507	-	-	0/1/1/1	-
4	EDO	A	515	-	-	0/1/1/1	-
4	EDO	D	602	-	-	0/1/1/1	-
4	EDO	K	506	-	-	0/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	A	513	-	-	0/1/1/1	-
5	GOL	P	509	-	-	0/4/4/4	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	A	517	-	-	1/1/1/1	-
4	EDO	V	601	-	-	0/1/1/1	-
5	GOL	X	601	-	-	0/4/4/4	-
4	EDO	A	511	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	510	-	-	1/1/1/1	-
4	EDO	I	507	-	-	0/1/1/1	-
4	EDO	Q	504	-	-	0/1/1/1	-
4	EDO	I	503	-	-	0/1/1/1	-
4	EDO	I	509	-	-	1/1/1/1	-
4	EDO	A	512	-	-	0/1/1/1	-
7	16P	A	509	-	-	2/8/8/17	-
4	EDO	B	508	-	-	0/1/1/1	-
4	EDO	B	514	-	-	1/1/1/1	-
4	EDO	P	511	-	-	0/1/1/1	-
4	EDO	P	507	-	-	0/1/1/1	-
5	GOL	D	601	-	-	0/4/4/4	-
4	EDO	Q	505	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

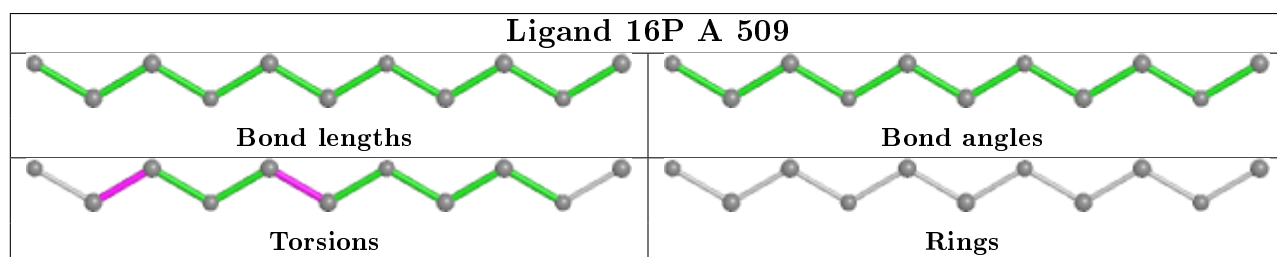
Mol	Chain	Res	Type	Atoms
7	A	509	16P	O3-C7-C8-O4
5	K	508	GOL	C1-C2-C3-O3
4	B	514	EDO	O1-C1-C2-O2
7	A	509	16P	O5-C10-C9-O4
4	B	509	EDO	O1-C1-C2-O2
4	B	510	EDO	O1-C1-C2-O2
4	B	515	EDO	O1-C1-C2-O2
4	P	508	EDO	O1-C1-C2-O2
4	A	511	EDO	O1-C1-C2-O2
4	P	505	EDO	O1-C1-C2-O2
5	K	508	GOL	O2-C2-C3-O3
4	A	506	EDO	O1-C1-C2-O2
4	A	514	EDO	O1-C1-C2-O2
4	A	510	EDO	O1-C1-C2-O2
4	K	503	EDO	O1-C1-C2-O2
4	A	504	EDO	O1-C1-C2-O2
4	A	517	EDO	O1-C1-C2-O2
4	K	505	EDO	O1-C1-C2-O2
4	I	508	EDO	O1-C1-C2-O2
4	I	509	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	504	EDO	1	0
4	I	511	EDO	1	0
6	I	505	SO4	1	0
5	K	508	GOL	1	0
4	A	514	EDO	2	0
4	B	513	EDO	1	0
5	X	601	GOL	1	0
4	I	507	EDO	1	0
6	Q	508	SO4	1	0
7	A	509	16P	5	0
5	D	601	GOL	1	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 i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	294/299 (98%)	0.09	2 (0%) 87 88	24, 32, 46, 82	0
1	B	294/299 (98%)	0.15	0 100 100	23, 32, 46, 73	0
1	I	294/299 (98%)	0.52	9 (3%) 49 51	35, 48, 63, 86	0
1	K	294/299 (98%)	0.23	4 (1%) 75 77	31, 43, 56, 76	0
1	P	294/299 (98%)	0.32	7 (2%) 59 62	31, 42, 57, 88	0
1	Q	294/299 (98%)	0.64	10 (3%) 45 48	34, 53, 70, 95	0
2	C	69/78 (88%)	0.28	3 (4%) 35 38	28, 44, 63, 77	0
2	D	65/78 (83%)	0.20	0 100 100	29, 41, 53, 63	0
2	U	65/78 (83%)	0.56	3 (4%) 32 35	41, 49, 73, 78	0
2	V	69/78 (88%)	0.67	5 (7%) 15 17	45, 61, 81, 85	0
2	W	68/78 (87%)	0.81	4 (5%) 22 25	40, 52, 79, 92	0
2	X	68/78 (87%)	0.61	5 (7%) 14 16	46, 57, 78, 96	0
All	All	2168/2262 (95%)	0.36	52 (2%) 59 62	23, 44, 67, 96	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	289	LEU	5.9
1	Q	146	ILE	4.2
2	C	513	LEU	4.0
1	Q	75	LEU	3.8
1	Q	188	ARG	3.5
1	I	75	LEU	3.3
2	W	580	PRO	3.2
2	U	525	TYR	3.2
1	P	299	ALA	3.1
2	W	538	ALA	3.1
2	X	547	ALA	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	P	7	LEU	3.1
2	X	570	LEU	3.0
2	W	513	LEU	2.9
1	P	225	PHE	2.9
1	P	235	PHE	2.8
2	C	580	PRO	2.8
2	X	514	ARG	2.8
1	K	274	GLY	2.7
1	P	289	LEU	2.7
2	V	528	VAL	2.7
2	V	525	TYR	2.7
1	P	188	ARG	2.7
1	K	299	ALA	2.6
2	C	525	TYR	2.6
2	V	513	LEU	2.6
1	Q	277	ASP	2.6
1	A	289	LEU	2.5
1	Q	89	PHE	2.5
1	I	293	PHE	2.5
1	I	282	MET	2.5
1	K	146	ILE	2.4
1	Q	133	ILE	2.4
1	I	7	LEU	2.4
1	I	277	ASP	2.4
2	X	519	LEU	2.3
2	V	580	PRO	2.3
2	U	533	ASP	2.3
1	A	40	LEU	2.3
1	I	299	ALA	2.2
1	Q	40	LEU	2.2
2	X	534	TYR	2.2
1	Q	48	SER	2.1
1	I	146	ILE	2.1
2	U	518	ILE	2.1
2	W	553	ILE	2.1
1	P	133	ILE	2.1
1	Q	108	LEU	2.1
1	I	38	LEU	2.1
1	I	6	SER	2.1
1	K	277	ASP	2.1
2	V	579	ARG	2.1



## 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
4	EDO	P	506	4/4	0.53	0.25	55,67,76,76	0
4	EDO	I	510	4/4	0.64	0.19	51,62,67,67	0
4	EDO	I	503	4/4	0.68	0.15	48,65,77,78	0
4	EDO	B	515	4/4	0.70	0.20	55,67,72,72	0
4	EDO	I	508	4/4	0.71	0.14	49,59,60,63	0
4	EDO	A	517	4/4	0.71	0.23	50,61,68,68	0
4	EDO	Q	503	4/4	0.72	0.21	54,65,77,80	0
4	EDO	B	506	4/4	0.73	0.21	41,49,55,55	0
5	GOL	X	601	6/6	0.73	0.25	49,63,75,77	0
5	GOL	K	508	6/6	0.74	0.24	39,47,63,63	0
4	EDO	P	505	4/4	0.75	0.20	42,53,60,64	0
4	EDO	B	512	4/4	0.75	0.22	35,54,62,75	0
6	SO4	P	513	5/5	0.76	0.17	54,63,80,87	0
4	EDO	P	511	4/4	0.77	0.24	46,55,64,64	0
7	16P	A	509	11/20	0.78	0.23	34,40,45,46	0
4	EDO	A	504	4/4	0.78	0.16	45,55,66,66	0
4	EDO	V	601	4/4	0.78	0.16	47,56,62,68	0
5	GOL	P	509	6/6	0.79	0.16	50,58,66,70	0
4	EDO	P	507	4/4	0.79	0.32	51,62,74,74	0
4	EDO	I	509	4/4	0.80	0.14	44,53,58,60	0
4	EDO	A	514	4/4	0.80	0.36	39,47,52,54	0
4	EDO	B	504	4/4	0.80	0.15	39,47,54,56	0
4	EDO	Q	506	4/4	0.82	0.13	53,63,70,70	0
4	EDO	K	505	4/4	0.82	0.20	52,63,66,72	0
4	EDO	Q	507	4/4	0.82	0.18	68,82,87,87	0
4	EDO	U	601	4/4	0.83	0.10	42,50,54,58	0
6	SO4	C	602	5/5	0.83	0.17	46,49,62,68	0

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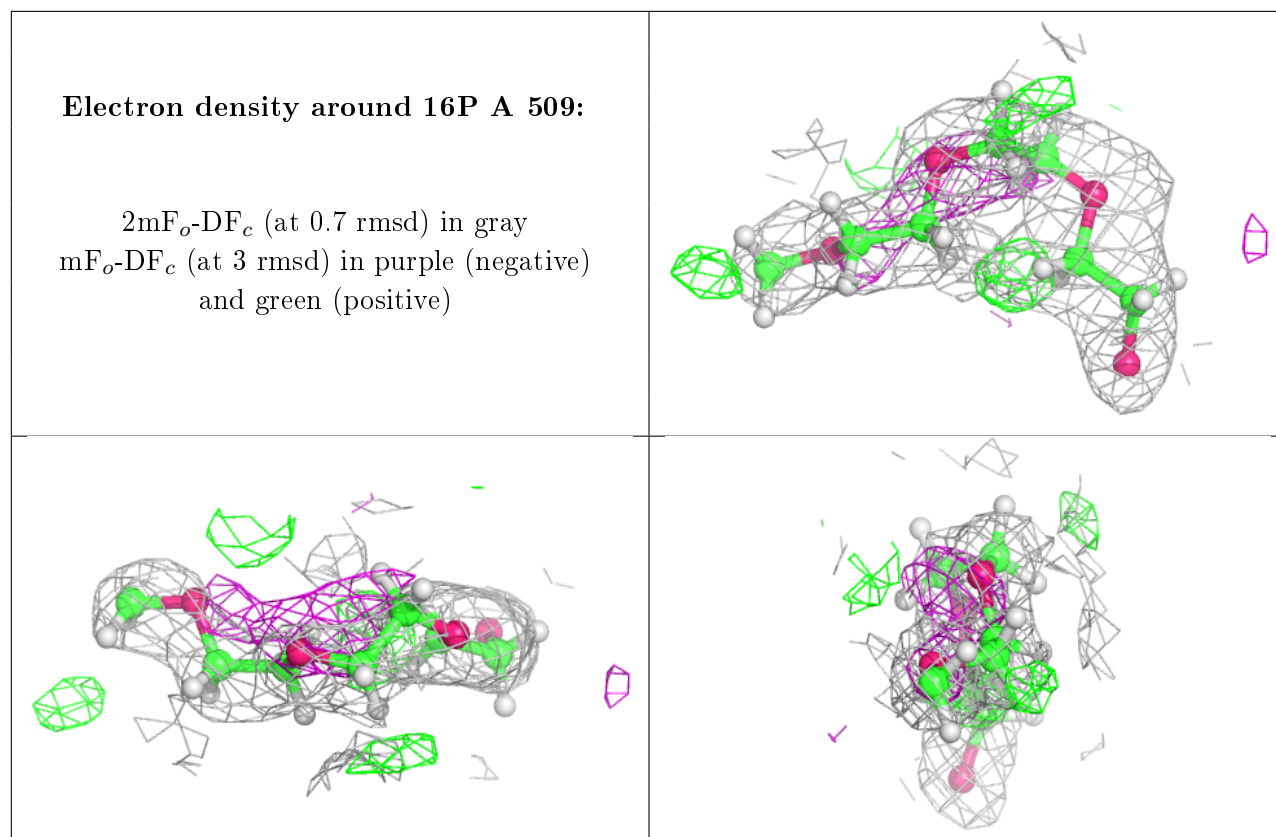
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	514	4/4	0.83	0.10	40,48,55,57	0
4	EDO	B	510	4/4	0.84	0.16	36,44,48,55	0
4	EDO	P	510	4/4	0.84	0.12	57,69,73,73	0
4	EDO	A	510	4/4	0.84	0.20	42,50,55,55	0
4	EDO	I	504	4/4	0.85	0.17	55,70,77,84	0
5	GOL	D	601	6/6	0.85	0.17	34,41,49,49	0
4	EDO	A	511	4/4	0.85	0.15	41,49,51,57	0
4	EDO	I	507	4/4	0.85	0.11	50,60,61,66	0
3	MN	Q	502	1/1	0.85	0.06	49,49,49,49	0
4	EDO	B	513	4/4	0.85	0.22	41,49,56,57	0
4	EDO	K	507	4/4	0.86	0.20	47,56,66,67	0
4	EDO	A	508	4/4	0.86	0.15	36,44,45,50	0
4	EDO	Q	504	4/4	0.87	0.13	58,70,73,73	0
4	EDO	K	503	4/4	0.87	0.10	52,62,71,71	0
4	EDO	B	511	4/4	0.88	0.24	39,48,56,61	0
4	EDO	A	506	4/4	0.88	0.08	39,48,55,55	0
4	EDO	A	515	4/4	0.89	0.16	32,40,47,48	0
4	EDO	A	513	4/4	0.89	0.10	46,57,68,68	0
4	EDO	P	508	4/4	0.90	0.18	46,55,57,59	0
4	EDO	K	506	4/4	0.90	0.24	47,57,65,69	0
4	EDO	D	602	4/4	0.90	0.17	40,49,52,57	0
4	EDO	B	505	4/4	0.90	0.10	41,49,51,53	0
4	EDO	A	507	4/4	0.91	0.10	42,50,57,58	0
4	EDO	B	507	4/4	0.91	0.17	36,44,44,50	0
4	EDO	A	516	4/4	0.91	0.26	40,49,58,58	0
4	EDO	Q	505	4/4	0.91	0.12	50,60,62,63	0
5	GOL	K	504	6/6	0.92	0.12	47,54,61,65	0
4	EDO	B	509	4/4	0.92	0.23	42,50,56,56	0
3	MN	P	502	1/1	0.92	0.06	43,43,43,43	0
4	EDO	B	503	4/4	0.92	0.17	33,40,42,50	0
6	SO4	K	509	5/5	0.92	0.10	35,36,41,44	0
6	SO4	I	506	5/5	0.93	0.13	66,66,71,73	0
4	EDO	B	508	4/4	0.93	0.08	38,46,56,56	0
6	SO4	D	603	5/5	0.93	0.12	42,46,51,53	0
3	MN	Q	501	1/1	0.93	0.15	39,39,39,39	0
6	SO4	V	602	5/5	0.93	0.09	60,70,73,79	0
4	EDO	P	503	4/4	0.93	0.16	37,45,48,50	0
6	SO4	P	512	5/5	0.93	0.12	38,39,42,49	0
4	EDO	P	504	4/4	0.94	0.16	37,45,47,47	0
6	SO4	W	601	5/5	0.94	0.09	60,61,74,79	0
6	SO4	Q	508	5/5	0.94	0.13	40,42,44,49	0
5	GOL	C	601	6/6	0.94	0.20	34,41,49,51	0

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*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	A	503	4/4	0.95	0.09	31,37,40,41	0
6	SO4	U	602	5/5	0.95	0.10	53,54,58,61	0
6	SO4	B	517	5/5	0.95	0.17	59,63,68,71	0
3	MN	B	501	1/1	0.95	0.17	36,36,36,36	0
4	EDO	A	505	4/4	0.95	0.13	32,38,42,44	0
4	EDO	I	511	4/4	0.96	0.23	50,60,62,65	0
6	SO4	A	518	5/5	0.96	0.09	32,32,34,35	0
3	MN	B	502	1/1	0.96	0.10	37,37,37,37	0
3	MN	A	502	1/1	0.97	0.04	37,37,37,37	0
3	MN	P	501	1/1	0.97	0.14	33,33,33,33	0
6	SO4	I	505	5/5	0.97	0.11	33,34,39,42	0
4	EDO	A	512	4/4	0.97	0.08	36,44,50,50	0
6	SO4	B	516	5/5	0.97	0.11	28,31,31,32	0
3	MN	I	501	1/1	0.98	0.14	34,34,34,34	0
3	MN	A	501	1/1	0.98	0.17	33,33,33,33	0
3	MN	I	502	1/1	0.98	0.03	45,45,45,45	0
3	MN	K	502	1/1	0.99	0.06	45,45,45,45	0
3	MN	K	501	1/1	0.99	0.09	32,32,32,32	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.