



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:25 am GMT

PDB ID : 4LE6  
Title : Crystal structure of the phosphotriesterase OPHC2 from *Pseudomonas pseudoalcaligenes*  
Authors : Gotthard, G.; Hiblot, J.; Chabriere, E.; Elias, M.  
Deposited on : 2013-06-25  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

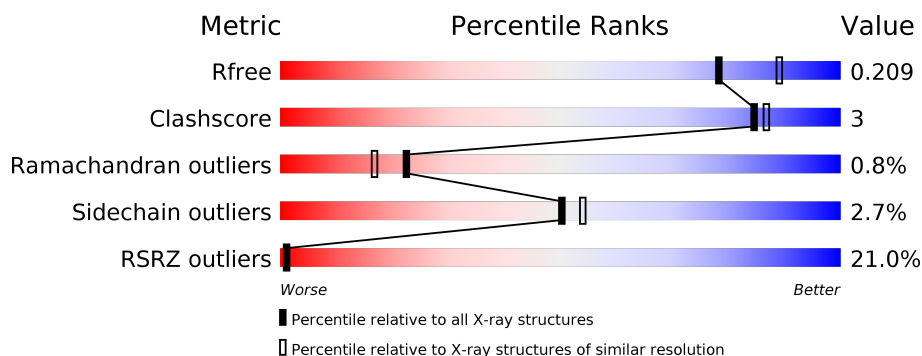
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	324	<div> <div>2%</div> <div>74%</div> <div>5%</div> <div>21%</div> </div>
1	B	324	<div> <div>3%</div> <div>73%</div> <div>5%</div> <div>21%</div> </div>
1	C	324	<div> <div>3%</div> <div>73%</div> <div>•</div> <div>22%</div> </div>
1	D	324	<div> <div>28%</div> <div>73%</div> <div>•</div> <div>23%</div> </div>
1	E	324	<div> <div>45%</div> <div>65%</div> <div>12%</div> <div>23%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	402	-	-	-	X
2	GOL	B	401[A]	-	-	-	X
2	GOL	B	401[B]	-	-	-	X
2	GOL	B	402[A]	-	-	-	X
2	GOL	B	402[B]	-	-	-	X
2	GOL	C	401	-	-	-	X
2	GOL	C	402	-	-	-	X
3	EDO	A	403	-	-	-	X
3	EDO	A	407	-	-	-	X
3	EDO	B	404	-	-	-	X
3	EDO	C	403	-	-	-	X
4	PGE	A	404[A]	-	-	-	X
4	PGE	A	404[B]	-	-	-	X

## 2 Entry composition [i](#)

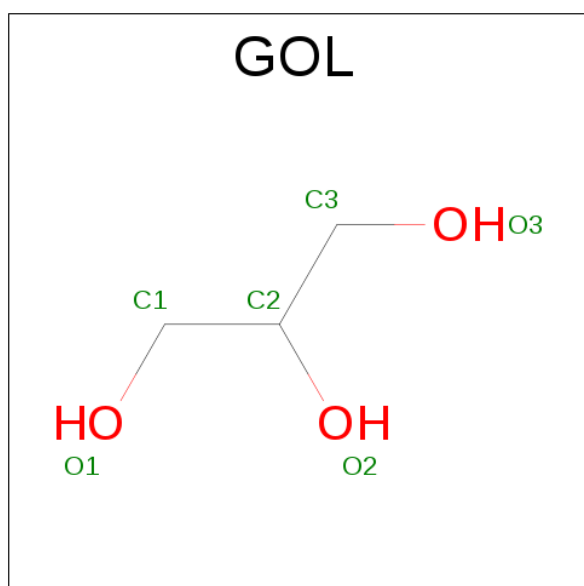
There are 6 unique types of molecules in this entry. The entry contains 20066 atoms, of which 9617 are hydrogens and 0 are deuteriums.

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 Organophosphorus hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	257	Total	C	H	N	O	S	0	3	0
			3903	1253	1936	336	374	4			
1	B	255	Total	C	H	N	O	S	0	1	0
			3850	1237	1908	333	368	4			
1	C	254	Total	C	H	N	O	S	0	1	0
			3831	1233	1896	329	369	4			
1	D	251	Total	C	H	N	O	S	0	1	0
			3792	1221	1879	325	363	4			
1	E	251	Total	C	H	N	O	S	0	0	0
			3770	1215	1866	323	362	4			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		

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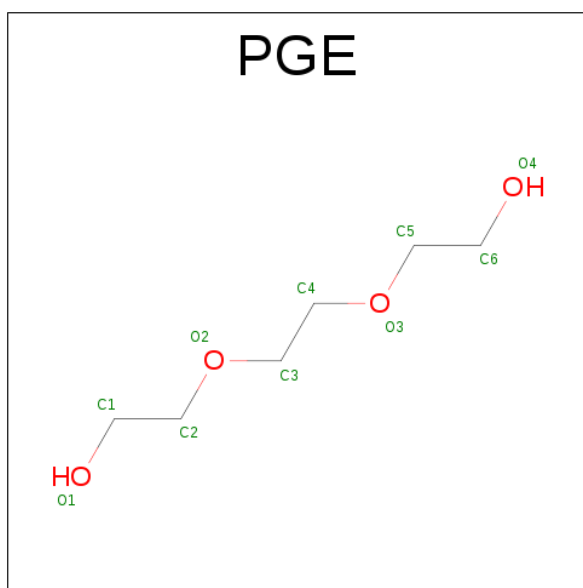
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	1
			28	6	16	6		
2	B	1	Total	C	H	O	0	1
			28	6	16	6		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 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
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	1
			48	12	28	8		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Zn	0	0
			2	2		
5	A	2	Total	Zn	0	0
			2	2		
5	D	2	Total	Zn	0	0
			2	2		
5	C	2	Total	Zn	0	0
			2	2		
5	E	2	Total	Zn	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	325	Total	O	0	0
			325	325		
6	B	167	Total	O	0	0
			167	167		
6	C	136	Total	O	0	0
			136	136		

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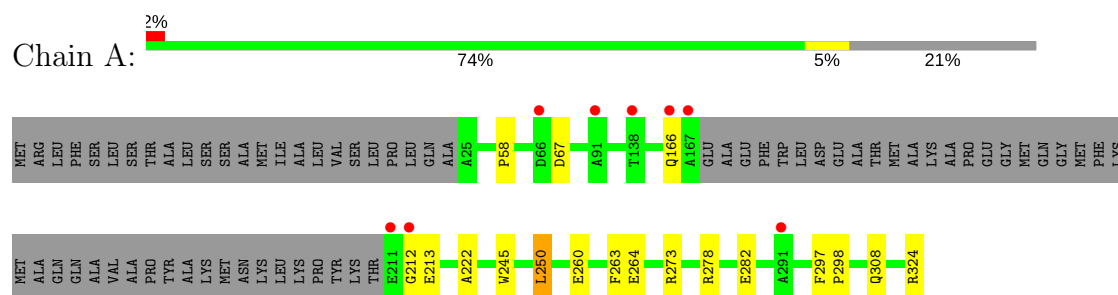
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	43	Total 43	O 43	0	0
6	E	11	Total 11	O 11	0	0

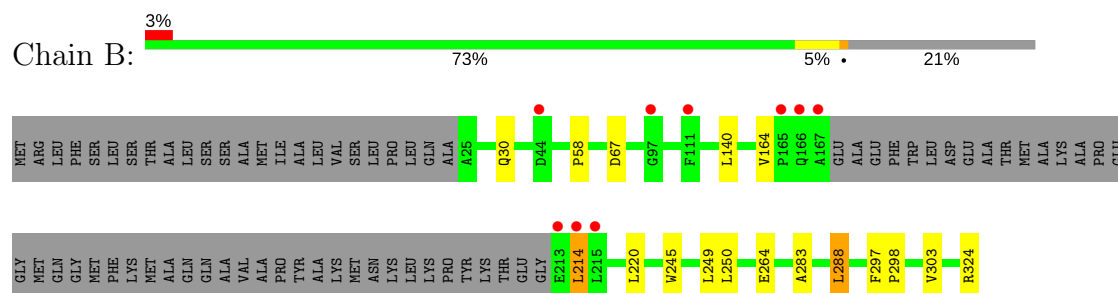
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

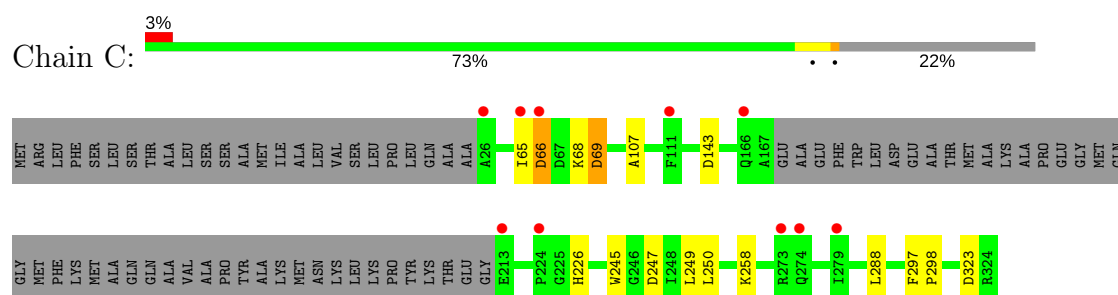
#### • Molecule 1: Organophosphorus hydrolase



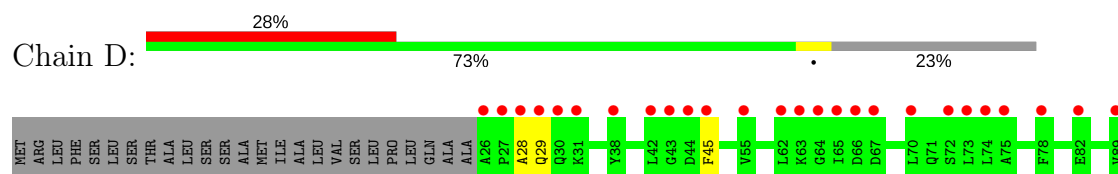
#### • Molecule 1: Organophosphorus hydrolase



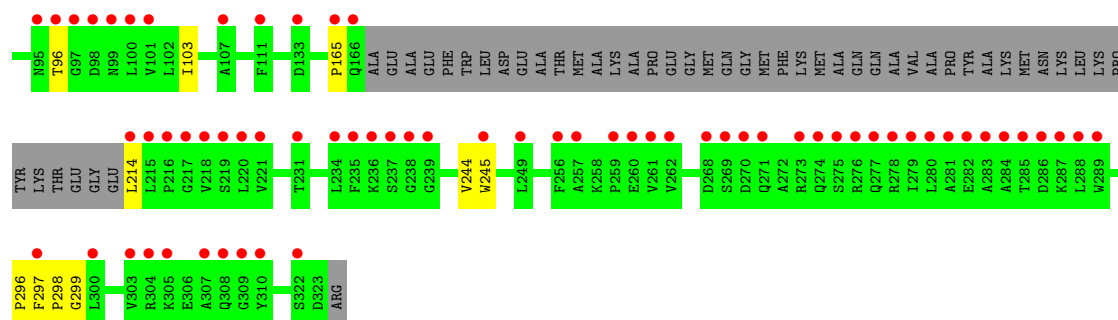
#### • Molecule 1: Organophosphorus hydrolase



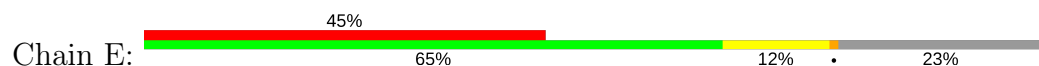
#### • Molecule 1: Organophosphorus hydrolase







• Molecule 1: Organophosphorus hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.91Å 63.85Å 221.26Å 90.00° 101.85° 90.00°	Depositor
Resolution (Å)	42.80 – 2.10 48.12 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.7 (42.80-2.10) 93.7 (48.12-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1352)	Depositor
R, $R_{free}$	0.173 , 0.210 0.172 , 0.209	Depositor DCC
$R_{free}$ test set	4125 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.016 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20066	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 5.94% 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, ZN, PGE, EDO

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	0.40	0/2023	0.57	0/2760
1	B	0.32	0/1992	0.52	0/2720
1	C	0.30	0/1985	0.51	0/2711
1	D	0.26	0/1960	0.46	0/2678
1	E	0.26	0/1951	0.46	0/2666
All	All	0.31	0/9911	0.51	0/13535

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	1967	1936	1933	12	0
1	B	1942	1908	1905	9	0
1	C	1935	1896	1893	7	0
1	D	1913	1879	1876	5	0
1	E	1904	1866	1863	20	0
2	A	12	16	16	1	0
2	B	30	40	40	2	0
2	C	12	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	6	8	8	0	0
3	A	8	12	12	1	0
3	B	4	6	6	0	0
3	C	4	6	6	0	0
4	A	20	28	28	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
6	A	325	0	0	5	0
6	B	167	0	0	2	0
6	C	136	0	0	1	0
6	D	43	0	0	0	0
6	E	11	0	0	3	0
All	All	10449	9617	9602	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (52) 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:29:GLN:NE2	1:E:44:ASP:O	2.17	0.77
1:A:278[B]:ARG:NH2	6:A:783:HOH:O	2.18	0.76
1:E:261:VAL:O	1:E:276:ARG:NH1	2.26	0.68
1:E:158:PRO:O	1:E:160:ALA:N	2.28	0.66
1:E:221:VAL:O	1:E:231:THR:OG1	2.16	0.63
1:E:247:ASP:OD1	1:E:247:ASP:N	2.33	0.61
1:A:67:ASP:OD1	6:A:761:HOH:O	2.16	0.59
1:E:57:LEU:O	1:E:85:VAL:N	2.34	0.59
1:E:98:ASP:O	1:E:99:ASN:ND2	2.37	0.57
1:E:104:ASP:OD2	1:E:144:HIS:ND1	2.40	0.54
1:E:223:SER:OG	6:E:511:HOH:O	2.18	0.54
1:B:283:ALA:HB3	1:B:303:VAL:HG11	1.90	0.53
1:A:297:PHE:CD1	1:A:298:PRO:HA	2.44	0.53
1:B:30:GLN:OE1	6:B:629:HOH:O	2.19	0.52
1:C:69:ASP:OD2	1:C:258:LYS:NZ	2.43	0.52
2:A:402:GOL:O3	2:B:401[A]:GOL:H11	2.10	0.52
1:A:264:GLU:HG2	1:B:58:PRO:HG3	1.93	0.50
1:D:297:PHE:CD1	1:D:298:PRO:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:ASP:OD2	1:E:107:ALA:N	2.47	0.47
1:E:143:ASP:OD2	6:E:510:HOH:O	2.20	0.47
1:B:297:PHE:CD1	1:B:298:PRO:HA	2.50	0.46
1:C:65:ILE:O	1:C:66:ASP:CB	2.63	0.46
1:E:118:VAL:O	1:E:122:LEU:N	2.49	0.46
1:A:260:GLU:HA	1:A:273:ARG:HD3	1.98	0.45
1:C:297:PHE:CD1	1:C:298:PRO:HA	2.52	0.45
2:B:402[A]:GOL:O1	6:B:603:HOH:O	2.10	0.45
1:C:323:ASP:OD2	6:C:594:HOH:O	2.21	0.45
1:A:324:ARG:NH1	6:A:752:HOH:O	2.50	0.44
1:A:58:PRO:HG3	1:B:264:GLU:HG2	1.99	0.44
1:A:222:ALA:HB1	3:A:403:EDO:H22	1.99	0.43
1:C:226:HIS:CD2	1:C:247:ASP:HB2	2.53	0.43
1:A:250:LEU:HD22	1:A:263:PHE:CE1	2.54	0.43
1:B:140:LEU:HD21	1:B:164:VAL:HG13	2.00	0.43
1:A:250:LEU:HD22	1:A:263:PHE:CD1	2.54	0.43
1:E:296:PRO:O	1:E:299:GLY:N	2.49	0.43
1:D:45:PHE:CD1	1:D:96:THR:HA	2.54	0.42
1:E:297:PHE:CD1	1:E:298:PRO:HA	2.54	0.42
1:C:107:ALA:HB2	1:C:143:ASP:HA	2.01	0.42
1:E:139:HIS:CD2	1:E:141:HIS:CG	3.08	0.42
1:E:215:LEU:HB3	1:E:216:PRO:HD2	2.02	0.42
1:A:166:GLN:N	6:A:723:HOH:O	2.52	0.42
1:D:296:PRO:O	1:D:299:GLY:N	2.53	0.42
1:D:103:ILE:HG21	1:D:244:VAL:HG11	2.02	0.41
1:E:227:THR:H	1:E:230:HIS:HB2	1.85	0.41
1:E:159:ASN:N	1:E:159:ASN:OD1	2.54	0.41
1:B:214:LEU:HD12	1:B:220:LEU:HD11	2.03	0.41
1:B:283:ALA:HA	1:B:288:LEU:HD11	2.02	0.41
1:A:282:GLU:OE2	6:A:788:HOH:O	2.22	0.41
1:E:266:ASP:N	6:E:508:HOH:O	2.54	0.40
1:C:65:ILE:O	1:C:66:ASP:HB2	2.21	0.40
1:E:52:ASP:OD1	1:E:117:VAL:N	2.50	0.40
1:B:283:ALA:CB	1:B:288:LEU:HD11	2.51	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	256/324 (79%)	249 (97%)	5 (2%)	2 (1%)	22	17
1	B	252/324 (78%)	247 (98%)	5 (2%)	0	100	100
1	C	251/324 (78%)	240 (96%)	10 (4%)	1 (0%)	38	35
1	D	248/324 (76%)	233 (94%)	13 (5%)	2 (1%)	22	17
1	E	247/324 (76%)	204 (83%)	38 (15%)	5 (2%)	9	4
All	All	1254/1620 (77%)	1173 (94%)	71 (6%)	10 (1%)	22	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	ASP
1	E	158	PRO
1	E	159	ASN
1	E	74	LEU
1	E	216	PRO
1	A	212	GLY
1	A	213	GLU
1	D	28	ALA
1	D	165	PRO
1	E	254	VAL

### 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	208/258 (81%)	205 (99%)	3 (1%)	71	78
1	B	205/258 (80%)	198 (97%)	7 (3%)	42	43
1	C	205/258 (80%)	199 (97%)	6 (3%)	48	51
1	D	203/258 (79%)	201 (99%)	2 (1%)	80	85
1	E	202/258 (78%)	193 (96%)	9 (4%)	32	30
All	All	1023/1290 (79%)	996 (97%)	27 (3%)	50	55

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	TRP
1	A	250	LEU
1	A	308	GLN
1	B	67	ASP
1	B	214	LEU
1	B	245	TRP
1	B	249	LEU
1	B	250	LEU
1	B	288	LEU
1	B	324	ARG
1	C	68	LYS
1	C	69	ASP
1	C	245	TRP
1	C	249	LEU
1	C	250	LEU
1	C	288	LEU
1	D	214	LEU
1	D	245	TRP
1	E	40	MET
1	E	42	LEU
1	E	56	ASP
1	E	148	LEU
1	E	159	ASN
1	E	220	LEU
1	E	245	TRP
1	E	247	ASP
1	E	282	GLU

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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	$\# Z  > 2$
2	GOL	A	401	-	5,5,5	0.38	0	5,5,5	0.22	0
2	GOL	A	402	-	5,5,5	0.23	0	5,5,5	0.59	0
3	EDO	A	403	-	3,3,3	0.41	0	2,2,2	0.29	0
4	PGE	A	404[A]	-	9,9,9	0.29	0	8,8,8	0.29	0
4	PGE	A	404[B]	-	9,9,9	0.31	0	8,8,8	0.33	0
3	EDO	A	407	-	3,3,3	0.43	0	2,2,2	0.50	0
2	GOL	B	401[A]	-	5,5,5	0.34	0	5,5,5	0.25	0
2	GOL	B	401[B]	-	5,5,5	0.33	0	5,5,5	0.23	0
2	GOL	B	402[A]	-	5,5,5	0.26	0	5,5,5	0.26	0
2	GOL	B	402[B]	-	5,5,5	0.32	0	5,5,5	0.31	0
2	GOL	B	403	-	5,5,5	0.38	0	5,5,5	0.19	0
3	EDO	B	404	-	3,3,3	0.29	0	2,2,2	0.20	0
2	GOL	C	401	-	5,5,5	0.38	0	5,5,5	0.47	0
2	GOL	C	402	-	5,5,5	0.35	0	5,5,5	0.38	0
3	EDO	C	403	-	3,3,3	0.48	0	2,2,2	0.19	0
2	GOL	D	401	-	5,5,5	0.37	0	5,5,5	0.15	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
2	GOL	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
3	EDO	A	403	-	-	0/1/1/1	0/0/0/0
4	PGE	A	404[A]	-	-	0/7/7/7	0/0/0/0
4	PGE	A	404[B]	-	-	0/7/7/7	0/0/0/0
3	EDO	A	407	-	-	0/1/1/1	0/0/0/0
2	GOL	B	401[A]	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401[B]	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402[A]	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402[B]	-	-	0/4/4/4	0/0/0/0
2	GOL	B	403	-	-	0/4/4/4	0/0/0/0
3	EDO	B	404	-	-	0/1/1/1	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	C	402	-	-	0/4/4/4	0/0/0/0
3	EDO	C	403	-	-	0/1/1/1	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	GOL	1	0
3	A	403	EDO	1	0
2	B	401[A]	GOL	1	0
2	B	402[A]	GOL	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	257/324 (79%)	0.61	8 (3%)	49	56	16, 27, 46, 122	3 (1%)
1	B	255/324 (78%)	0.37	9 (3%)	44	51	27, 42, 68, 147	1 (0%)
1	C	254/324 (78%)	0.44	10 (3%)	40	47	30, 50, 78, 106	1 (0%)
1	D	251/324 (77%)	1.92	92 (36%)	0	0	48, 81, 119, 142	2 (0%)
1	E	251/324 (77%)	2.79	147 (58%)	0	0	64, 115, 149, 168	5 (1%)
All	All	1268/1620 (78%)	1.22	266 (20%)	1	1	16, 56, 130, 168	12 (0%)

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	GLN	12.0
1	B	167	ALA	10.2
1	E	134	THR	10.0
1	D	70	LEU	10.0
1	E	218	VAL	9.9
1	D	27	PRO	9.6
1	E	100	LEU	9.5
1	D	215	LEU	9.5
1	D	28	ALA	8.8
1	E	140	LEU	8.4
1	E	165	PRO	7.4
1	E	257	ALA	7.2
1	E	166	GLN	7.2
1	E	75	ALA	7.1
1	E	67	ASP	7.1
1	D	220	LEU	7.0
1	D	307	ALA	6.9
1	E	72	SER	6.8
1	E	219	SER	6.6
1	E	45	PHE	6.6

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Mol	Chain	Res	Type	RSRZ
1	E	220	LEU	6.6
1	E	132	VAL	6.5
1	E	26	ALA	6.5
1	E	99	ASN	6.5
1	E	128	GLN	6.3
1	E	217	GLY	6.2
1	E	260	GLU	6.2
1	D	285	THR	6.1
1	D	44	ASP	6.1
1	D	237	SER	6.0
1	E	101	VAL	5.9
1	E	162	VAL	5.9
1	D	308	GLN	5.9
1	E	274	GLN	5.9
1	E	155	PRO	5.8
1	D	216	PRO	5.7
1	E	272	ALA	5.7
1	E	157	TYR	5.7
1	E	28	ALA	5.7
1	E	214	LEU	5.7
1	E	70	LEU	5.7
1	E	161	THR	5.6
1	D	279	ILE	5.6
1	E	68	LYS	5.6
1	D	97	GLY	5.5
1	D	257	ALA	5.5
1	E	216	PRO	5.5
1	D	281	ALA	5.5
1	A	211	GLU	5.5
1	E	261	VAL	5.5
1	D	309	GLY	5.4
1	E	127	TYR	5.4
1	D	26	ALA	5.4
1	D	219	SER	5.4
1	D	287	LYS	5.3
1	E	65	ILE	5.3
1	E	275	SER	5.2
1	E	215	LEU	5.1
1	E	160	ALA	5.1
1	E	154	SER	5.0
1	E	97	GLY	5.0
1	E	164	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	214	LEU	4.9
1	E	309	GLY	4.9
1	D	218	VAL	4.8
1	D	98	ASP	4.8
1	D	43	GLY	4.8
1	E	93	LEU	4.8
1	E	69	ASP	4.8
1	E	27	PRO	4.8
1	E	221	VAL	4.7
1	E	279	ILE	4.7
1	A	212	GLY	4.7
1	E	96	THR	4.6
1	E	310	TYR	4.6
1	E	222	ALA	4.6
1	E	263	PHE	4.6
1	D	283	ALA	4.5
1	E	280	LEU	4.5
1	D	65	ILE	4.5
1	D	96	THR	4.4
1	E	131	GLN	4.4
1	D	284	ALA	4.4
1	D	288	LEU	4.4
1	E	42	LEU	4.4
1	D	217	GLY	4.4
1	E	136	LEU	4.3
1	E	270	ASP	4.3
1	E	80	ALA	4.2
1	E	265	PHE	4.2
1	D	270	ASP	4.2
1	E	159	ASN	4.2
1	C	66	ASP	4.1
1	D	256	PHE	4.1
1	E	249	LEU	4.1
1	E	130	GLU	4.1
1	D	310	TYR	4.1
1	E	55	VAL	4.1
1	E	44	ASP	4.1
1	E	98	ASP	4.1
1	E	243	LEU	4.0
1	D	322	SER	4.0
1	D	235	PHE	4.0
1	B	214	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	286	ASP	4.0
1	E	149	VAL	4.0
1	E	133	ASP	3.9
1	E	129	PRO	3.9
1	E	117	VAL	3.9
1	D	305	LYS	3.9
1	E	287	LYS	3.8
1	D	278	ARG	3.8
1	E	268	ASP	3.8
1	D	66	ASP	3.8
1	D	234	LEU	3.8
1	E	116	GLY	3.7
1	E	66	ASP	3.7
1	D	238	GLY	3.7
1	E	264	GLU	3.7
1	D	101	VAL	3.6
1	E	303	VAL	3.6
1	D	274	GLN	3.6
1	E	122	LEU	3.6
1	E	254	VAL	3.6
1	E	307	ALA	3.6
1	D	239	GLY	3.5
1	E	120	THR	3.5
1	E	137	LEU	3.5
1	D	42	LEU	3.5
1	D	280	LEU	3.5
1	D	268	ASP	3.4
1	D	277	GLN	3.4
1	E	238	GLY	3.4
1	E	248	ILE	3.4
1	E	102	LEU	3.4
1	D	236	LYS	3.4
1	D	273	ARG	3.4
1	E	234	LEU	3.4
1	E	152	ASP	3.4
1	E	138	THR	3.4
1	D	221	VAL	3.4
1	E	57	LEU	3.3
1	C	213	GLU	3.3
1	E	103	ILE	3.3
1	D	282	GLU	3.2
1	D	100	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	267	VAL	3.2
1	E	158	PRO	3.2
1	E	59	ALA	3.2
1	C	166	GLN	3.2
1	E	73	LEU	3.2
1	E	245	TRP	3.2
1	D	275	SER	3.1
1	C	274	GLN	3.1
1	E	320	ILE	3.1
1	D	74	LEU	3.1
1	E	228	PRO	3.0
1	D	289	TRP	3.0
1	D	45	PHE	3.0
1	D	82	GLU	3.0
1	E	60	SER	3.0
1	E	262	VAL	3.0
1	B	166	GLN	3.0
1	B	165	PRO	3.0
1	E	95	ASN	3.0
1	D	99	ASN	2.9
1	E	146	CYS	2.9
1	D	64	GLY	2.9
1	E	83	LYS	2.9
1	E	278	ARG	2.9
1	E	58	PRO	2.9
1	D	231	THR	2.9
1	E	242	LEU	2.9
1	E	232	SER	2.9
1	E	153	GLY	2.9
1	C	65	ILE	2.8
1	E	271	GLN	2.8
1	E	56	ASP	2.8
1	B	215	LEU	2.8
1	E	81	SER	2.8
1	E	82	GLU	2.8
1	E	240	GLN	2.8
1	D	29	GLN	2.7
1	E	233	TYR	2.7
1	C	279	ILE	2.7
1	B	111	PHE	2.7
1	D	276	ARG	2.7
1	A	167	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	259	PRO	2.7
1	D	262	VAL	2.7
1	D	63	LYS	2.7
1	D	133	ASP	2.7
1	E	288	LEU	2.6
1	D	271	GLN	2.6
1	D	303	VAL	2.6
1	E	123	LYS	2.6
1	C	26	ALA	2.6
1	E	255	GLN	2.6
1	E	230	HIS	2.6
1	E	150	ASN	2.6
1	E	89	VAL	2.6
1	C	273	ARG	2.5
1	E	92	TYR	2.5
1	E	156	ALA	2.5
1	D	75	ALA	2.5
1	E	41	ALA	2.5
1	A	291	ALA	2.5
1	E	109	GLN	2.5
1	E	147	GLY	2.5
1	D	260	GLU	2.4
1	D	165	PRO	2.4
1	D	72	SER	2.4
1	E	126	GLY	2.4
1	E	29	GLN	2.4
1	D	95	ASN	2.4
1	D	78	PHE	2.4
1	D	269	SER	2.4
1	E	78	PHE	2.4
1	E	322	SER	2.4
1	E	43	GLY	2.4
1	E	119	GLN	2.4
1	A	66	ASP	2.4
1	E	62	LEU	2.3
1	E	256	PHE	2.3
1	E	163	GLU	2.3
1	D	297	PHE	2.3
1	E	74	LEU	2.3
1	E	231	THR	2.3
1	E	306	GLU	2.3
1	D	261	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	97	GLY	2.2
1	E	223	SER	2.2
1	E	259	PRO	2.2
1	D	38	TYR	2.2
1	D	89	VAL	2.2
1	E	135	VAL	2.2
1	E	266	ASP	2.2
1	D	31	LYS	2.2
1	E	235	PHE	2.2
1	E	276	ARG	2.2
1	D	304	ARG	2.2
1	A	166	GLN	2.1
1	C	224	PRO	2.2
1	D	55	VAL	2.1
1	D	111	PHE	2.1
1	D	107	ALA	2.1
1	E	229	GLY	2.1
1	E	284	ALA	2.1
1	B	213	GLU	2.1
1	A	91	ALA	2.1
1	A	138	THR	2.1
1	D	249	LEU	2.1
1	B	44	ASP	2.1
1	D	62	LEU	2.1
1	C	111	PHE	2.1
1	D	73	LEU	2.0
1	E	250	LEU	2.0
1	E	47	VAL	2.0
1	E	281	ALA	2.0
1	D	67	ASP	2.0
1	D	245	TRP	2.0
1	D	300	LEU	2.0
1	E	295	LEU	2.0
1	E	151	ALA	2.0
1	E	241	SER	2.0
1	D	30	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	C	403	4/4	0.83	0.76	52.30	32,38,43,44	10
2	GOL	C	402	6/6	0.79	1.21	32.92	29,35,40,43	14
2	GOL	A	402	6/6	0.59	1.00	27.38	32,38,40,41	14
3	EDO	A	407	4/4	0.90	0.71	22.86	41,49,51,51	10
4	PGE	A	404[B]	10/10	0.80	0.90	21.66	31,38,44,45	24
4	PGE	A	404[A]	10/10	0.80	0.90	21.46	31,39,45,46	24
2	GOL	B	401[B]	6/6	0.65	0.69	15.10	35,42,46,49	14
2	GOL	B	401[A]	6/6	0.65	0.69	14.75	35,42,46,46	14
3	EDO	B	404	4/4	0.94	0.36	12.84	20,24,26,31	10
2	GOL	B	402[B]	6/6	0.66	0.55	10.33	38,49,56,59	14
2	GOL	B	402[A]	6/6	0.66	0.55	10.33	30,46,53,56	14
3	EDO	A	403	4/4	0.84	0.54	7.94	20,26,37,44	10
2	GOL	C	401	6/6	0.87	0.35	7.34	23,29,36,44	14
5	ZN	B	405	1/1	0.99	0.16	0.66	34,34,34,34	0
2	GOL	B	403	6/6	0.94	0.14	0.46	33,41,51,56	0
2	GOL	D	401	6/6	0.94	0.17	0.04	56,68,80,82	0
5	ZN	B	406	1/1	1.00	0.14	-0.00	31,31,31,31	0
2	GOL	A	401	6/6	0.96	0.14	-0.43	24,31,41,45	0
5	ZN	C	405	1/1	0.97	0.14	-0.89	42,42,42,42	0
5	ZN	C	404	1/1	0.99	0.13	-1.06	43,43,43,43	0
5	ZN	A	405	1/1	0.99	0.17	-2.19	24,24,24,24	0
5	ZN	E	401	1/1	0.78	0.10	-2.21	97,97,97,97	0
5	ZN	D	403	1/1	0.97	0.10	-2.24	56,56,56,56	0
5	ZN	E	402	1/1	0.96	0.10	-2.27	98,98,98,98	0
5	ZN	D	402	1/1	0.97	0.09	-3.00	53,53,53,53	0
5	ZN	A	406	1/1	1.00	0.15	-3.62	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.