



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:49 PM UTC

PDB ID : 4LE6 / pdb_00004le6
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

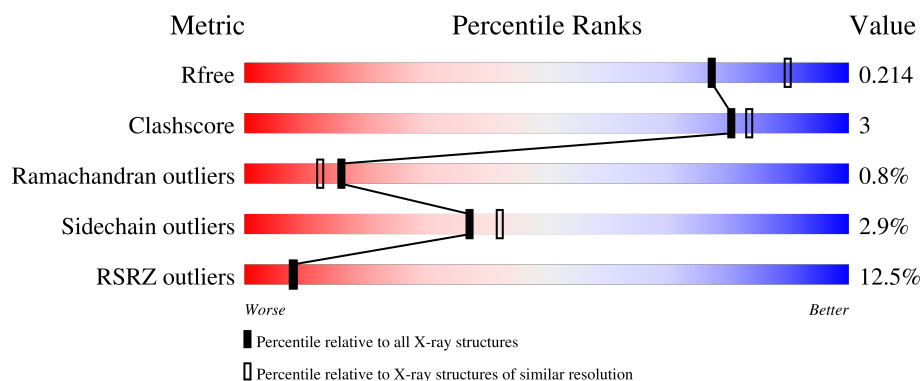
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	324	2% 74% 5% 21%
1	B	324	2% 73% 6% 21%
1	C	324	2% 73% 5% 22%
1	D	324	10% 73% • 23%
1	E	324	34% 64% 12% 23%

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	C	402	-	-	-	X

2 Entry composition [i](#)

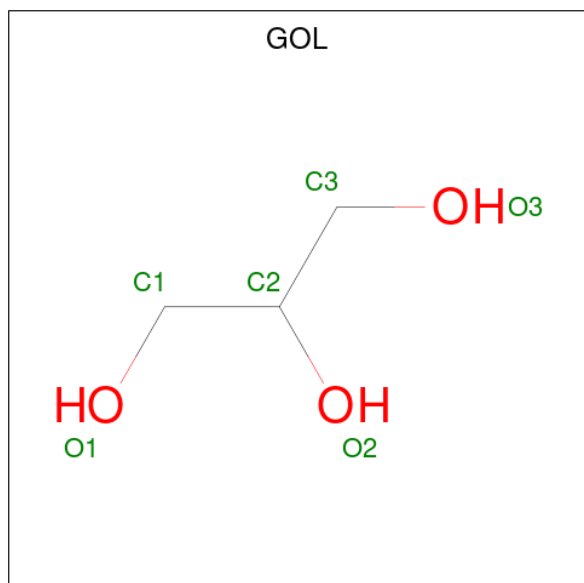
There are 6 unique types of molecules in this entry. The entry contains 20066 atoms, of which 9617 are hydrogens and 0 are deuteriums.

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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

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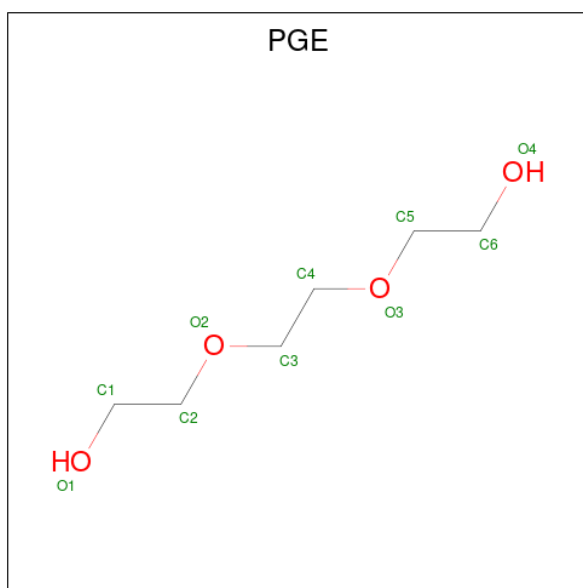
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	1
			28	6	16	6		
2	B	1	Total	C	H	O	0	1
			28	6	16	6		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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 (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	B	2	Total	Zn	0	0
			2	2		
5	C	2	Total	Zn	0	0
			2	2		
5	D	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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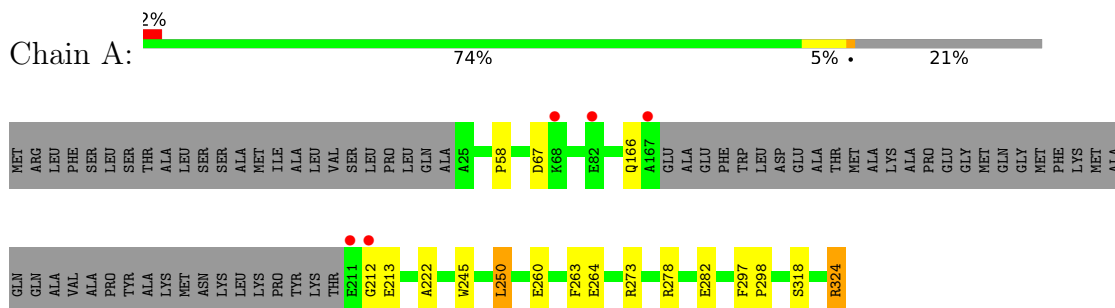
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	43	Total 43	O 43	0	0
6	E	11	Total 11	O 11	0	0

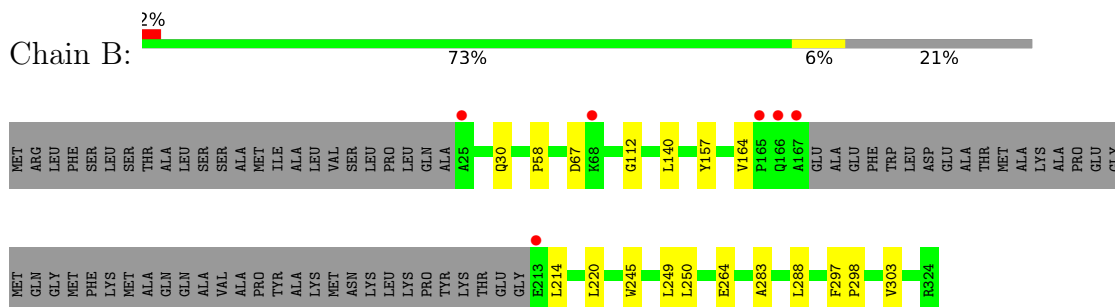
3 Residue-property plots

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.

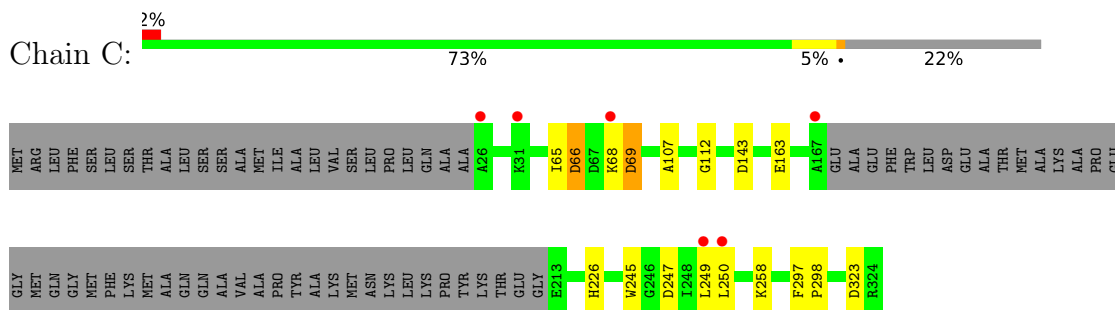
- Molecule 1: Organophosphorus hydrolase



- 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, α , β , γ	109.91Å 63.85Å 221.26Å 90.00° 101.85° 90.00°	Depositor
Resolution (Å)	42.80 – 2.10 42.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.7 (42.80-2.10) 93.7 (42.80-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1352)	Depositor
R, R_{free}	0.173 , 0.210 0.178 , 0.214	Depositor DCC
R_{free} test set	4127 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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	0.95	EDS
Total number of atoms	20066	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PGE, ZN, EDO, GOL

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	0.50	0/2023	0.76	2/2760 (0.1%)
1	B	0.40	0/1992	0.75	4/2720 (0.1%)
1	C	0.38	0/1985	0.77	2/2711 (0.1%)
1	D	0.33	0/1960	0.72	0/2678
1	E	0.34	0/1951	0.73	2/2666 (0.1%)
All	All	0.39	0/9911	0.74	10/13535 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	112	GLY	CA-C-N	7.80	127.98	119.87
1	C	112	GLY	C-N-CA	7.80	127.98	119.87
1	B	157	TYR	CA-C-N	5.45	125.07	119.56
1	B	157	TYR	C-N-CA	5.45	125.07	119.56
1	A	318	SER	CA-C-N	-5.35	115.07	120.21
1	A	318	SER	C-N-CA	-5.35	115.07	120.21
1	B	112	GLY	CA-C-N	5.17	126.19	120.45
1	B	112	GLY	C-N-CA	5.17	126.19	120.45
1	E	215	LEU	CA-C-N	5.14	126.26	119.84
1	E	215	LEU	C-N-CA	5.14	126.26	119.84

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	0	0
2	B	30	40	40	1	0
2	C	12	16	16	0	0
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	51	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 (51) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:402[A]:GOL:O1	6:B:603:HOH:O	2.10	0.52
1:C:69:ASP:OD2	1:C:258:LYS:NZ	2.43	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
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
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:OD1	1:E:159:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	256/324 (79%)	249 (97%)	5 (2%)	2 (1%)	16	12
1	B	252/324 (78%)	247 (98%)	5 (2%)	0	100	100
1	C	251/324 (78%)	240 (96%)	10 (4%)	1 (0%)	30	28
1	D	248/324 (76%)	233 (94%)	13 (5%)	2 (1%)	16	12
1	E	247/324 (76%)	204 (83%)	38 (15%)	5 (2%)	6	2
All	All	1254/1620 (77%)	1173 (94%)	71 (6%)	10 (1%)	16	12

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%)	59	67
1	B	205/258 (80%)	201 (98%)	4 (2%)	48	56
1	C	205/258 (80%)	198 (97%)	7 (3%)	32	35
1	D	203/258 (79%)	200 (98%)	3 (2%)	57	65
1	E	202/258 (78%)	189 (94%)	13 (6%)	16	14
All	All	1023/1290 (79%)	993 (97%)	30 (3%)	37	42

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	TRP
1	A	250	LEU
1	A	324	ARG
1	B	67	ASP
1	B	245	TRP
1	B	249	LEU
1	B	250	LEU
1	C	68	LYS
1	C	69	ASP
1	C	163[A]	GLU
1	C	163[B]	GLU
1	C	245	TRP
1	C	249	LEU
1	C	250	LEU
1	D	214	LEU
1	D	245	TRP
1	D	290	VAL
1	E	40	MET
1	E	42	LEU
1	E	56	ASP
1	E	62	LEU
1	E	65	ILE
1	E	122	LEU

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Mol	Chain	Res	Type
1	E	148	LEU
1	E	159	ASN
1	E	220	LEU
1	E	244	VAL
1	E	245	TRP
1	E	247	ASP
1	E	282	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	B	99	ASN
1	B	119	GLN
1	B	150	ASN
1	B	271	GLN
1	C	90	ASN
1	C	99	ASN
1	C	119	GLN
1	C	302	HIS
1	D	90	ASN
1	D	271	GLN
1	E	271	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	EDO	B	404	-	3,3,3	0.26	0	2,2,2	0.22	0
4	PGE	A	404[B]	-	9,9,9	0.31	0	8,8,8	0.33	0
2	GOL	B	401[B]	-	5,5,5	0.37	0	5,5,5	0.26	0
2	GOL	B	402[A]	-	5,5,5	0.31	0	5,5,5	0.28	0
2	GOL	C	402	-	5,5,5	0.38	0	5,5,5	0.44	0
3	EDO	C	403	-	3,3,3	0.45	0	2,2,2	0.21	0
4	PGE	A	404[A]	-	9,9,9	0.30	0	8,8,8	0.28	0
2	GOL	A	402	-	5,5,5	0.30	0	5,5,5	0.63	0
2	GOL	D	401	-	5,5,5	0.40	0	5,5,5	0.13	0
2	GOL	A	401	-	5,5,5	0.43	0	5,5,5	0.21	0
3	EDO	A	403	-	3,3,3	0.38	0	2,2,2	0.31	0
3	EDO	A	407	-	3,3,3	0.41	0	2,2,2	0.51	0
2	GOL	C	401	-	5,5,5	0.41	0	5,5,5	0.51	0
2	GOL	B	401[A]	-	5,5,5	0.36	0	5,5,5	0.28	0
2	GOL	B	402[B]	-	5,5,5	0.36	0	5,5,5	0.32	0
2	GOL	B	403	-	5,5,5	0.42	0	5,5,5	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	404	-	-	0/1/1/1	-
4	PGE	A	404[B]	-	-	4/7/7/7	-
2	GOL	B	401[B]	-	-	4/4/4/4	-
2	GOL	B	402[A]	-	-	2/4/4/4	-
2	GOL	C	402	-	-	1/4/4/4	-
3	EDO	C	403	-	-	0/1/1/1	-
4	PGE	A	404[A]	-	-	3/7/7/7	-
2	GOL	A	402	-	-	2/4/4/4	-
2	GOL	D	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
3	EDO	A	403	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	407	-	-	1/1/1/1	-
2	GOL	C	401	-	-	0/4/4/4	-
2	GOL	B	401[A]	-	-	0/4/4/4	-
2	GOL	B	402[B]	-	-	3/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	O1-C1-C2-C3
2	B	401[B]	GOL	O1-C1-C2-C3
2	B	401[B]	GOL	O2-C2-C3-O3
2	B	402[A]	GOL	O1-C1-C2-O2
2	B	402[A]	GOL	O1-C1-C2-C3
2	B	402[B]	GOL	O1-C1-C2-O2
2	B	402[B]	GOL	O1-C1-C2-C3
2	B	401[B]	GOL	O1-C1-C2-O2
4	A	404[B]	PGE	O1-C1-C2-O2
2	B	401[B]	GOL	C1-C2-C3-O3
2	D	401	GOL	O1-C1-C2-C3
2	A	402	GOL	O1-C1-C2-O2
4	A	404[A]	PGE	O2-C3-C4-O3
4	A	404[A]	PGE	O1-C1-C2-O2
4	A	404[B]	PGE	O3-C5-C6-O4
4	A	404[A]	PGE	O3-C5-C6-O4
2	D	401	GOL	O1-C1-C2-O2
2	C	402	GOL	O1-C1-C2-O2
4	A	404[B]	PGE	C1-C2-O2-C3
4	A	404[B]	PGE	C4-C3-O2-C2
3	A	403	EDO	O1-C1-C2-O2
3	A	407	EDO	O1-C1-C2-O2
2	B	402[B]	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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, 95th 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 ²)	Q<0.9
1	A	257/324 (79%)	-0.58	5 (1%) 66 69	18, 30, 54, 132	6 (2%)
1	B	255/324 (78%)	-0.11	6 (2%) 59 62	29, 47, 74, 160	2 (0%)
1	C	254/324 (78%)	0.06	6 (2%) 59 62	32, 55, 85, 116	2 (0%)
1	D	251/324 (77%)	1.12	31 (12%) 8 8	42, 89, 130, 157	3 (1%)
1	E	251/324 (77%)	1.98	110 (43%) 0 1	39, 125, 162, 186	5 (1%)
All	All	1268/1620 (78%)	0.49	158 (12%) 8 8	18, 60, 142, 186	18 (1%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	GLN	10.7
1	E	166	GLN	9.7
1	E	83	LYS	9.2
1	D	68	LYS	8.2
1	E	68	LYS	7.8
1	E	82	GLU	6.9
1	E	308	GLN	6.7
1	E	263	PHE	6.1
1	C	68	LYS	6.0
1	A	212	GLY	5.9
1	B	167	ALA	5.3
1	E	265	PHE	5.3
1	A	167	ALA	5.1
1	B	68	LYS	5.0
1	D	214	LEU	5.0
1	E	134	THR	5.0
1	E	245	TRP	4.8
1	E	220	LEU	4.5
1	D	70	LEU	4.3
1	E	165	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	140	LEU	4.1
1	E	161	THR	3.9
1	E	250	LEU	3.8
1	D	258[A]	LYS	3.8
1	E	257	ALA	3.8
1	D	220	LEU	3.8
1	E	215	LEU	3.8
1	E	55	VAL	3.7
1	C	167	ALA	3.7
1	E	222	ALA	3.7
1	E	101	VAL	3.7
1	E	261	VAL	3.6
1	E	249	LEU	3.6
1	E	307	ALA	3.5
1	E	62	LEU	3.5
1	E	162	VAL	3.5
1	D	249	LEU	3.4
1	E	74	LEU	3.4
1	E	164	VAL	3.4
1	E	293	ALA	3.4
1	E	267	VAL	3.3
1	D	26	ALA	3.3
1	E	75	ALA	3.3
1	E	248	ILE	3.3
1	E	235	PHE	3.2
1	B	166	GLN	3.2
1	E	42	LEU	3.2
1	E	234	LEU	3.2
1	E	137	LEU	3.1
1	E	47	VAL	3.1
1	A	68	LYS	3.1
1	E	251	ASN	3.1
1	E	290	VAL	3.1
1	E	221	VAL	3.0
1	E	100	LEU	3.0
1	D	27	PRO	3.0
1	E	310	TYR	3.0
1	E	272	ALA	2.9
1	E	26	ALA	2.9
1	E	223	SER	2.9
1	C	26	ALA	2.9
1	E	244	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	243	LEU	2.8
1	E	110	CYS	2.8
1	D	303	VAL	2.8
1	E	155	PRO	2.8
1	E	111	PHE	2.8
1	E	59	ALA	2.8
1	D	235	PHE	2.7
1	D	28	ALA	2.7
1	E	256	PHE	2.7
1	E	58	PRO	2.7
1	D	97	GLY	2.7
1	D	291	ALA	2.7
1	E	41	ALA	2.7
1	E	255	GLN	2.7
1	E	279	ILE	2.7
1	E	219	SER	2.6
1	E	254	VAL	2.6
1	A	82	GLU	2.6
1	C	250	LEU	2.6
1	D	248	ILE	2.6
1	B	165	PRO	2.6
1	E	157	TYR	2.6
1	B	25	ALA	2.6
1	E	253	ALA	2.6
1	E	93	LEU	2.6
1	E	242	LEU	2.5
1	E	218	VAL	2.5
1	E	294	HIS	2.5
1	D	81	SER	2.5
1	E	322	SER	2.5
1	D	288	LEU	2.5
1	E	45	PHE	2.5
1	E	229	GLY	2.5
1	D	135	VAL	2.5
1	E	303	VAL	2.5
1	E	67	ASP	2.5
1	D	222	ALA	2.5
1	D	221	VAL	2.4
1	D	279	ILE	2.5
1	A	211	GLU	2.4
1	E	314	PRO	2.4
1	D	57	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	57	LEU	2.4
1	E	232	SER	2.4
1	D	165	PRO	2.4
1	E	246	GLY	2.4
1	E	264	GLU	2.4
1	D	254	VAL	2.4
1	E	92	TYR	2.4
1	E	132	VAL	2.4
1	E	149	VAL	2.4
1	E	323	ASP	2.3
1	B	213	GLU	2.3
1	E	289	TRP	2.3
1	E	116	GLY	2.3
1	E	89	VAL	2.3
1	E	109	GLN	2.3
1	E	73	LEU	2.3
1	C	31	LYS	2.3
1	E	288	LEU	2.3
1	E	233	TYR	2.3
1	D	111	PHE	2.2
1	E	214	LEU	2.2
1	E	285	THR	2.2
1	D	257	ALA	2.2
1	D	300	LEU	2.2
1	E	280	LEU	2.2
1	E	295	LEU	2.2
1	E	60	SER	2.2
1	E	87	THR	2.2
1	E	104	ASP	2.2
1	E	80	ALA	2.2
1	E	160	ALA	2.2
1	E	230	HIS	2.2
1	D	215	LEU	2.2
1	D	231	THR	2.2
1	E	148	LEU	2.1
1	E	228	PRO	2.1
1	E	65	ILE	2.1
1	E	85	VAL	2.1
1	E	262	VAL	2.1
1	E	309	GLY	2.1
1	E	284	ALA	2.1
1	E	252	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	78	PHE	2.1
1	C	249	LEU	2.1
1	E	54	TYR	2.1
1	E	158	PRO	2.1
1	E	227	THR	2.1
1	E	231	THR	2.1
1	E	103	ILE	2.1
1	E	117	VAL	2.1
1	D	101	VAL	2.0
1	E	107	ALA	2.0
1	E	61	LEU	2.0
1	E	138	THR	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
2	GOL	C	402	6/6	0.53	0.52	29,35,40,43	14
2	GOL	A	402	6/6	0.58	0.36	32,38,40,41	14
3	EDO	C	403	4/4	0.66	0.39	32,38,43,44	10
2	GOL	B	402[A]	6/6	0.74	0.26	30,46,53,56	14
2	GOL	B	402[B]	6/6	0.74	0.26	38,49,56,59	14
2	GOL	B	401[A]	6/6	0.74	0.36	35,42,46,46	14
2	GOL	B	401[B]	6/6	0.74	0.36	35,42,46,49	14
3	EDO	A	407	4/4	0.78	0.39	41,49,51,51	10
4	PGE	A	404[A]	10/10	0.85	0.22	31,39,45,46	24
4	PGE	A	404[B]	10/10	0.85	0.22	31,38,44,45	24
2	GOL	C	401	6/6	0.89	0.19	23,29,36,44	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	403	4/4	0.89	0.16	20,26,37,44	10
3	EDO	B	404	4/4	0.92	0.11	20,24,26,31	10
2	GOL	D	401	6/6	0.94	0.09	56,68,80,82	0
5	ZN	E	402	1/1	0.95	0.07	98,98,98,98	0
5	ZN	E	401	1/1	0.96	0.06	97,97,97,97	0
2	GOL	B	403	6/6	0.96	0.07	33,41,51,56	0
2	GOL	A	401	6/6	0.97	0.06	24,31,41,45	0
5	ZN	D	403	1/1	0.97	0.04	56,56,56,56	0
5	ZN	D	402	1/1	0.99	0.04	53,53,53,53	0
5	ZN	A	405	1/1	0.99	0.03	24,24,24,24	0
5	ZN	C	404	1/1	0.99	0.02	43,43,43,43	0
5	ZN	C	405	1/1	0.99	0.03	42,42,42,42	0
5	ZN	A	406	1/1	1.00	0.01	20,20,20,20	0
5	ZN	B	405	1/1	1.00	0.04	34,34,34,34	0
5	ZN	B	406	1/1	1.00	0.02	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.