



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2025 – 01:15 pm BST

PDB ID : 7ZJO / pdb_00007zjo
Title : Phosphorylated Thalassospira sp. esterase
Authors : Lund, B.A.
Deposited on : 2022-04-11
Resolution : 1.95 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

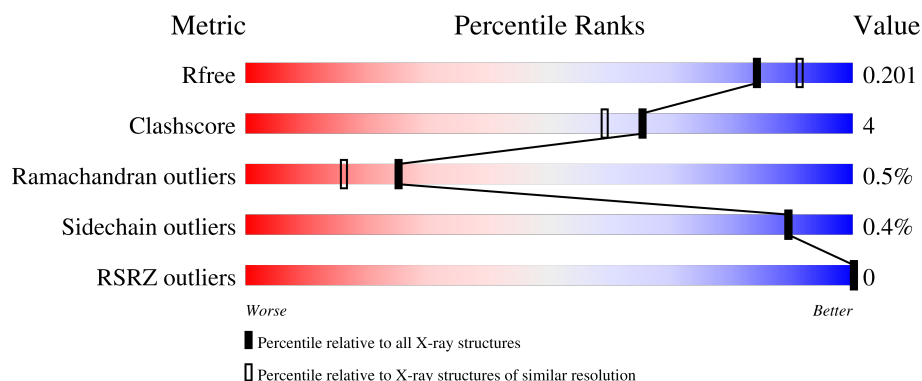
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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	317	<div> <div style="width: 90%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> <div>90% 9% .</div>
1	B	317	<div> <div style="width: 94%;"></div> <div style="width: 4%;"></div> <div style="width: 2%;"></div> </div> <div>94% . .</div>
1	C	317	<div> <div style="width: 91%;"></div> <div style="width: 7%;"></div> <div style="width: 2%;"></div> </div> <div>91% 7% .</div>
1	D	317	<div> <div style="width: 92%;"></div> <div style="width: 8%;"></div> </div> <div>92% 8%</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
4	SO4	B	405	-	-	X	-

2 Entry composition [i](#)

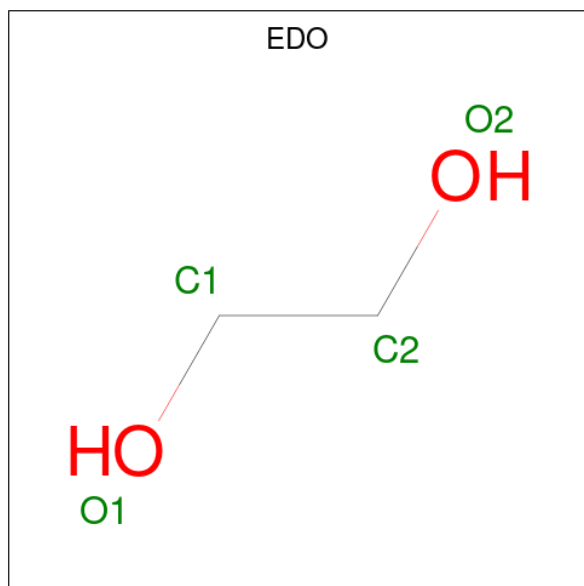
There are 6 unique types of molecules in this entry. The entry contains 20006 atoms, of which 9474 are hydrogens and 0 are deuteriums.

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 Lipase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	315	Total	C	H	N	O	P	S	0	4	0
			4747	1515	2339	412	476	1	4			
1	B	314	Total	C	H	N	O	P	S	0	2	0
			4717	1506	2323	410	473	1	4			
1	C	314	Total	C	H	N	O	P	S	0	4	0
			4733	1510	2332	411	475	1	4			
1	D	316	Total	C	H	N	O	P	S	0	6	0
			4779	1524	2355	414	480	1	5			

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



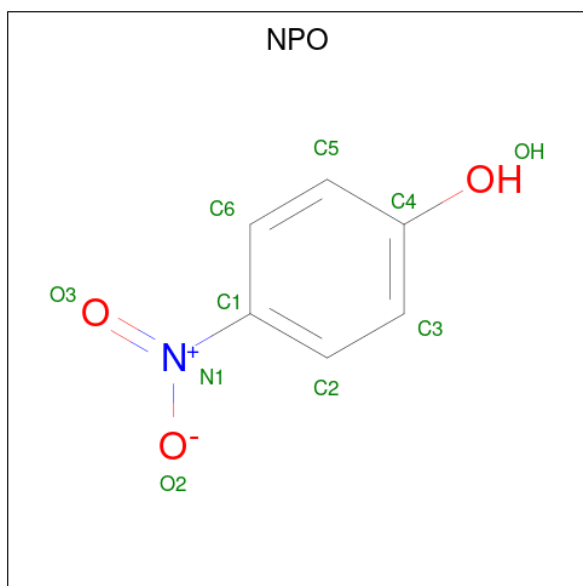
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		

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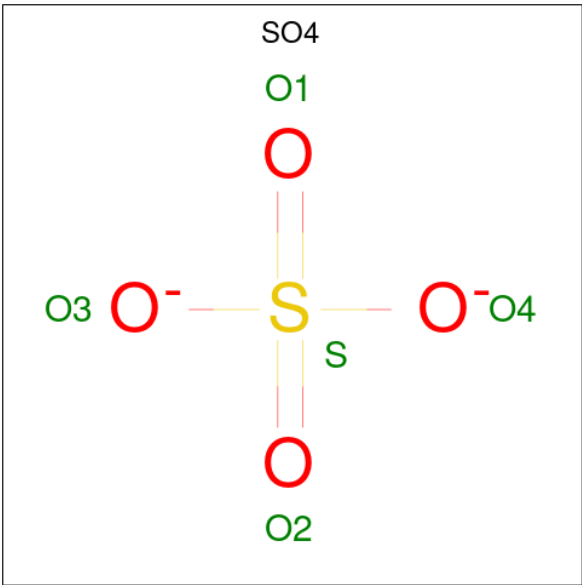
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	1
			20	4	12	4		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	1
			20	4	12	4		

- Molecule 3 is P-NITROPHENOL (CCD ID: NPO) (formula: $C_6H_5NO_3$).



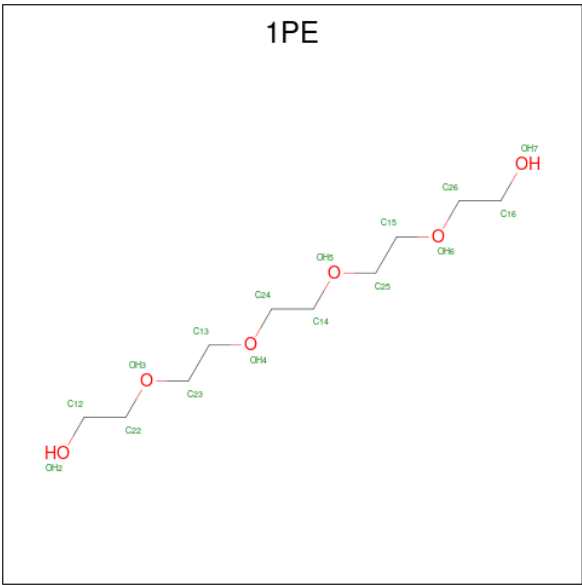
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
3	C	1	Total	C	H	N	O	0	0
			15	6	5	1	3		
3	D	1	Total	C	H	N	O	0	0
			15	6	5	1	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			38	10	22	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			38	10	22	6		

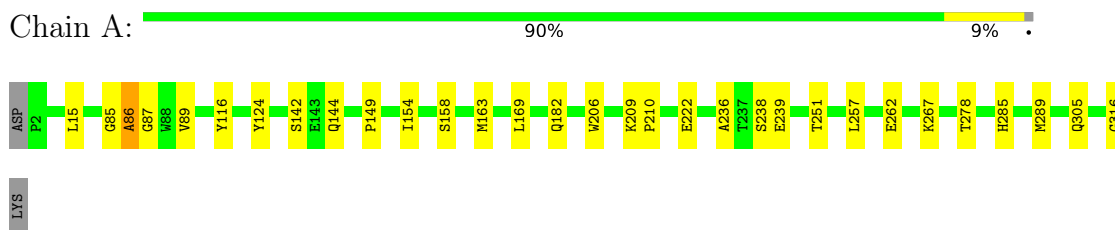
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	190	Total	O	0	0
			190	190		
6	B	203	Total	O	0	0
			203	203		
6	C	218	Total	O	0	0
			218	218		
6	D	173	Total	O	0	0
			173	173		

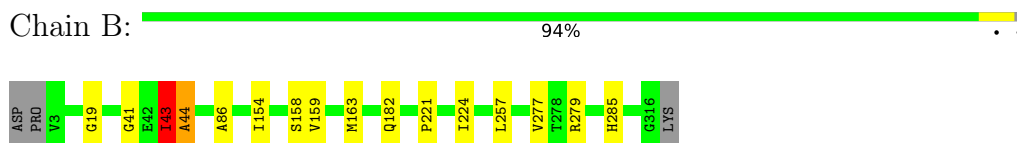
3 Residue-property plots [i](#)

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.

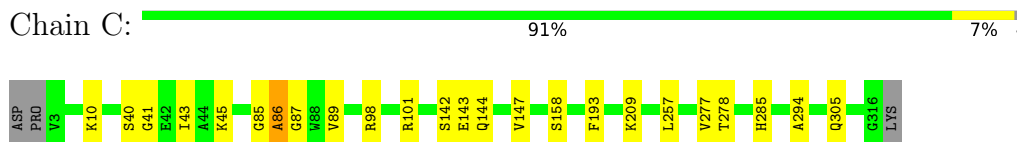
- Molecule 1: Lipase



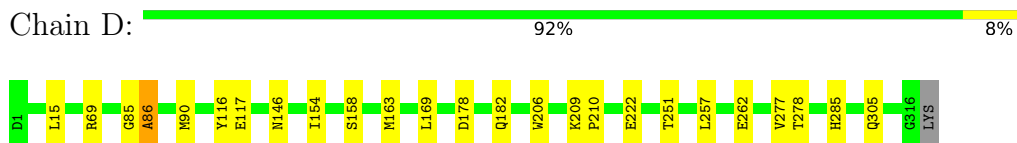
- Molecule 1: Lipase



- Molecule 1: Lipase



- Molecule 1: Lipase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.21Å 115.77Å 87.55Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	64.10 – 1.95 64.10 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.8 (64.10-1.95) 96.5 (64.10-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.167 , 0.198 0.168 , 0.201	Depositor DCC
R_{free} test set	1658 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.447 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20006	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: SO4, 1PE, NPO, SEP, 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	0/2470	0.50	0/3380
1	B	0.46	0/2444	0.54	0/3345
1	C	0.44	0/2462	0.53	0/3369
1	D	0.39	0/2490	0.50	0/3407
All	All	0.42	0/9866	0.52	0/13501

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	2408	2339	2316	23	0
1	B	2394	2323	2314	12	0
1	C	2401	2332	2308	19	0
1	D	2424	2355	2328	18	0
2	A	4	6	6	0	0
2	B	16	24	24	0	0
2	C	16	24	24	0	0
2	D	8	12	12	1	0
3	B	10	5	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	10	5	5	0	0
3	D	10	5	5	2	0
4	B	10	0	0	3	0
4	C	5	0	0	1	0
5	B	16	22	22	1	0
5	C	16	22	22	0	0
6	A	190	0	0	5	1
6	B	203	0	0	2	1
6	C	218	0	0	1	1
6	D	173	0	0	2	0
All	All	10532	9474	9391	71	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (71) 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:222:GLU:OE1	6:D:501:HOH:O	1.99	0.80
1:A:238:SER:OG	6:A:501:HOH:O	2.01	0.77
1:D:178:ASP:OD1	6:D:502:HOH:O	2.06	0.73
1:A:239:GLU:O	6:A:502:HOH:O	2.08	0.71
1:B:279:ARG:NH2	4:B:405:SO4:O3	2.26	0.68
1:C:143:GLU:OE1	1:C:144:GLN:OE1	2.14	0.66
1:A:316:GLY:O	6:A:503:HOH:O	2.15	0.64
4:C:503:SO4:O4	6:C:601:HOH:O	2.15	0.64
5:B:404:1PE:OH7	5:B:404:1PE:OH2	2.16	0.64
4:B:405:SO4:S	6:B:501:HOH:O	2.56	0.60
4:B:405:SO4:O4	6:B:501:HOH:O	2.16	0.59
1:A:278[A]:THR:HG21	1:A:305:GLN:HE22	1.67	0.59
1:D:90[B]:MET:HE1	3:D:401:NPO:C2	2.36	0.56
1:B:43:ILE:O	1:B:44:ALA:C	2.48	0.56
1:B:159:VAL:O	1:B:163:MET:HG3	2.04	0.56
1:D:222:GLU:H	1:D:222:GLU:CD	2.14	0.56
1:C:43:ILE:HD11	1:C:294:ALA:CB	2.36	0.56
1:C:43:ILE:HD11	1:C:294:ALA:HB3	1.87	0.55
1:D:278[A]:THR:HG21	1:D:305:GLN:HE22	1.71	0.55
1:B:43:ILE:N	1:C:40:SER:HB2	2.23	0.54
1:C:45:LYS:HE3	1:C:101:ARG:CZ	2.37	0.54
1:D:90[B]:MET:HE1	3:D:401:NPO:H2	1.89	0.54
1:A:222:GLU:H	1:A:222:GLU:CD	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:GLU:HA	2:D:402[B]:EDO:H11	1.92	0.51
1:B:43:ILE:HA	1:C:40:SER:HB2	1.93	0.50
1:A:267:LYS:NZ	6:A:511:HOH:O	2.44	0.50
1:C:43:ILE:HG12	1:C:98:ARG:HD3	1.94	0.49
1:A:15:LEU:HD11	1:A:206:TRP:CE3	2.48	0.49
1:A:144:GLN:OE1	1:A:144:GLN:N	2.31	0.49
1:D:116:TYR:CZ	1:D:163:MET:HE1	2.47	0.49
1:A:144:GLN:OE1	6:A:504:HOH:O	2.18	0.48
1:C:143:GLU:H	1:C:143:GLU:CD	2.22	0.47
1:A:85:GLY:O	1:A:86:ALA:CB	2.62	0.47
1:A:251:THR:HG21	1:A:262:GLU:HG3	1.95	0.47
1:C:10:LYS:HE3	1:C:10:LYS:HB2	1.66	0.47
1:D:85:GLY:O	1:D:86:ALA:CB	2.62	0.47
1:D:15:LEU:HD11	1:D:206:TRP:CE3	2.50	0.47
1:D:251:THR:HG21	1:D:262:GLU:HG3	1.96	0.46
1:B:43:ILE:CA	1:C:40:SER:HB2	2.46	0.46
1:B:41:GLY:CA	1:C:41:GLY:O	2.64	0.46
1:A:116:TYR:CZ	1:A:163:MET:HE1	2.51	0.46
1:D:69:ARG:NH2	1:D:146:ASN:O	2.50	0.45
1:C:278[A]:THR:HG21	1:C:305:GLN:HE22	1.81	0.45
1:D:85:GLY:O	1:D:86:ALA:HB3	2.16	0.45
1:C:278[B]:THR:HG21	1:C:305:GLN:HE22	1.81	0.45
1:C:193:PHE:O	1:C:209:LYS:HE2	2.17	0.45
1:B:257:LEU:HD12	1:B:285:HIS:CE1	2.53	0.44
1:A:257:LEU:HD12	1:A:285:HIS:CE1	2.52	0.44
1:D:15:LEU:HD11	1:D:206:TRP:HE3	1.83	0.44
1:C:257:LEU:HD12	1:C:285:HIS:CE1	2.53	0.44
1:B:221:PRO:O	1:B:224:ILE:HG22	2.18	0.44
1:D:257:LEU:HD12	1:D:285:HIS:CE1	2.53	0.43
1:D:169:LEU:HD23	1:D:169:LEU:C	2.43	0.43
1:A:15:LEU:HD11	1:A:206:TRP:HE3	1.83	0.43
1:C:85:GLY:O	1:C:86:ALA:CB	2.67	0.43
1:C:142:SER:HB2	1:C:147:VAL:O	2.19	0.43
1:D:209:LYS:HB3	1:D:210:PRO:HD3	2.01	0.43
1:B:154:ILE:O	1:B:182:GLN:HA	2.20	0.41
1:D:154:ILE:O	1:D:182:GLN:HA	2.20	0.41
1:A:85:GLY:O	1:A:86:ALA:HB3	2.21	0.41
1:C:85:GLY:O	1:C:86:ALA:HB3	2.21	0.41
1:A:154:ILE:O	1:A:182:GLN:HA	2.20	0.41
1:A:209:LYS:HB3	1:A:210:PRO:HD3	2.01	0.41
1:A:142:SER:HB2	1:A:149:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TYR:O	1:B:19:GLY:HA2	2.21	0.41
1:A:289:MET:HE3	1:A:289:MET:HB3	2.00	0.41
1:C:87:GLY:C	1:C:89:VAL:H	2.29	0.40
1:A:87:GLY:C	1:A:89:VAL:H	2.30	0.40
1:A:236:ALA:O	1:A:267:LYS:NZ	2.55	0.40
1:A:169:LEU:HD23	1:A:169:LEU:C	2.46	0.40
1:B:43:ILE:N	1:B:43:ILE:HD13	2.36	0.40

All (2) 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)
6:B:556:HOH:O	6:B:683:HOH:O[2_656]	2.03	0.17
6:A:600:HOH:O	6:C:817:HOH:O[4_546]	2.17	0.03

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	316/317 (100%)	306 (97%)	9 (3%)	1 (0%)	37	29
1	B	313/317 (99%)	302 (96%)	8 (3%)	3 (1%)	13	5
1	C	315/317 (99%)	305 (97%)	9 (3%)	1 (0%)	37	29
1	D	319/317 (101%)	312 (98%)	6 (2%)	1 (0%)	37	29
All	All	1263/1268 (100%)	1225 (97%)	32 (2%)	6 (0%)	25	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ALA
1	B	86	ALA

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Mol	Chain	Res	Type
1	C	86	ALA
1	D	86	ALA
1	B	44	ALA
1	B	43	ILE

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	252/250 (101%)	252 (100%)	0	100	100
1	B	249/250 (100%)	247 (99%)	2 (1%)	79	78
1	C	251/250 (100%)	250 (100%)	1 (0%)	89	89
1	D	254/250 (102%)	253 (100%)	1 (0%)	89	89
All	All	1006/1000 (101%)	1002 (100%)	4 (0%)	89	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	ILE
1	B	277	VAL
1	C	277	VAL
1	D	277	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	305	GLN
1	B	71	GLN
1	B	305	GLN
1	C	305	GLN
1	D	9	GLN
1	D	218	GLN
1	D	305	GLN

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Mol	Chain	Res	Type
1	D	308	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	C	158	1	8,9,10	1.65	2 (25%)	8,12,14	1.05	0
1	SEP	D	158	1	8,9,10	1.67	1 (12%)	8,12,14	1.22	1 (12%)
1	SEP	B	158	1	8,9,10	1.82	1 (12%)	8,12,14	1.12	1 (12%)
1	SEP	A	158	1	8,9,10	1.68	1 (12%)	8,12,14	1.42	2 (25%)

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
1	SEP	C	158	1	-	4/5/8/10	-
1	SEP	D	158	1	-	2/5/8/10	-
1	SEP	B	158	1	-	4/5/8/10	-
1	SEP	A	158	1	-	1/5/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	SEP	P-O1P	4.57	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	SEP	P-O1P	4.15	1.63	1.50
1	D	158	SEP	P-O1P	3.87	1.63	1.50
1	C	158	SEP	P-O2P	3.06	1.66	1.54
1	C	158	SEP	P-O1P	2.37	1.58	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	SEP	P-OG-CB	-3.17	109.56	118.30
1	D	158	SEP	P-OG-CB	-2.51	111.37	118.30
1	B	158	SEP	OG-CB-CA	2.10	110.19	108.14
1	A	158	SEP	OG-CB-CA	2.03	110.12	108.14

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	158	SEP	CB-OG-P-O2P
1	B	158	SEP	CB-OG-P-O3P
1	C	158	SEP	CB-OG-P-O2P
1	C	158	SEP	CB-OG-P-O3P
1	C	158	SEP	CB-OG-P-O1P
1	A	158	SEP	N-CA-CB-OG
1	B	158	SEP	N-CA-CB-OG
1	C	158	SEP	N-CA-CB-OG
1	D	158	SEP	N-CA-CB-OG
1	B	158	SEP	CB-OG-P-O1P
1	D	158	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NPO	C	501	-	9,10,10	0.75	0	11,13,13	0.56	0
3	NPO	D	401	-	9,10,10	1.00	1 (11%)	11,13,13	0.46	0
2	EDO	C	506	-	3,3,3	0.43	0	2,2,2	0.35	0
3	NPO	B	401	-	9,10,10	0.92	0	11,13,13	0.58	0
2	EDO	B	406[A]	-	3,3,3	0.60	0	2,2,2	0.41	0
2	EDO	B	407	-	3,3,3	0.49	0	2,2,2	0.19	0
4	SO4	B	405	-	4,4,4	0.18	0	6,6,6	0.24	0
2	EDO	D	402[B]	-	3,3,3	0.57	0	2,2,2	0.56	0
5	1PE	C	502	-	15,15,15	0.51	0	14,14,14	0.37	0
2	EDO	B	402	-	3,3,3	0.47	0	2,2,2	0.24	0
2	EDO	C	507	-	3,3,3	0.53	0	2,2,2	0.34	0
2	EDO	A	401	-	3,3,3	0.59	0	2,2,2	0.19	0
2	EDO	B	406[B]	-	3,3,3	0.37	0	2,2,2	0.82	0
2	EDO	C	505	-	3,3,3	0.50	0	2,2,2	0.33	0
2	EDO	C	504	-	3,3,3	0.78	0	2,2,2	0.26	0
4	SO4	B	403	-	4,4,4	0.13	0	6,6,6	0.16	0
4	SO4	C	503	-	4,4,4	0.35	0	6,6,6	0.14	0
5	1PE	B	404	-	15,15,15	0.54	0	14,14,14	0.33	0
2	EDO	D	402[A]	-	3,3,3	0.42	0	2,2,2	0.31	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	NPO	C	501	-	-	0/2/4/4	0/1/1/1
2	EDO	C	505	-	-	0/1/1/1	-
2	EDO	D	402[B]	-	-	1/1/1/1	-
5	1PE	C	502	-	-	5/13/13/13	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	C	507	-	-	0/1/1/1	-
2	EDO	C	504	-	-	0/1/1/1	-
3	NPO	D	401	-	-	0/2/4/4	0/1/1/1
2	EDO	A	401	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	506	-	-	0/1/1/1	-
3	NPO	B	401	-	-	0/2/4/4	0/1/1/1
2	EDO	B	406[A]	-	-	0/1/1/1	-
2	EDO	D	402[A]	-	-	1/1/1/1	-
5	1PE	B	404	-	-	5/13/13/13	-
2	EDO	B	407	-	-	1/1/1/1	-
2	EDO	B	406[B]	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NPO	O3-N1	-2.68	1.18	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	404	1PE	OH4-C13-C23-OH3
5	C	502	1PE	OH5-C14-C24-OH4
2	D	402[B]	EDO	O1-C1-C2-O2
5	B	404	1PE	OH7-C16-C26-OH6
5	C	502	1PE	OH7-C16-C26-OH6
5	B	404	1PE	C24-C14-OH5-C25
5	B	404	1PE	C16-C26-OH6-C15
5	C	502	1PE	C15-C25-OH5-C14
5	C	502	1PE	C12-C22-OH3-C23
2	B	406[B]	EDO	O1-C1-C2-O2
5	C	502	1PE	OH6-C15-C25-OH5
2	D	402[A]	EDO	O1-C1-C2-O2
2	B	407	EDO	O1-C1-C2-O2
5	B	404	1PE	OH6-C15-C25-OH5

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	NPO	2	0
4	B	405	SO4	3	0
2	D	402[B]	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	SO4	1	0
5	B	404	1PE	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 [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, 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	314/317 (99%)	-1.33	0 100 100	14, 35, 56, 89	3 (0%)
1	B	313/317 (98%)	-1.38	0 100 100	16, 29, 44, 115	2 (0%)
1	C	313/317 (98%)	-1.38	0 100 100	15, 29, 46, 95	2 (0%)
1	D	315/317 (99%)	-1.32	0 100 100	14, 34, 55, 88	3 (0%)
All	All	1255/1268 (98%)	-1.35	0 100 100	14, 32, 51, 115	10 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	SEP	B	158	10/11	0.99	0.03	20,23,25,29	0
1	SEP	C	158	10/11	0.99	0.03	21,23,28,28	0
1	SEP	D	158	10/11	0.99	0.03	24,29,33,35	0
1	SEP	A	158	10/11	1.00	0.02	24,28,33,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	EDO	D	402[A]	4/4	0.95	0.10	33,40,43,43	10
2	EDO	D	402[B]	4/4	0.95	0.10	31,38,44,44	10
2	EDO	B	406[B]	4/4	0.98	0.13	25,30,32,33	10
2	EDO	B	407	4/4	0.98	0.05	42,51,54,57	0
2	EDO	A	401	4/4	0.98	0.05	39,47,56,57	0
2	EDO	B	406[A]	4/4	0.98	0.13	19,26,31,31	10
3	NPO	B	401	10/10	0.98	0.05	38,43,52,52	0
3	NPO	D	401	10/10	0.98	0.12	78,88,105,106	0
4	SO4	B	405	5/5	0.98	0.05	81,87,94,112	0
5	1PE	B	404	16/16	0.98	0.07	62,80,94,100	0
2	EDO	C	504	4/4	0.99	0.05	26,38,44,46	0
2	EDO	C	505	4/4	0.99	0.05	38,46,54,57	0
3	NPO	C	501	10/10	0.99	0.04	33,41,49,52	0
2	EDO	C	506	4/4	0.99	0.06	32,38,45,45	0
4	SO4	B	403	5/5	0.99	0.04	38,42,61,71	0
2	EDO	C	507	4/4	0.99	0.04	39,48,57,63	0
4	SO4	C	503	5/5	0.99	0.03	41,42,60,74	0
2	EDO	B	402	4/4	0.99	0.04	34,42,49,53	0
5	1PE	C	502	16/16	0.99	0.06	49,62,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.