



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:38 AM GMT

PDB ID : 3O4P  
Title : DFPase at 0.85 Angstrom resolution (H atoms included)  
Authors : Liebschner, D.; Elias, M.; Koepke, J.; Lecomte, C.; Guillot, B.; Jelsch, C.; Chabriere, E.  
Deposited on : 2010-07-27  
Resolution : 0.85 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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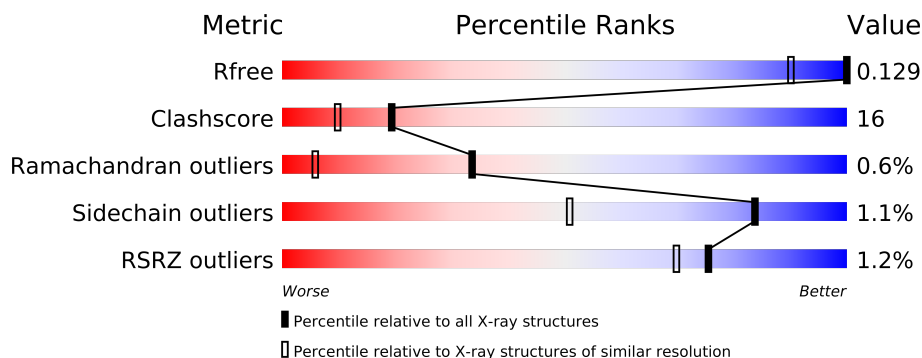
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 0.85 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))
$R_{free}$	66092	1084 (1.12-0.62)
Clashscore	79885	1127 (1.10-0.62)
Ramachandran outliers	78287	1051 (1.10-0.62)
Sidechain outliers	78261	1050 (1.10-0.62)
RSRZ outliers	66119	1084 (1.12-0.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	314	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	403	-	X
3	MES	A	411	-	X
3	MES	A	412	-	X
4	EDO	A	421	-	X
4	EDO	A	422	-	X
4	EDO	A	423	-	X
4	EDO	A	426	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	A	427	-	X
4	EDO	A	428	-	X
5	PGE	A	433	-	X
5	PGE	A	434	-	X
6	DXE	A	442	-	X
6	DXE	A	443	-	X
7	MXE	A	451	-	X
7	MXE	A	452	-	X
8	PEG	A	461	-	X
8	PEG	A	462	-	X
9	ME2	A	471	-	X

## 2 Entry composition i

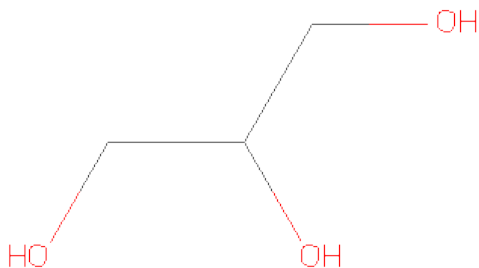
There are 11 unique types of molecules in this entry. The entry contains 5370 atoms, of which 2096 are hydrogens and 0 are deuterium.

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 Diisopropyl-fluorophosphatase.

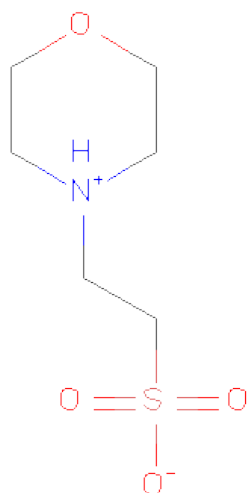
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	314	4722	1688	2065	456	495	18	0	46	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



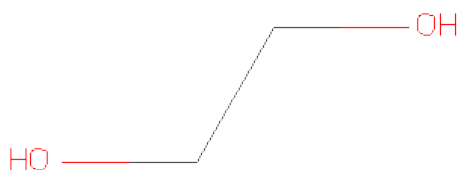
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



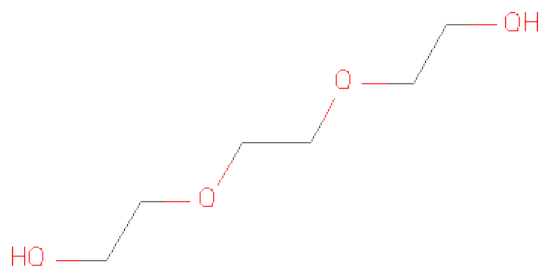
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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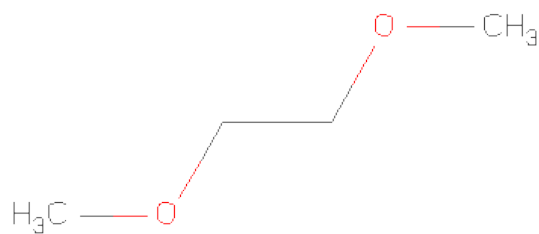
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



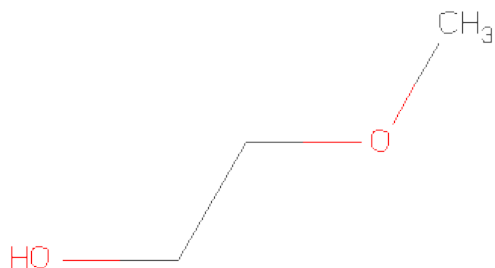
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula:  $C_4H_{10}O_2$ ).



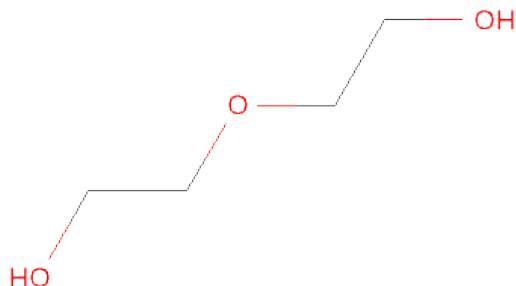
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		
6	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 7 is 2-METHOXYETHANOL (three-letter code: MXE) (formula:  $C_3H_8O_2$ ).



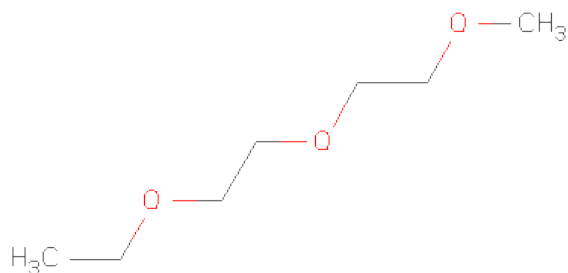
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			5	3	2		
7	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is 1-ETHOXY-2-(2-METHOXYETHOXY)ETHANE (three-letter code: ME2) (formula:  $C_7H_{16}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	Ca	0	0
			2	2		

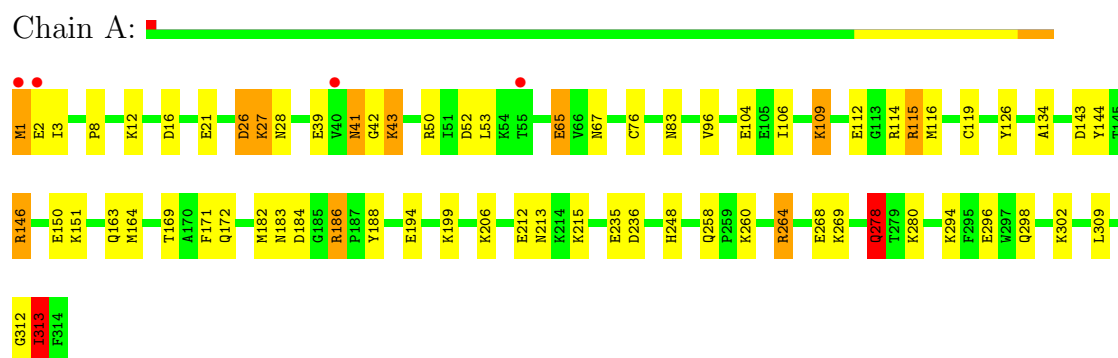
- Molecule 11 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	466	Total	H	O	0	15
			512	31	481		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Diisopropyl-fluorophosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.11Å 81.85Å 86.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.80 – 0.85 20.92 – 0.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.80-0.85) 86.3 (20.92-0.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 0.83Å)	Xtriage
Refinement program	MoPro	Depositor
R, $R_{free}$	0.103 , 0.121 0.116 , 0.129	Depositor DCC
$R_{free}$ test set	2462 reflections (1.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	6.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 78.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 255775 reflections	Xtriage
$F_o, F_c$ correlation	0.99	EDS
Total number of atoms	5370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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, PGE, CA, EDO, MES, ME2, DXE, PEG, MXE

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	1.59	37/2949 (1.3%)	1.67	53/3975 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	ARG	NE-CZ	-22.21	1.04	1.33
1	A	278	GLN	CD-OE1	19.77	1.67	1.24
1	A	39	GLU	CD-OE1	19.76	1.47	1.25
1	A	41	ASN	CB-CG	17.99	1.92	1.51
1	A	41	ASN	CG-OD1	17.60	1.62	1.24
1	A	112	GLU	CD-OE2	-16.37	1.07	1.25
1	A	150	GLU	CD-OE2	15.62	1.42	1.25
1	A	264	ARG	CZ-NH2	13.17	1.50	1.33
1	A	109	LYS	CD-CE	11.89	1.80	1.51
1	A	27	LYS	CE-NZ	-10.46	1.23	1.49
1	A	67	ASN	CG-OD1	10.46	1.47	1.24
1	A	65	GLU	CD-OE2	10.26	1.36	1.25
1	A	298	GLN	CD-OE1	-9.54	1.02	1.24
1	A	150	GLU	CG-CD	-9.16	1.38	1.51
1	A	28	ASN	CG-OD1	9.11	1.44	1.24
1	A	183	ASN	CG-ND2	8.39	1.53	1.32
1	A	41	ASN	CA-CB	8.23	1.74	1.53
1	A	264	ARG	CD-NE	7.65	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	LYS	CE-NZ	7.63	1.68	1.49
1	A	112	GLU	CB-CG	7.50	1.66	1.52
1	A	42	GLY	C-O	-7.09	1.12	1.23
1	A	104	GLU	CG-CD	-7.07	1.41	1.51
1	A	278	GLN	CG-CD	-6.94	1.35	1.51
1	A	235	GLU	CG-CD	6.60	1.61	1.51
1	A	183	ASN	CG-OD1	-6.56	1.09	1.24
1	A	39	GLU	CD-OE2	-6.52	1.18	1.25
1	A	109	LYS	CE-NZ	6.21	1.64	1.49
1	A	104	GLU	CD-OE1	5.95	1.32	1.25
1	A	199	LYS	CE-NZ	-5.92	1.34	1.49
1	A	52	ASP	CG-OD1	-5.88	1.11	1.25
1	A	28	ASN	CG-ND2	-5.72	1.18	1.32
1	A	183	ASN	CB-CG	5.65	1.64	1.51
1	A	67	ASN	CG-ND2	-5.61	1.18	1.32
1	A	112	GLU	CA-CB	5.39	1.65	1.53
1	A	16	ASP	CG-OD2	5.14	1.37	1.25
1	A	39	GLU	CG-CD	-5.08	1.44	1.51
1	A	12	LYS	CD-CE	-5.04	1.38	1.51

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ARG	NE-CZ-NH1	24.49	132.54	120.30
1	A	186[A]	ARG	NE-CZ-NH2	18.20	129.40	120.30
1	A	186[B]	ARG	NE-CZ-NH2	18.20	129.40	120.30
1	A	43	LYS	CG-CD-CE	16.62	161.75	111.90
1	A	115[A]	ARG	CD-NE-CZ	15.70	145.57	123.60
1	A	115[B]	ARG	CD-NE-CZ	15.70	145.57	123.60
1	A	115[A]	ARG	NE-CZ-NH2	15.44	128.02	120.30
1	A	115[B]	ARG	NE-CZ-NH2	15.44	128.02	120.30
1	A	186[A]	ARG	CD-NE-CZ	14.30	143.62	123.60
1	A	186[B]	ARG	CD-NE-CZ	14.30	143.62	123.60
1	A	41	ASN	OD1-CG-ND2	11.83	149.11	121.90
1	A	43	LYS	CD-CE-NZ	11.40	137.91	111.70
1	A	112	GLU	CG-CD-OE1	-10.72	96.86	118.30
1	A	264	ARG	NH1-CZ-NH2	-10.64	107.70	119.40
1	A	114[A]	ARG	CD-NE-CZ	9.87	137.42	123.60
1	A	114[B]	ARG	CD-NE-CZ	9.87	137.42	123.60
1	A	186[A]	ARG	NE-CZ-NH1	-9.58	115.51	120.30
1	A	186[B]	ARG	NE-CZ-NH1	-9.58	115.51	120.30
1	A	41	ASN	CB-CG-ND2	-9.57	93.73	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143[A]	ASP	CB-CG-OD1	-8.65	110.52	118.30
1	A	143[B]	ASP	CB-CG-OD1	-8.65	110.52	118.30
1	A	1[A]	MET	C-N-CA	8.50	142.95	121.70
1	A	1[B]	MET	C-N-CA	8.50	142.95	121.70
1	A	169[A]	THR	CA-CB-CG2	-7.94	101.28	112.40
1	A	169[B]	THR	CA-CB-CG2	-7.94	101.28	112.40
1	A	182	MET	CG-SD-CE	-7.76	87.78	100.20
1	A	236	ASP	CB-CG-OD2	-7.74	111.34	118.30
1	A	146[A]	ARG	CB-CA-C	-7.59	95.22	110.40
1	A	146[B]	ARG	CB-CA-C	-7.59	95.22	110.40
1	A	114[A]	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	114[B]	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	112	GLU	OE1-CD-OE2	6.72	131.37	123.30
1	A	126	TYR	CB-CG-CD2	6.61	124.97	121.00
1	A	150	GLU	CG-CD-OE1	6.57	131.44	118.30
1	A	115[A]	ARG	NH1-CZ-NH2	-6.54	112.20	119.40
1	A	115[B]	ARG	NH1-CZ-NH2	-6.54	112.20	119.40
1	A	235	GLU	OE1-CD-OE2	6.38	130.96	123.30
1	A	112	GLU	CG-CD-OE2	6.10	130.50	118.30
1	A	67	ASN	CB-CG-OD1	-5.99	109.62	121.60
1	A	309	LEU	CB-CG-CD2	5.93	121.07	111.00
1	A	184	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	188	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	A	150	GLU	OE1-CD-OE2	-5.76	116.38	123.30
1	A	114[A]	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	114[B]	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	52	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	188	TYR	CD1-CG-CD2	5.49	123.94	117.90
1	A	184	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	143[A]	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	143[B]	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	144	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	188	TYR	CG-CD2-CE2	-5.11	117.21	121.30
1	A	26	ASP	CB-CG-OD2	-5.08	113.73	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	GLN	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2657	2065	0	66	4
2	A	12	0	0	0	0
3	A	24	0	0	3	0
4	A	32	0	0	11	0
5	A	20	0	0	4	0
6	A	12	0	0	6	0
7	A	10	0	0	6	0
8	A	14	0	0	3	0
9	A	10	0	0	3	0
10	A	2	0	0	0	0
11	A	481	31	0	27	4
All	All	3274	2096	0	79	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (79) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:LYS:CD	1:A:109:LYS:CE	1.81	1.58
1:A:41:ASN:CB	1:A:41:ASN:CA	1.74	1.57
1:A:43:LYS:NZ	1:A:43:LYS:CE	1.68	1.55
1:A:41:ASN:CB	1:A:41:ASN:CG	1.92	1.38
1:A:278:GLN:OE1	1:A:278:GLN:CD	1.67	1.32
1:A:215[C]:LYS:CE	11:A:1046:HOH:O	1.65	1.32
1:A:50[C]:ARG:CZ	11:A:1039:HOH:O	1.78	1.27
1:A:146[B]:ARG:NH2	11:A:948:HOH:O	1.70	1.22
1:A:43:LYS:HZ2	3:A:411:MES:C3	1.52	1.22
1:A:2[B]:GLU:CA	11:A:861:HOH:O	1.88	1.21
4:A:423:EDO:O1	11:A:959:HOH:O	1.57	1.20
8:A:462:PEG:C3	8:A:462:PEG:O1	1.90	1.18
1:A:50[C]:ARG:NH1	11:A:1042:HOH:O	1.87	1.08
1:A:50[A]:ARG:NH2	11:A:1040:HOH:O	1.95	0.97
1:A:43:LYS:NZ	3:A:411:MES:C3	2.28	0.96
1:A:50[C]:ARG:NH2	11:A:1039:HOH:O	1.83	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:50[A]:ARG:CZ	11:A:1040:HOH:O	2.19	0.90
1:A:115[B]:ARG:CD	4:A:423:EDO:O2	2.22	0.88
1:A:41:ASN:CB	1:A:41:ASN:ND2	2.38	0.85
1:A:151[B]:LYS:CE	7:A:452:MXE:C3	2.59	0.81
1:A:312[B]:GLY:O	1:A:313[B]:ILE:CG1	2.29	0.80
1:A:109:LYS:CG	1:A:109:LYS:CE	2.58	0.80
1:A:296:GLU:O	6:A:443:DXE:C4	2.29	0.80
5:A:434:PGE:C6	11:A:544:HOH:O	2.28	0.79
4:A:428:EDO:C1	11:A:1082:HOH:O	2.30	0.78
1:A:312[B]:GLY:C	1:A:313[B]:ILE:CG1	2.52	0.77
1:A:268[A]:GLU:OE1	11:A:1014:HOH:O	2.01	0.77
1:A:116[A]:MET:CE	1:A:164:MET:HG2	2.14	0.77
1:A:260[B]:LYS:NZ	4:A:427:EDO:C2	2.47	0.77
1:A:163[B]:GLN:NE2	11:A:978:HOH:O	2.19	0.76
4:A:425:EDO:C2	11:A:876:HOH:O	2.35	0.75
1:A:50[A]:ARG:NE	11:A:1040:HOH:O	2.22	0.71
6:A:443:DXE:C4	11:A:770:HOH:O	2.40	0.69
1:A:26:ASP:HB2	1:A:83:ASN:HD22	1.58	0.68
1:A:41:ASN:CB	1:A:41:ASN:C	2.59	0.68
1:A:171[B]:PHE:CD2	7:A:452:MXE:C2	2.77	0.67
1:A:264:ARG:HH11	9:A:471:ME2:C5	2.08	0.66
1:A:258:GLN:NE2	4:A:425:EDO:O1	2.30	0.64
1:A:41:ASN:CB	1:A:41:ASN:N	2.59	0.63
1:A:215[C]:LYS:NZ	11:A:1046:HOH:O	2.08	0.63
4:A:421:EDO:C2	11:A:859:HOH:O	2.51	0.59
9:A:471:ME2:C6	9:A:471:ME2:O2	2.51	0.59
1:A:8:PRO:HB3	6:A:443:DXE:C4	2.33	0.58
1:A:106[B]:ILE:CD1	8:A:461:PEG:C4	2.82	0.58
1:A:151[A]:LYS:NZ	7:A:452:MXE:C3	2.68	0.57
1:A:27:LYS:H	1:A:83:ASN:ND2	2.02	0.56
1:A:2[B]:GLU:N	11:A:861:HOH:O	2.24	0.55
1:A:27:LYS:H	1:A:83:ASN:HD22	1.55	0.54
1:A:280[B]:LYS:CE	5:A:434:PGE:O3	2.56	0.53
1:A:248:HIS:NE2	9:A:471:ME2:C5	2.73	0.52
1:A:41:ASN:CB	1:A:41:ASN:HD21	2.23	0.51
1:A:269:LYS:HZ2	6:A:442:DXE:C1	2.23	0.50
7:A:451:MXE:C3	11:A:859:HOH:O	2.60	0.49
1:A:27:LYS:NZ	11:A:862[B]:HOH:O	2.45	0.49
1:A:258:GLN:HE22	4:A:425:EDO:C1	2.26	0.49
1:A:76:CYS:H	11:A:614:HOH:H2	1.60	0.48
1:A:258:GLN:H	4:A:427:EDO:C1	2.27	0.47
4:A:422:EDO:C1	11:A:517:HOH:O	2.63	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:296:GLU:HB2	6:A:443:DXE:C4	2.46	0.45
1:A:8:PRO:CB	6:A:443:DXE:C4	2.95	0.45
1:A:96[A]:VAL:CG2	1:A:106[A]:ILE:CD1	2.94	0.45
1:A:65:GLU:HG3	8:A:462:PEG:C4	2.48	0.44
1:A:41:ASN:CB	1:A:41:ASN:O	2.66	0.43
1:A:53:LEU:HD22	1:A:53:LEU:HA	1.79	0.43
1:A:302[B]:LYS:NZ	11:A:655:HOH:O	2.51	0.43
3:A:412:MES:O2S	11:A:1129:HOH:O	2.19	0.43
1:A:194:GLU:OE1	7:A:452:MXE:C3	2.68	0.42
1:A:163[B]:GLN:CD	11:A:978:HOH:O	2.54	0.42
4:A:426:EDO:C1	5:A:433:PGE:O4	2.68	0.42
1:A:171[B]:PHE:CE2	7:A:452:MXE:C2	3.03	0.42
1:A:119:CYS:HA	1:A:134:ALA:HA	2.01	0.41
1:A:212[A]:GLU:OE2	11:A:997:HOH:O	2.20	0.41
1:A:41:ASN:HD21	1:A:41:ASN:CA	2.33	0.41
1:A:151[B]:LYS:NZ	1:A:172:GLN:OE1	2.55	0.40

All (4) 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	Distance(Å)	Clash(Å)
1:A:213[B]:ASN:OD1	11:A:1011:HOH:O[2_554]	1.00	1.20
1:A:50[A]:ARG:NH1	11:A:1114:HOH:O[2_555]	1.82	0.38
1:A:186[A]:ARG:NH1	11:A:968:HOH:O[1_655]	1.85	0.35
1:A:294[B]:LYS:NZ	11:A:978:HOH:O[3_645]	2.08	0.12

## 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	360/314 (115%)	343 (95%)	13 (4%)	4 (1%)	21 2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3[A]	ILE
1	A	3[B]	ILE
1	A	313[A]	ILE
1	A	313[B]	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	307/263 (117%)	302 (98%)	5 (2%)	75	35

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	206[A]	LYS
1	A	206[B]	LYS
1	A	313[A]	ILE
1	A	313[B]	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	41	ASN
1	A	83	ASN
1	A	189	GLN
1	A	258	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	4.03	3 (60%)	5,5,5	2.52	2 (40%)
2	GOL	A	403	-	5,5,5	3.70	4 (80%)	5,5,5	1.16	1 (20%)
3	MES	A	411	-	12,12,12	2.27	4 (33%)	16,16,16	3.21	10 (62%)
3	MES	A	412	-	12,12,12	1.75	2 (16%)	16,16,16	3.01	7 (43%)
4	EDO	A	421	-	3,3,3	0.64	0	2,2,2	0.59	0
4	EDO	A	422	-	3,3,3	0.66	0	2,2,2	2.53	2 (100%)
4	EDO	A	423	-	3,3,3	0.94	0	2,2,2	1.91	1 (50%)
4	EDO	A	424	-	3,3,3	1.00	0	2,2,2	0.04	0
4	EDO	A	425	-	3,3,3	0.82	0	2,2,2	0.76	0
4	EDO	A	426	-	3,3,3	1.24	0	2,2,2	0.59	0
4	EDO	A	427	-	3,3,3	0.58	0	2,2,2	2.00	1 (50%)
4	EDO	A	428	-	3,3,3	0.98	0	2,2,2	0.40	0
5	PGE	A	433	-	9,9,9	0.97	0	8,8,8	1.64	2 (25%)
5	PGE	A	434	-	9,9,9	1.07	0	8,8,8	2.03	4 (50%)
6	DXE	A	442	-	5,5,5	0.53	0	4,4,4	2.59	3 (75%)
6	DXE	A	443	-	5,5,5	0.66	0	4,4,4	1.54	1 (25%)
7	MXE	A	451	-	4,4,4	0.86	0	3,3,3	4.46	3 (100%)
7	MXE	A	452	-	4,4,4	0.41	0	3,3,3	3.10	2 (66%)
8	PEG	A	461	-	6,6,6	0.69	0	5,5,5	3.03	3 (60%)
8	PEG	A	462	-	6,6,6	1.16	0	5,5,5	1.89	1 (20%)
9	ME2	A	471	-	9,9,9	0.96	0	8,8,8	0.96	1 (12%)

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	403	-	-	0/4/4/4	0/0/0/0
3	MES	A	411	-	-	0/6/14/14	0/1/1/1
3	MES	A	412	-	-	0/6/14/14	1/1/1/1
4	EDO	A	421	-	-	0/1/1/1	0/0/0/0
4	EDO	A	422	-	-	0/1/1/1	0/0/0/0
4	EDO	A	423	-	-	0/1/1/1	0/0/0/0
4	EDO	A	424	-	-	0/1/1/1	0/0/0/0
4	EDO	A	425	-	-	0/1/1/1	0/0/0/0
4	EDO	A	426	-	-	0/1/1/1	0/0/0/0
4	EDO	A	427	-	-	0/1/1/1	0/0/0/0
4	EDO	A	428	-	-	0/1/1/1	0/0/0/0
5	PGE	A	433	-	-	0/7/7/7	0/0/0/0
5	PGE	A	434	-	-	0/7/7/7	0/0/0/0
6	DXE	A	442	-	-	0/3/3/3	0/0/0/0
6	DXE	A	443	-	-	0/3/3/3	0/0/0/0
7	MXE	A	451	-	-	0/2/2/2	0/0/0/0
7	MXE	A	452	-	-	0/2/2/2	0/0/0/0
8	PEG	A	461	-	-	0/4/4/4	0/0/0/0
8	PEG	A	462	-	-	0/4/4/4	0/0/0/0
9	ME2	A	471	-	-	0/7/7/7	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GOL	C3-C2	-7.59	1.21	1.52
2	A	403	GOL	C3-C2	-6.57	1.25	1.52
3	A	411	MES	O2S-S	5.27	1.57	1.45
3	A	412	MES	O1S-S	-4.40	1.35	1.45
3	A	411	MES	O3S-S	-3.70	1.37	1.45
2	A	403	GOL	O3-C3	3.49	1.57	1.42
2	A	401	GOL	O1-C1	3.17	1.56	1.42
3	A	412	MES	C5-N4	2.92	1.56	1.49
2	A	401	GOL	O3-C3	2.84	1.54	1.42
2	A	403	GOL	O1-C1	2.81	1.54	1.42
3	A	411	MES	C8-S	2.75	1.83	1.78
2	A	403	GOL	C1-C2	-2.16	1.43	1.52
3	A	411	MES	O1S-S	2.02	1.50	1.45

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	411	MES	O3S-S-O1S	7.51	131.79	112.48
3	A	412	MES	C2-C3-N4	-6.45	101.69	109.96
7	A	451	MXE	C3-O2-C2	5.77	154.61	113.24
3	A	412	MES	C8-C7-N4	-5.47	103.08	112.44
8	A	461	PEG	O2-C2-C1	4.94	134.38	110.61
3	A	411	MES	C2-C3-N4	-4.59	104.07	109.96
3	A	411	MES	O3S-S-C8	-4.26	95.00	105.99
7	A	452	MXE	C3-O2-C2	4.20	143.40	113.24
3	A	412	MES	C7-N4-C5	-4.12	100.89	111.66
7	A	451	MXE	O1-C1-C2	3.97	137.56	111.80
2	A	401	GOL	O2-C2-C3	3.96	126.25	108.22
8	A	462	PEG	O2-C3-C4	3.81	128.91	110.61
3	A	412	MES	C5-N4-C3	-3.50	102.81	109.75
5	A	434	PGE	O2-C2-C1	3.46	127.27	110.61
5	A	433	PGE	C5-O3-C4	3.41	128.39	113.38
6	A	442	DXE	O1-C2-C3	3.33	139.62	111.19
3	A	412	MES	O1-C6-C5	-3.32	107.39	111.34
3	A	411	MES	O1S-S-C8	-3.29	96.23	106.36
7	A	451	MXE	O2-C2-C1	3.28	139.14	111.20
2	A	401	GOL	O3-C3-C2	3.18	125.22	109.71
6	A	442	DXE	C1-O1-C2	3.13	135.73	113.24
8	A	461	PEG	C3-O2-C2	3.11	127.06	113.38
7	A	452	MXE	O1-C1-C2	3.11	131.94	111.80
3	A	411	MES	C6-C5-N4	3.10	113.93	109.96
3	A	411	MES	C7-N4-C5	-3.10	103.56	111.66
3	A	412	MES	O1-C2-C3	3.05	114.97	111.34
3	A	411	MES	O2S-S-O1S	2.90	118.03	112.44
3	A	411	MES	C7-N4-C3	-2.88	104.12	111.66
4	A	422	EDO	O1-C1-C2	2.75	131.34	112.13
8	A	461	PEG	O2-C3-C4	2.66	123.42	110.61
3	A	411	MES	O3S-S-O2S	-2.66	105.65	112.48
5	A	434	PGE	O3-C4-C3	2.54	122.01	110.47
3	A	411	MES	C8-C7-N4	-2.50	108.16	112.44
4	A	423	EDO	O1-C1-C2	2.41	129.01	112.13
6	A	442	DXE	O2-C3-C2	2.41	131.75	111.19
6	A	443	DXE	O1-C2-C3	2.37	131.42	111.19
4	A	427	EDO	O1-C1-C2	2.37	128.68	112.13
4	A	422	EDO	O2-C2-C1	2.29	128.17	112.13
2	A	403	GOL	O2-C2-C3	2.26	118.50	108.22
3	A	412	MES	C7-C8-S	-2.15	106.64	112.49
9	A	471	ME2	O1-C2-C3	2.14	129.49	111.19
5	A	434	PGE	O2-C3-C4	2.13	120.14	110.47
5	A	434	PGE	O1-C1-C2	2.09	125.35	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	433	PGE	O2-C2-C1	2.00	120.24	110.61

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	412	MES	C2-C3-C5-C6-N4-O1

## 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	314/314 (100%)	-0.71	4 (1%) 74 69	4, 8, 18, 41	21 (6%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1[A]	MET	6.7
1	A	2[A]	GLU	5.2
1	A	55	THR	3.0
1	A	40	VAL	2.1

### 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	DXE	A	442	6/6	0.23	23.52	15,30,31,34	6

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	DXE	A	443	6/6	0.26	23.19	22,40,44,49	5
8	PEG	A	462	7/7	0.31	19.41	37,40,48,52	7
4	EDO	A	428	4/4	0.22	11.17	55,65,74,77	0
4	EDO	A	422	4/4	0.11	10.99	8,11,16,23	4
8	PEG	A	461	7/7	0.19	7.21	24,37,52,52	7
9	ME2	A	471	10/10	0.20	7.12	22,33,40,41	10
3	MES	A	412	12/12	0.20	7.12	16,33,43,44	12
5	PGE	A	433	10/10	0.16	6.80	16,25,30,30	10
7	MXE	A	452	5/5	0.12	6.32	13,16,22,27	5
3	MES	A	411	12/12	0.17	6.26	10,24,31,32	12
7	MXE	A	451	5/5	0.14	6.08	13,15,24,24	5
4	EDO	A	421	4/4	0.13	5.00	24,26,32,34	4
5	PGE	A	434	10/10	0.14	4.60	12,22,34,35	10
2	GOL	A	403	6/6	0.13	4.51	10,13,16,19	6
4	EDO	A	423	4/4	0.15	4.21	18,30,30,43	4
4	EDO	A	427	4/4	0.15	3.47	22,27,32,36	4
4	EDO	A	426	4/4	0.13	3.47	22,22,29,54	4
4	EDO	A	424	4/4	0.08	0.89	14,16,22,24	0
2	GOL	A	401	6/6	0.05	0.19	12,18,22,24	0
4	EDO	A	425	4/4	0.10	0.16	22,24,29,39	4
10	CA	A	491	1/1	0.03	-0.92	4,4,4,4	0
10	CA	A	492	1/1	0.02	-1.65	4,4,4,4	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.