



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:33 PM GMT

PDB ID : 1PJX  
Title : 0.85 ANGSTROM STRUCTURE OF SQUID GANGLION DFPASE  
Authors : Koepke, J.; Rueterjans, H.; Luecke, C.; Fritzsche, G.  
Deposited on : 2003-06-04  
Resolution : 0.85 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

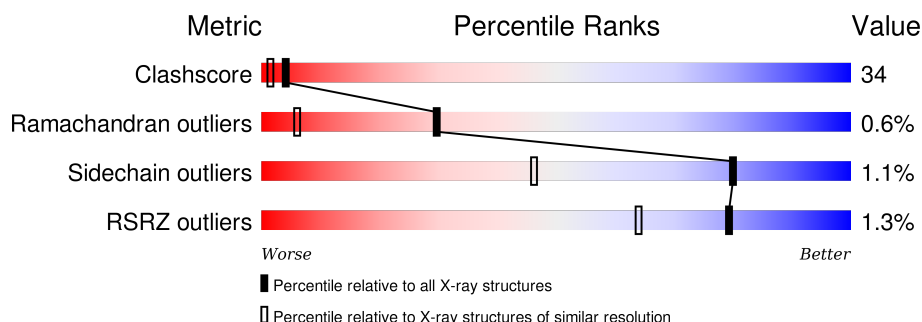
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
Clashscore	102246	1090 (1.08-0.64)
Ramachandran outliers	100387	1016 (1.08-0.64)
Sidechain outliers	100360	1018 (1.08-0.64)
RSRZ outliers	91569	1009 (1.08-0.64)

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	314	

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
10	PEG	A	461	-	-	X	X
10	PEG	A	462	-	-	-	X
3	ME2	A	471	-	-	X	X
4	MES	A	411	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MES	A	412	-	-	X	X
5	EDO	A	422	-	-	-	X
5	EDO	A	423	-	-	X	X
5	EDO	A	424	-	-	-	X
5	EDO	A	425	-	-	X	-
5	EDO	A	426	-	-	-	X
5	EDO	A	427	-	-	X	-
5	EDO	A	428	-	-	X	-
6	PGE	A	433	-	-	X	X
6	PGE	A	434	-	-	X	X
7	DXE	A	441	-	-	X	X
7	DXE	A	443	-	-	X	X
8	MXE	A	451	-	-	X	X
8	MXE	A	452	-	-	X	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 3295 atoms, of which 0 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.

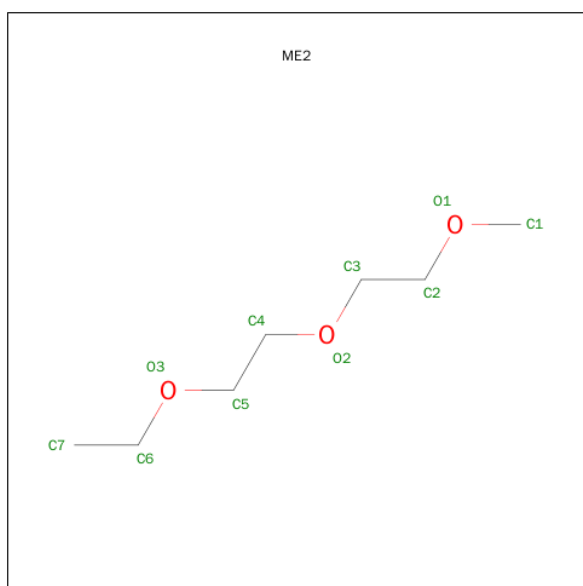
- Molecule 1 is a protein called DIISOPROPYLFLUOROPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	46	0
			2657	1688	456	495	18			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

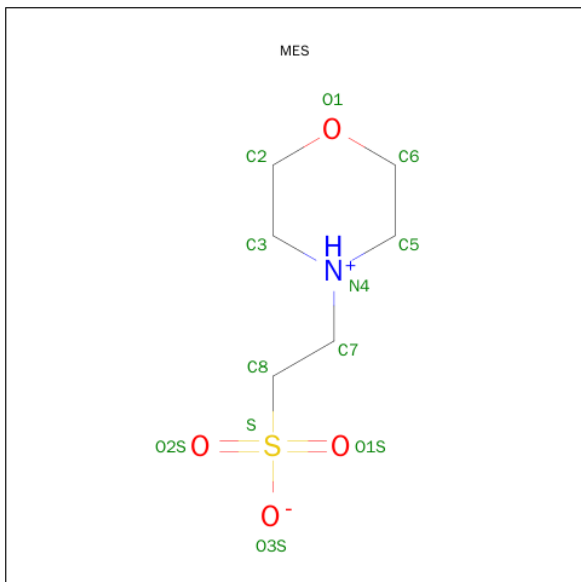
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 1-ETHOXY-2-(2-METHOXYETHOXY)ETHANE (three-letter code: ME2) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



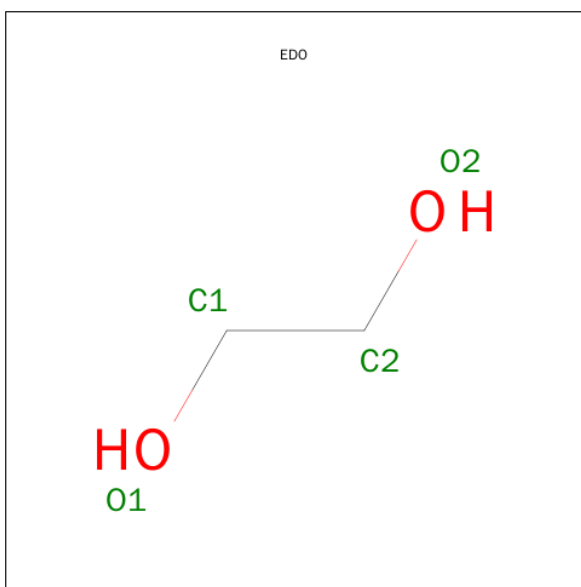
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	7	3		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



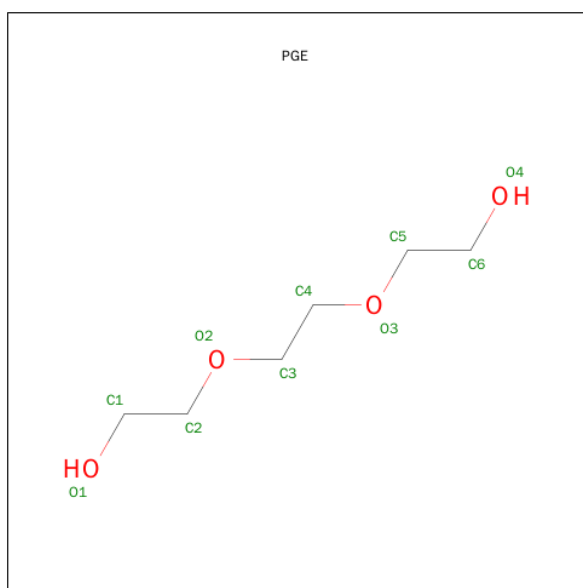
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



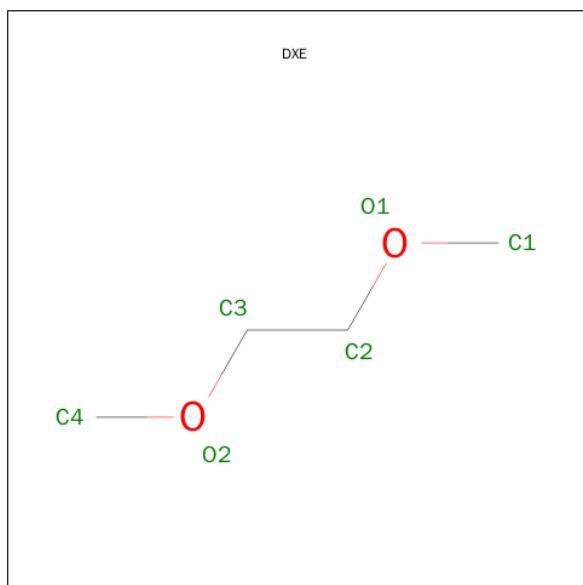
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



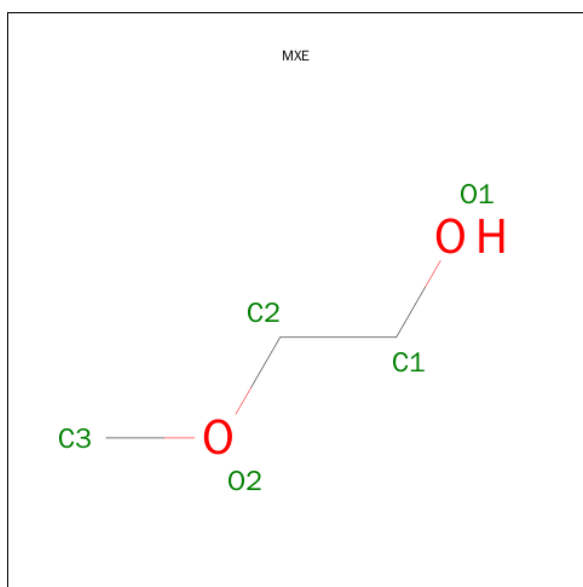
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0

- Molecule 7 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula:  $C_4H_{10}O_2$ ).



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

- Molecule 8 is 2-METHOXYETHANOL (three-letter code: MXE) (formula:  $C_3H_8O_2$ ).



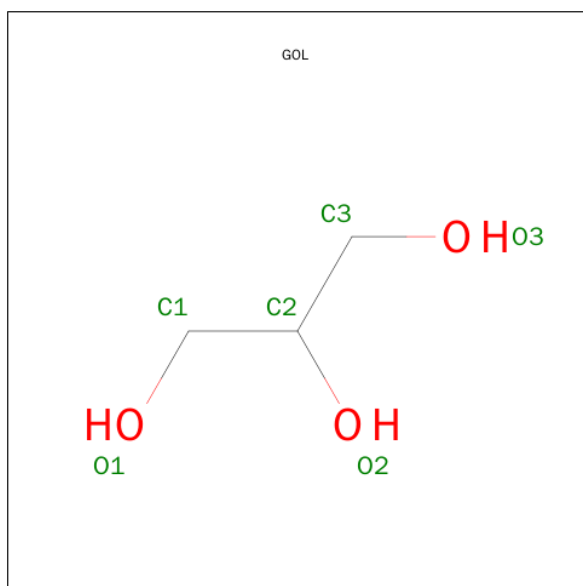
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			5	3	2		

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

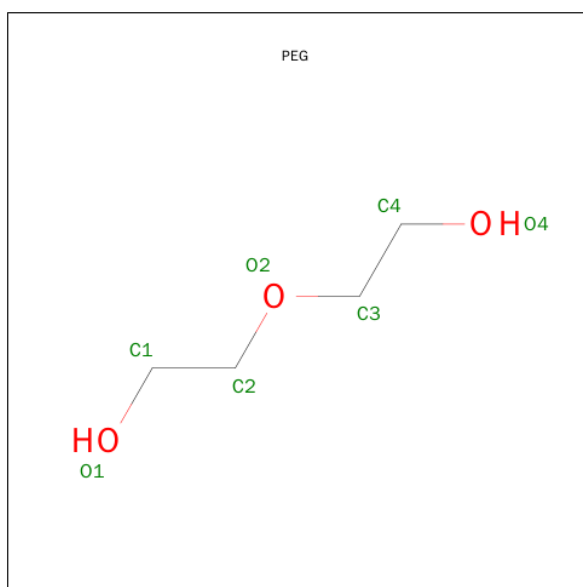
- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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





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

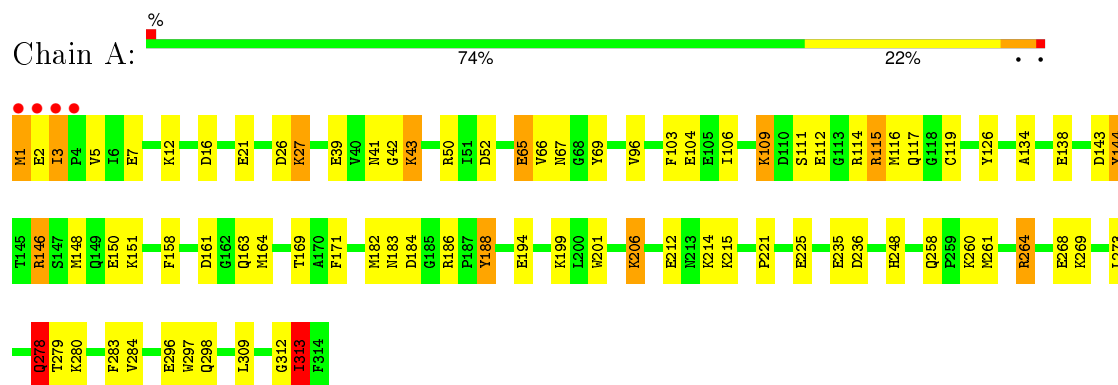
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	479	Total	O	0	17
			496	496		

### 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 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 ( $\text{RSRZ} > 2$ ). 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: DIISOPROPYLFLUOROPHOSPHATASE



## 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)	10.00 – 0.85 10.00 – 0.85	Depositor EDS
% Data completeness (in resolution range)	90.8 (10.00-0.85) 87.0 (10.00-0.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 0.85Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.111 , 0.128 0.161 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	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> )	0.36 , 91.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 242977 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	1.53	33/2949 (1.1%)	1.67	55/3975 (1.4%)

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	2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	ARG	NE-CZ	-23.31	1.02	1.33
1	A	278	GLN	CD-OE1	21.50	1.71	1.24
1	A	39	GLU	CD-OE1	20.33	1.48	1.25
1	A	150	GLU	CD-OE2	15.97	1.43	1.25
1	A	112	GLU	CD-OE2	-15.57	1.08	1.25
1	A	264	ARG	CZ-NH2	14.11	1.51	1.33
1	A	109	LYS	CD-CE	12.91	1.83	1.51
1	A	109	LYS	CE-NZ	12.57	1.80	1.49
1	A	27	LYS	CE-NZ	-11.46	1.20	1.49
1	A	150	GLU	CG-CD	-10.68	1.35	1.51
1	A	298	GLN	CD-OE1	-10.18	1.01	1.24
1	A	65	GLU	CD-OE2	10.08	1.36	1.25
1	A	183	ASN	CG-ND2	9.07	1.55	1.32
1	A	264	ARG	CD-NE	8.73	1.61	1.46
1	A	112	GLU	CB-CG	7.18	1.65	1.52
1	A	42	GLY	C-O	-7.12	1.12	1.23
1	A	104	GLU	CD-OE1	6.78	1.33	1.25
1	A	39	GLU	CD-OE2	-6.61	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	GLU	CG-CD	6.59	1.61	1.51
1	A	278	GLN	CG-CD	-6.56	1.35	1.51
1	A	104	GLU	CG-CD	-6.50	1.42	1.51
1	A	183	ASN	CG-OD1	-6.44	1.09	1.24
1	A	199	LYS	CE-NZ	-6.08	1.33	1.49
1	A	52	ASP	CG-OD1	-5.89	1.11	1.25
1	A	183	ASN	CB-CG	5.58	1.63	1.51
1	A	112	GLU	CA-CB	5.57	1.66	1.53
1	A	111	SER	CA-CB	5.44	1.61	1.52
1	A	41	ASN	C-N	5.40	1.42	1.33
1	A	67	ASN	CG-ND2	5.39	1.46	1.32
1	A	16	ASP	CG-OD2	5.27	1.37	1.25
1	A	161	ASP	CB-CG	-5.10	1.41	1.51
1	A	43	LYS	CG-CD	-5.00	1.35	1.52
1	A	39	GLU	CG-CD	-5.00	1.44	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ARG	NE-CZ-NH1	25.43	133.02	120.30
1	A	43	LYS	CG-CD-CE	19.11	169.22	111.90
1	A	186[A]	ARG	NE-CZ-NH2	17.94	129.27	120.30
1	A	186[B]	ARG	NE-CZ-NH2	17.94	129.27	120.30
1	A	115[A]	ARG	CD-NE-CZ	16.26	146.36	123.60
1	A	115[B]	ARG	CD-NE-CZ	16.26	146.36	123.60
1	A	186[A]	ARG	CD-NE-CZ	15.45	145.23	123.60
1	A	186[B]	ARG	CD-NE-CZ	15.45	145.23	123.60
1	A	115[A]	ARG	NE-CZ-NH2	15.15	127.88	120.30
1	A	115[B]	ARG	NE-CZ-NH2	15.15	127.88	120.30
1	A	43	LYS	CD-CE-NZ	14.61	145.29	111.70
1	A	264	ARG	NH1-CZ-NH2	-10.47	107.88	119.40
1	A	112	GLU	CG-CD-OE1	-10.47	97.36	118.30
1	A	114[A]	ARG	CD-NE-CZ	9.77	137.28	123.60
1	A	114[B]	ARG	CD-NE-CZ	9.77	137.28	123.60
1	A	1[A]	MET	C-N-CA	8.59	143.19	121.70
1	A	1[B]	MET	C-N-CA	8.59	143.19	121.70
1	A	143[A]	ASP	CB-CG-OD1	-8.43	110.72	118.30
1	A	143[B]	ASP	CB-CG-OD1	-8.43	110.72	118.30
1	A	186[A]	ARG	NE-CZ-NH1	-8.41	116.09	120.30
1	A	186[B]	ARG	NE-CZ-NH1	-8.41	116.09	120.30
1	A	236	ASP	CB-CG-OD2	-7.96	111.13	118.30
1	A	169[A]	THR	CA-CB-CG2	-7.86	101.40	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169[B]	THR	CA-CB-CG2	-7.86	101.40	112.40
1	A	150	GLU	OE1-CD-OE2	-7.83	113.90	123.30
1	A	112	GLU	OE1-CD-OE2	7.76	132.61	123.30
1	A	182	MET	CG-SD-CE	-7.60	88.03	100.20
1	A	146[A]	ARG	CB-CA-C	-7.53	95.33	110.40
1	A	146[B]	ARG	CB-CA-C	-7.53	95.33	110.40
1	A	150	GLU	CG-CD-OE1	6.70	131.69	118.30
1	A	235	GLU	OE1-CD-OE2	6.46	131.06	123.30
1	A	126	TYR	CB-CG-CD2	6.46	124.87	121.00
1	A	184	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	115[A]	ARG	NH1-CZ-NH2	-6.39	112.37	119.40
1	A	115[B]	ARG	NH1-CZ-NH2	-6.39	112.37	119.40
1	A	114[A]	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	114[B]	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	188	TYR	CB-CG-CD1	-6.13	117.33	121.00
1	A	52	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	309	LEU	CB-CG-CD2	5.79	120.84	111.00
1	A	27	LYS	CD-CE-NZ	5.74	124.91	111.70
1	A	188	TYR	CD1-CG-CD2	5.70	124.17	117.90
1	A	114[A]	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	114[B]	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	184	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	111	SER	O-C-N	-5.36	114.12	122.70
1	A	26	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	225	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	A	284[A]	VAL	CG1-CB-CG2	-5.07	102.80	110.90
1	A	284[B]	VAL	CG1-CB-CG2	-5.07	102.80	110.90
1	A	188	TYR	CG-CD2-CE2	-5.06	117.25	121.30
1	A	143[A]	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	143[B]	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	12	LYS	CB-CG-CD	5.06	124.75	111.60
1	A	144	TYR	CB-CG-CD1	-5.02	117.99	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	TYR	Sidechain
1	A	278	GLN	Sidechain

## 5.2 Too-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 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	2657	0	2566	139	0
2	A	2	0	0	0	0
3	A	10	0	16	11	0
4	A	24	0	26	17	0
5	A	32	0	48	33	0
6	A	20	0	28	16	0
7	A	18	0	30	28	0
8	A	10	0	16	37	0
9	A	12	0	9	0	0
10	A	14	0	20	7	0
11	A	496	0	0	57	0
All	All	3295	0	2759	191	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 34.

All (191) 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:A:109:LYS:CD	1:A:109:LYS:CE	1.83	1.57
1:A:109:LYS:NZ	1:A:109:LYS:CE	1.80	1.41
1:A:43:LYS:NZ	4:A:411:MES:H31	1.34	1.37
1:A:278:GLN:OE1	1:A:278:GLN:CD	1.71	1.28
1:A:264:ARG:HG2	11:A:1047:HOH:O	1.19	1.26
1:A:50[C]:ARG:CZ	11:A:1039:HOH:O	1.80	1.25
1:A:146[B]:ARG:NH2	11:A:948:HOH:O	1.70	1.23
8:A:452:MXE:H11	11:A:694:HOH:O	1.06	1.23
1:A:264:ARG:CG	11:A:1047:HOH:O	1.77	1.21
1:A:2[B]:GLU:CA	11:A:861:HOH:O	1.90	1.19
1:A:214[B]:LYS:CE	11:A:694:HOH:O	1.87	1.18
1:A:115[B]:ARG:HD3	5:A:423:EDO:O2	1.39	1.17
1:A:96[A]:VAL:HG23	1:A:106[A]:ILE:HD11	1.16	1.16
1:A:296:GLU:HB2	7:A:443:DXE:H42	1.27	1.13
7:A:441:DXE:C4	8:A:451:MXE:H31	1.81	1.11
1:A:50[A]:ARG:NH1	11:A:1114:HOH:O	1.81	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151[A]:LYS:HZ3	8:A:452:MXE:H31	1.13	1.10
1:A:2[B]:GLU:CA	1:A:3[B]:ILE:HB	1.82	1.09
1:A:260[B]:LYS:NZ	5:A:427:EDO:H22	1.64	1.09
8:A:452:MXE:C1	11:A:694:HOH:O	1.68	1.08
1:A:215[C]:LYS:HE2	11:A:1046:HOH:O	0.90	1.08
7:A:441:DXE:H41	8:A:451:MXE:H31	1.33	1.05
1:A:151[B]:LYS:HE3	8:A:452:MXE:H32	1.36	1.05
1:A:312[B]:GLY:C	1:A:313[B]:ILE:HG13	1.74	1.03
1:A:280[B]:LYS:HE2	6:A:434:PGE:O3	1.60	1.01
1:A:264:ARG:HH11	3:A:471:ME2:H51	1.21	1.01
1:A:296:GLU:O	7:A:443:DXE:H41	1.58	1.00
1:A:214[B]:LYS:HE2	11:A:694:HOH:O	1.50	0.98
1:A:296:GLU:O	7:A:443:DXE:C4	2.09	0.98
1:A:43:LYS:HZ3	4:A:411:MES:H31	1.18	0.98
1:A:50[A]:ARG:NH2	11:A:1040:HOH:O	1.94	0.97
1:A:43:LYS:NZ	4:A:411:MES:C3	2.27	0.96
5:A:425:EDO:H21	11:A:876:HOH:O	1.63	0.96
1:A:50[C]:ARG:NH2	11:A:1039:HOH:O	1.84	0.96
1:A:264:ARG:CD	11:A:1047:HOH:O	2.02	0.95
1:A:312[B]:GLY:O	1:A:313[B]:ILE:HG13	1.64	0.95
1:A:96[A]:VAL:CG2	1:A:106[A]:ILE:HD11	1.98	0.94
1:A:50[A]:ARG:CZ	11:A:1040:HOH:O	2.19	0.90
1:A:43:LYS:HZ2	4:A:411:MES:H31	1.08	0.89
1:A:151[B]:LYS:HE3	8:A:452:MXE:C3	2.02	0.88
1:A:151[A]:LYS:NZ	8:A:452:MXE:H31	1.86	0.88
1:A:115[B]:ARG:CD	5:A:423:EDO:O2	2.22	0.88
3:A:471:ME2:H62	3:A:471:ME2:O2	1.74	0.86
1:A:65:GLU:O	4:A:412:MES:H61	1.76	0.85
1:A:214[B]:LYS:NZ	11:A:694:HOH:O	2.03	0.84
1:A:116[A]:MET:HE3	1:A:164:MET:HG2	1.59	0.84
1:A:260[B]:LYS:HZ2	5:A:427:EDO:H22	1.43	0.84
1:A:215[C]:LYS:CE	11:A:1046:HOH:O	1.65	0.83
1:A:296:GLU:CB	7:A:443:DXE:H42	2.07	0.82
1:A:43:LYS:HZ2	4:A:411:MES:C3	1.88	0.82
5:A:428:EDO:C1	11:A:1082:HOH:O	2.28	0.82
1:A:214[A]:LYS:HE3	11:A:670:HOH:O	1.77	0.82
1:A:171[B]:PHE:CD2	8:A:452:MXE:H21	2.15	0.81
1:A:312[B]:GLY:O	1:A:313[B]:ILE:CG1	2.29	0.80
1:A:264:ARG:NH1	3:A:471:ME2:H51	1.96	0.80
7:A:443:DXE:H43	11:A:770:HOH:O	1.80	0.79
6:A:434:PGE:C6	11:A:544:HOH:O	2.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:423:EDO:O1	11:A:959:HOH:O	1.53	0.78
1:A:116[A]:MET:CE	1:A:164:MET:HG2	2.13	0.78
1:A:151[B]:LYS:CE	8:A:452:MXE:C3	2.62	0.78
1:A:109:LYS:CG	1:A:109:LYS:CE	2.61	0.77
1:A:106[B]:ILE:HD12	10:A:461:PEG:C4	2.15	0.77
1:A:312[B]:GLY:C	1:A:313[B]:ILE:CG1	2.52	0.77
1:A:103:PHE:CZ	4:A:412:MES:H52	2.20	0.77
7:A:441:DXE:C1	8:A:452:MXE:H31	2.15	0.77
1:A:260[B]:LYS:HZ3	5:A:427:EDO:H22	1.46	0.77
7:A:441:DXE:H41	8:A:451:MXE:C3	2.12	0.77
5:A:428:EDO:H12	11:A:1082:HOH:O	1.84	0.76
1:A:43:LYS:HZ3	4:A:411:MES:C3	1.94	0.76
1:A:163[B]:GLN:NE2	11:A:978:HOH:O	2.19	0.75
1:A:268[A]:GLU:OE1	11:A:1014:HOH:O	2.04	0.74
5:A:424:EDO:H11	6:A:433:PGE:H42	1.70	0.74
1:A:151[B]:LYS:HE2	8:A:452:MXE:H31	1.69	0.74
7:A:441:DXE:H11	8:A:452:MXE:H31	1.72	0.72
6:A:434:PGE:H62	11:A:544:HOH:O	1.89	0.72
1:A:50[A]:ARG:NE	11:A:1040:HOH:O	2.22	0.72
1:A:151[A]:LYS:HZ3	7:A:441:DXE:H11	1.54	0.72
8:A:452:MXE:O1	11:A:670:HOH:O	2.07	0.71
1:A:103:PHE:CE1	4:A:412:MES:H52	2.24	0.71
8:A:452:MXE:H33	11:A:531:HOH:O	1.89	0.71
1:A:260[A]:LYS:HE3	11:A:942:HOH:O	1.88	0.71
5:A:428:EDO:H11	11:A:1082:HOH:O	1.90	0.70
7:A:441:DXE:O1	8:A:452:MXE:C3	2.40	0.69
5:A:421:EDO:H22	11:A:859:HOH:O	1.90	0.69
1:A:221:PRO:HA	5:A:425:EDO:H11	1.74	0.69
6:A:433:PGE:H5	11:A:644:HOH:O	1.92	0.68
1:A:260[B]:LYS:CE	5:A:427:EDO:H22	2.24	0.68
1:A:151[B]:LYS:CE	8:A:452:MXE:H32	2.19	0.67
1:A:171[B]:PHE:CD2	8:A:452:MXE:C2	2.78	0.67
1:A:151[B]:LYS:CE	8:A:452:MXE:H31	2.23	0.67
1:A:65:GLU:HG3	10:A:462:PEG:H42	1.76	0.66
1:A:214[A]:LYS:NZ	8:A:452:MXE:H11	2.09	0.66
1:A:258:GLN:NE2	5:A:425:EDO:O1	2.27	0.66
1:A:248:HIS:NE2	3:A:471:ME2:H52	2.10	0.66
1:A:151[A]:LYS:HZ3	8:A:452:MXE:C3	2.01	0.66
1:A:260[B]:LYS:NZ	5:A:427:EDO:C2	2.53	0.66
1:A:115[B]:ARG:HD2	1:A:138[B]:GLU:OE2	1.95	0.66
1:A:106[B]:ILE:CD1	10:A:461:PEG:C4	2.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLN:H	5:A:427:EDO:H11	1.61	0.65
5:A:426:EDO:H11	6:A:433:PGE:O4	1.97	0.64
7:A:441:DXE:C1	8:A:452:MXE:C3	2.76	0.64
5:A:424:EDO:H11	6:A:433:PGE:C4	2.29	0.63
1:A:69:TYR:CD1	4:A:411:MES:H81	2.33	0.62
6:A:434:PGE:H42	11:A:735:HOH:O	1.98	0.62
1:A:260[B]:LYS:HZ2	5:A:427:EDO:C2	2.11	0.62
1:A:215[C]:LYS:NZ	11:A:1046:HOH:O	2.10	0.61
7:A:441:DXE:H11	8:A:452:MXE:C3	2.31	0.60
1:A:151[A]:LYS:HZ3	7:A:441:DXE:C1	2.14	0.59
7:A:441:DXE:H43	8:A:451:MXE:H31	1.82	0.59
1:A:279:THR:HB	6:A:434:PGE:H2	1.84	0.58
5:A:422:EDO:H21	11:A:517:HOH:O	2.03	0.58
1:A:66:VAL:HG22	4:A:412:MES:H22	1.84	0.58
1:A:264:ARG:NH1	11:A:1047:HOH:O	2.37	0.57
1:A:115[B]:ARG:HD3	5:A:423:EDO:C2	2.33	0.57
8:A:451:MXE:H33	11:A:859:HOH:O	2.05	0.57
1:A:106[B]:ILE:CD1	10:A:461:PEG:H41	2.36	0.56
5:A:428:EDO:O2	11:A:1126:HOH:O	1.86	0.56
4:A:412:MES:O2S	11:A:1129:HOH:O	2.17	0.56
5:A:425:EDO:C2	11:A:876:HOH:O	2.37	0.56
1:A:258:GLN:N	5:A:427:EDO:H11	2.21	0.55
8:A:452:MXE:H12	11:A:694:HOH:O	1.67	0.55
1:A:264:ARG:HH11	3:A:471:ME2:C5	2.08	0.55
1:A:214[B]:LYS:HZ3	7:A:441:DXE:H41	1.72	0.54
7:A:443:DXE:H43	11:A:532:HOH:O	2.08	0.54
1:A:296:GLU:O	7:A:443:DXE:H42	2.03	0.54
1:A:214[B]:LYS:HZ3	7:A:441:DXE:C4	2.21	0.54
1:A:69:TYR:CE1	4:A:411:MES:H81	2.44	0.53
5:A:421:EDO:C2	11:A:859:HOH:O	2.53	0.53
7:A:441:DXE:C1	8:A:452:MXE:O2	2.56	0.53
1:A:214[B]:LYS:HZ1	8:A:452:MXE:C1	2.22	0.53
3:A:471:ME2:C6	3:A:471:ME2:O2	2.52	0.52
1:A:258:GLN:HE22	5:A:425:EDO:C1	2.23	0.52
1:A:7[B]:GLU:OE1	3:A:471:ME2:H21	2.09	0.52
1:A:106[B]:ILE:HD12	10:A:461:PEG:H42	1.90	0.52
1:A:248:HIS:NE2	3:A:471:ME2:C5	2.72	0.52
1:A:2[B]:GLU:N	11:A:861:HOH:O	2.28	0.51
1:A:214[A]:LYS:HZ1	8:A:452:MXE:H11	1.75	0.51
1:A:264:ARG:CZ	11:A:1047:HOH:O	2.59	0.50
1:A:148[A]:MET:HG3	6:A:433:PGE:O4	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:451:MXE:C3	11:A:859:HOH:O	2.61	0.49
7:A:441:DXE:H13	11:A:977:HOH:O	2.12	0.49
1:A:27:LYS:NZ	11:A:862[B]:HOH:O	2.45	0.49
1:A:206[B]:LYS:HE3	1:A:212[B]:GLU:OE1	2.13	0.49
1:A:151[A]:LYS:NZ	8:A:452:MXE:C3	2.68	0.48
1:A:5:VAL:O	3:A:471:ME2:H13	2.12	0.48
1:A:43:LYS:CE	4:A:411:MES:H71	2.44	0.47
1:A:296:GLU:CA	7:A:443:DXE:H42	2.45	0.47
1:A:258:GLN:H	5:A:427:EDO:C1	2.25	0.47
1:A:116[A]:MET:HE1	1:A:164:MET:HG2	1.94	0.47
1:A:116[A]:MET:HB2	1:A:116[A]:MET:HE2	1.73	0.46
5:A:422:EDO:C1	11:A:517:HOH:O	2.63	0.46
1:A:297:TRP:O	7:A:443:DXE:H13	2.16	0.46
7:A:443:DXE:H32	11:A:770:HOH:O	2.15	0.46
1:A:65:GLU:HG3	10:A:462:PEG:C4	2.45	0.45
1:A:258:GLN:O	5:A:427:EDO:H21	2.16	0.45
7:A:441:DXE:C1	11:A:977:HOH:O	2.64	0.44
1:A:269:LYS:HZ3	7:A:442:DXE:C1	2.29	0.44
1:A:50[C]:ARG:NH1	11:A:1042:HOH:O	1.87	0.44
1:A:7[B]:GLU:HG3	3:A:471:ME2:H12	1.98	0.44
1:A:106[B]:ILE:CD1	10:A:461:PEG:H42	2.45	0.44
6:A:434:PGE:H4	6:A:434:PGE:H62	1.68	0.44
1:A:144:TYR:OH	1:A:146[A]:ARG:HD3	2.18	0.44
1:A:69:TYR:CE1	4:A:411:MES:H51	2.53	0.43
1:A:296:GLU:OE2	6:A:434:PGE:H22	2.19	0.43
1:A:201:TRP:CH2	7:A:441:DXE:H21	2.54	0.43
1:A:194:GLU:OE1	8:A:452:MXE:C3	2.68	0.42
1:A:194:GLU:OE1	8:A:452:MXE:H32	2.19	0.42
1:A:158:PHE:CE2	5:A:422:EDO:H12	2.54	0.42
1:A:163[B]:GLN:CD	11:A:978:HOH:O	2.55	0.42
1:A:171[B]:PHE:CE2	8:A:452:MXE:C2	3.03	0.42
1:A:261[B]:MET:HE2	1:A:261[B]:MET:HB2	1.65	0.41
1:A:260[B]:LYS:HD3	5:A:427:EDO:C2	2.51	0.41
1:A:212[A]:GLU:HG3	11:A:997:HOH:O	2.19	0.41
3:A:471:ME2:C5	11:A:1047:HOH:O	2.68	0.41
1:A:103:PHE:O	4:A:412:MES:H72	2.21	0.41
4:A:412:MES:H51	4:A:412:MES:H81	1.27	0.40
1:A:116[A]:MET:HG3	1:A:117:GLN:N	2.36	0.40
5:A:426:EDO:C1	6:A:433:PGE:O4	2.67	0.40
1:A:119:CYS:HA	1:A:134:ALA:HA	2.03	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	360/314 (115%)	343 (95%)	13 (4%)	4 (1%)	17 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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	307/263 (117%)	302 (98%)	5 (2%)	70 31

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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	258	GLN

### 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 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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$
9	GOL	A	401	-	5,5,5	4.30	3 (60%)	5,5,5	2.45	2 (40%)
9	GOL	A	403	1	5,5,5	3.89	4 (80%)	5,5,5	1.11	1 (20%)
4	MES	A	411	-	11,12,12	2.11	4 (36%)	14,16,16	4.87	8 (57%)
4	MES	A	412	-	11,12,12	1.83	4 (36%)	14,16,16	2.71	6 (42%)
5	EDO	A	421	-	3,3,3	0.55	0	2,2,2	0.53	0
5	EDO	A	422	-	3,3,3	0.63	0	2,2,2	2.26	2 (100%)
5	EDO	A	423	-	3,3,3	0.91	0	2,2,2	1.72	1 (50%)
5	EDO	A	424	-	3,3,3	0.93	0	2,2,2	0.06	0
5	EDO	A	425	-	3,3,3	0.72	0	2,2,2	0.70	0
5	EDO	A	426	-	3,3,3	1.17	0	2,2,2	0.57	0
5	EDO	A	427	-	3,3,3	0.52	0	2,2,2	1.87	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	428	-	3,3,3	0.89	0	2,2,2	0.42	0
6	PGE	A	433	-	9,9,9	0.99	0	8,8,8	1.71	2 (25%)
6	PGE	A	434	-	9,9,9	1.07	0	8,8,8	2.11	5 (62%)
7	DXE	A	441	8	5,5,5	0.93	0	4,4,4	1.06	0
7	DXE	A	442	-	5,5,5	0.54	0	4,4,4	2.67	3 (75%)
7	DXE	A	443	-	5,5,5	0.67	0	4,4,4	1.64	1 (25%)
8	MXE	A	451	-	4,4,4	0.89	0	3,3,3	4.68	3 (100%)
8	MXE	A	452	7	4,4,4	0.44	0	3,3,3	3.32	2 (66%)
10	PEG	A	461	-	6,6,6	0.68	0	5,5,5	2.89	3 (60%)
10	PEG	A	462	-	6,6,6	1.19	0	5,5,5	2.06	2 (40%)
3	ME2	A	471	-	9,9,9	0.96	0	8,8,8	1.00	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
9	GOL	A	401	-	-	0/4/4/4	0/0/0/0
9	GOL	A	403	1	-	0/4/4/4	0/0/0/0
4	MES	A	411	-	-	0/6/14/14	0/1/1/1
4	MES	A	412	-	-	0/6/14/14	0/1/1/1
5	EDO	A	421	-	-	0/1/1/1	0/0/0/0
5	EDO	A	422	-	-	0/1/1/1	0/0/0/0
5	EDO	A	423	-	-	0/1/1/1	0/0/0/0
5	EDO	A	424	-	-	0/1/1/1	0/0/0/0
5	EDO	A	425	-	-	0/1/1/1	0/0/0/0
5	EDO	A	426	-	-	0/1/1/1	0/0/0/0
5	EDO	A	427	-	-	0/1/1/1	0/0/0/0
5	EDO	A	428	-	-	0/1/1/1	0/0/0/0
6	PGE	A	433	-	-	0/7/7/7	0/0/0/0
6	PGE	A	434	-	-	0/7/7/7	0/0/0/0
7	DXE	A	441	8	-	0/3/3/3	0/0/0/0
7	DXE	A	442	-	-	0/3/3/3	0/0/0/0
7	DXE	A	443	-	-	0/3/3/3	0/0/0/0
8	MXE	A	451	-	-	0/2/2/2	0/0/0/0
8	MXE	A	452	7	-	0/2/2/2	0/0/0/0
10	PEG	A	461	-	-	0/4/4/4	0/0/0/0
10	PEG	A	462	-	-	0/4/4/4	0/0/0/0
3	ME2	A	471	-	-	0/7/7/7	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	401	GOL	C3-C2	-8.25	1.20	1.52
9	A	403	GOL	C3-C2	-7.06	1.25	1.52
4	A	411	MES	O3S-S	-3.47	1.37	1.46
4	A	412	MES	O1S-S	-3.25	1.35	1.45
9	A	403	GOL	C1-C2	-2.28	1.43	1.52
4	A	411	MES	C3-N4	2.08	1.52	1.46
4	A	412	MES	C7-N4	2.12	1.52	1.47
4	A	412	MES	C3-N4	2.24	1.53	1.46
9	A	401	GOL	O3-C3	2.84	1.54	1.42
9	A	403	GOL	O1-C1	2.85	1.54	1.42
4	A	411	MES	C7-N4	3.01	1.54	1.47
9	A	401	GOL	O1-C1	3.20	1.56	1.42
9	A	403	GOL	O3-C3	3.48	1.57	1.42
4	A	412	MES	C5-N4	3.64	1.56	1.46
4	A	411	MES	O2S-S	4.02	1.57	1.45

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	411	MES	O1S-S-C8	-12.50	96.24	106.91
4	A	411	MES	O2S-S-C8	-7.25	100.72	106.91
4	A	412	MES	C2-C3-N4	-5.80	101.34	110.12
4	A	412	MES	C7-N4-C5	-4.29	100.27	111.27
4	A	411	MES	C2-C3-N4	-4.10	103.91	110.12
4	A	412	MES	O2S-S-C8	-3.72	103.73	106.91
4	A	411	MES	C7-N4-C5	-2.89	103.86	111.27
4	A	411	MES	C7-N4-C3	-2.87	103.92	111.27
4	A	412	MES	C5-N4-C3	-2.79	102.86	108.90
4	A	411	MES	O3S-S-O2S	-2.42	105.97	111.61
4	A	412	MES	O1-C6-C5	-2.21	106.78	111.84
10	A	462	PEG	C3-O2-C2	-2.05	104.50	113.31
6	A	434	PGE	O1-C1-C2	2.05	124.67	112.03
6	A	434	PGE	O3-C5-C6	2.10	120.09	110.43
9	A	403	GOL	O2-C2-C3	2.15	118.51	108.65
5	A	422	EDO	O2-C2-C1	2.17	128.09	112.54
5	A	423	EDO	O1-C1-C2	2.17	128.12	112.54
6	A	434	PGE	O2-C3-C4	2.21	120.19	110.36
6	A	433	PGE	O2-C2-C1	2.23	120.69	110.43
3	A	471	ME2	O1-C2-C3	2.23	130.16	111.29
5	A	427	EDO	O1-C1-C2	2.25	128.70	112.54
5	A	422	EDO	O1-C1-C2	2.35	129.36	112.54
7	A	443	DXE	O1-C2-C3	2.42	131.76	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	442	DXE	O2-C3-C2	2.48	132.24	111.29
6	A	434	PGE	O3-C4-C3	2.54	121.63	110.36
10	A	461	PEG	O2-C3-C4	2.70	122.86	110.43
4	A	411	MES	C6-C5-N4	2.70	114.22	110.12
9	A	401	GOL	O3-C3-C2	3.02	124.84	110.18
10	A	461	PEG	C3-O2-C2	3.18	126.97	113.31
4	A	412	MES	O1S-S-C8	3.22	109.65	106.91
8	A	452	MXE	O1-C1-C2	3.26	132.13	112.03
8	A	451	MXE	O2-C2-C1	3.27	138.95	111.31
7	A	442	DXE	C1-O1-C2	3.29	134.69	113.09
7	A	442	DXE	O1-C2-C3	3.36	139.72	111.29
6	A	434	PGE	O2-C2-C1	3.72	127.56	110.43
6	A	433	PGE	C5-O3-C4	3.77	129.52	113.31
9	A	401	GOL	O2-C2-C3	3.78	126.00	108.65
8	A	451	MXE	O1-C1-C2	4.05	137.04	112.03
10	A	462	PEG	O2-C3-C4	4.12	129.42	110.43
10	A	461	PEG	O2-C2-C1	4.51	131.21	110.43
8	A	452	MXE	C3-O2-C2	4.56	143.07	113.09
8	A	451	MXE	C3-O2-C2	6.22	153.96	113.09
4	A	411	MES	O3S-S-O1S	8.51	131.41	111.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 135 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	411	MES	10	0
4	A	412	MES	7	0
5	A	421	EDO	2	0
5	A	422	EDO	3	0
5	A	423	EDO	4	0
5	A	424	EDO	2	0
5	A	425	EDO	5	0
5	A	426	EDO	2	0
5	A	427	EDO	11	0
5	A	428	EDO	4	0
6	A	433	PGE	6	0
6	A	434	PGE	10	0
7	A	441	DXE	17	0
7	A	442	DXE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	443	DXE	10	0
8	A	451	MXE	8	0
8	A	452	MXE	29	0
10	A	461	PEG	5	0
10	A	462	PEG	2	0
3	A	471	ME2	11	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, 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%)	-0.18	4 (1%)	79 64	4, 8, 18, 42	21 (6%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1[A]	MET	7.2
1	A	2[A]	GLU	7.0
1	A	3[A]	ILE	3.9
1	A	4	PRO	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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
7	DXE	A	443	6/6	0.70	0.34	19.77	22,42,50,51	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	PEG	A	462	7/7	0.35	0.36	14.57	39,42,50,53	7
6	PGE	A	433	10/10	0.77	0.19	7.98	16,25,29,30	10
4	MES	A	412	12/12	0.81	0.22	4.89	16,34,44,45	12
6	PGE	A	434	10/10	0.88	0.17	4.20	12,22,34,36	10
8	MXE	A	452	5/5	0.90	0.13	4.08	13,15,22,25	5
5	EDO	A	426	4/4	0.76	0.15	3.95	23,23,29,56	4
3	ME2	A	471	10/10	0.74	0.23	3.51	23,34,40,41	10
10	PEG	A	461	7/7	0.69	0.15	3.30	24,37,50,53	7
7	DXE	A	441	6/6	0.81	0.14	3.00	14,24,26,29	6
4	MES	A	411	12/12	0.81	0.18	3.00	10,24,31,32	12
5	EDO	A	424	4/4	0.93	0.13	2.71	14,16,22,25	0
5	EDO	A	423	4/4	0.80	0.16	2.56	18,30,30,40	4
5	EDO	A	422	4/4	0.95	0.11	2.26	8,11,16,24	4
8	MXE	A	451	5/5	0.85	0.14	2.06	13,16,24,25	5
5	EDO	A	427	4/4	0.86	0.15	1.84	22,27,32,37	4
9	GOL	A	403	6/6	0.86	0.14	1.80	10,13,16,19	6
5	EDO	A	421	4/4	0.72	0.13	1.71	24,26,33,35	4
9	GOL	A	401	6/6	0.81	0.13	1.61	12,18,22,24	0
5	EDO	A	425	4/4	0.85	0.10	-0.05	22,24,29,41	4
2	CA	A	491	1/1	1.00	0.03	-2.38	4,4,4,4	0
2	CA	A	492	1/1	1.00	0.02	-2.84	4,4,4,4	0
5	EDO	A	428	4/4	0.55	0.22	-	56,67,75,78	0
7	DXE	A	442	6/6	0.68	0.20	-	15,30,31,34	6

## 6.5 Other polymers [i](#)

There are no such residues in this entry.