



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2025 – 09:32 PM EDT

PDB ID : 9C4S / pdb\_00009c4s  
Title : Menin mutant G331R in complex with MLL peptide  
Authors : Clegg, B.D.; Cierpicki, T.; Grembecka, J.  
Deposited on : 2024-06-05  
Resolution : 1.54 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

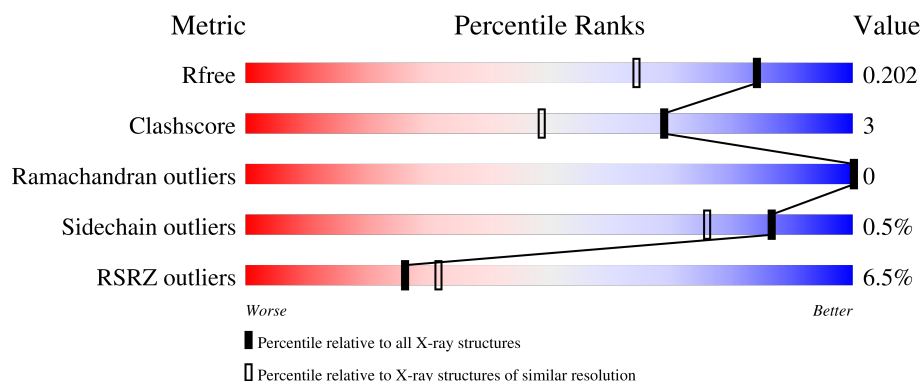
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.54 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	3511 (1.56-1.52)
Clashscore	180529	3784 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)
RSRZ outliers	164620	3510 (1.56-1.52)

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  $\geq 3$ , 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	489	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div></div> </div> </div>
2	B	14	<div> <div>57%</div> <div>43%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8144 atoms, of which 3861 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 Menin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	468	Total	C	H	N	O	S	124	20	0
			7475	2396	3729	640	693	17			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP O00255
A	-3	GLY	-	expression tag	UNP O00255
A	-2	SER	-	expression tag	UNP O00255
A	-1	SER	-	expression tag	UNP O00255
A	0	SER	-	expression tag	UNP O00255
A	?	-	ILE	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	THR	deletion	UNP O00255
A	?	-	ASN	deletion	UNP O00255
A	?	-	VAL	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	LEU	deletion	UNP O00255
A	?	-	THR	deletion	UNP O00255
A	?	-	PHE	deletion	UNP O00255
A	?	-	GLN	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	SER	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	ALA	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	ASP	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	326	ARG	GLY	engineered mutation	UNP O00255
A	?	-	GLU	deletion	UNP O00255

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP O00255
A	?	-	ARG	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	GLN	deletion	UNP O00255
A	?	-	SER	deletion	UNP O00255
A	?	-	GLN	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	?	-	THR	deletion	UNP O00255
A	?	-	GLN	deletion	UNP O00255
A	541	ALA	THR	variant	UNP O00255

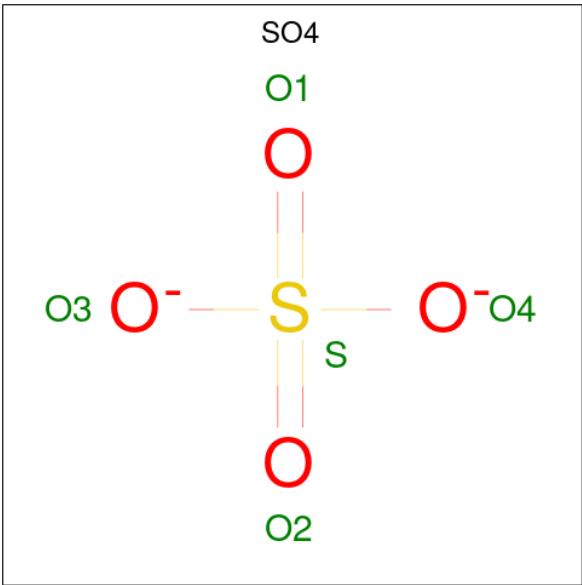
- Molecule 2 is a protein called MLL cleavage product N320.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	H	N	O	5	0	1
			203	65	100	23	15			

There are 3 discrepancies between the modelled and reference sequences:

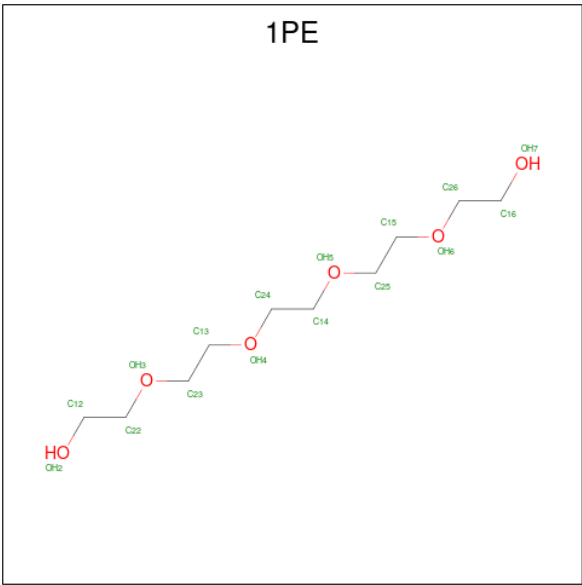
Chain	Residue	Modelled	Actual	Comment	Reference
B	3	ACE	-	acetylation	UNP Q03164
B	5	ALA	CYS	engineered mutation	UNP Q03164
B	16	NH2	-	amidation	UNP Q03164

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



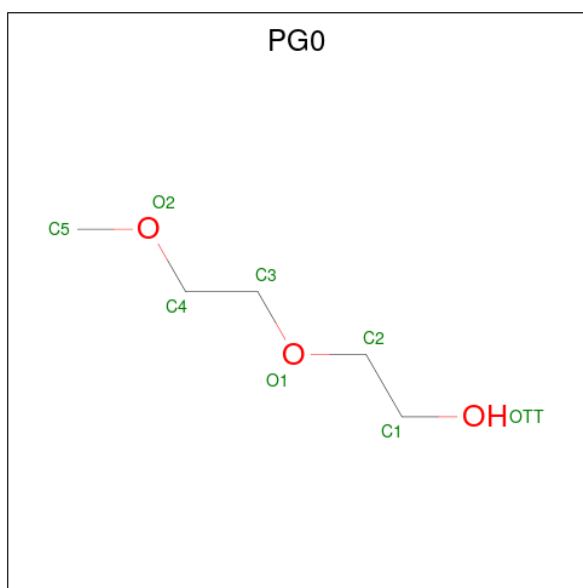
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



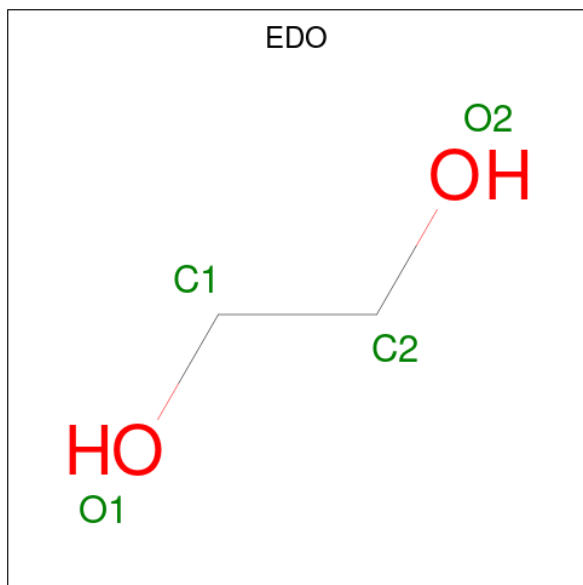
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	3	0
			26	7	15	4		

- Molecule 5 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula:  $C_5H_{12}O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	3	0
			19	5	11	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	384	Total 384	O 384	0	0
7	B	12	Total 12	O 12	0	0



- Molecule 1: Menin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.70Å 80.01Å 124.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.29 – 1.54 67.29 – 1.54	Depositor EDS
% Data completeness (in resolution range)	100.0 (67.29-1.54) 100.0 (67.29-1.54)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.172 , 0.202 0.172 , 0.202	Depositor DCC
$R_{free}$ test set	3710 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 1PE, PG0, ACE, EDO, NH2

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	0.73	0/3908	1.15	10/5305 (0.2%)
2	B	1.12	0/104	1.85	3/141 (2.1%)
All	All	0.74	0/4012	1.17	13/5446 (0.2%)

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	5
2	B	0	1
All	All	0	6

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	14	GLY	O-C-N	11.62	134.48	122.86
1	A	205	ASP	CA-CB-CG	8.22	120.82	112.60
2	B	4	SER	O-C-N	6.28	133.04	123.00
1	A	282	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	285	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	207	ARG	NE-CZ-NH2	-5.54	114.21	119.20
1	A	31	GLU	CB-CA-C	-5.19	102.23	110.02
2	B	12	ARG	CG-CD-NE	-5.18	100.60	112.00
1	A	232	ARG	CD-NE-CZ	5.12	131.56	124.40
1	A	568	THR	CA-CB-OG1	-5.11	101.94	109.60
1	A	186	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	355	ARG	N-CA-C	5.06	118.23	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	GLU	CB-CG-CD	5.00	121.10	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	PHE	Peptide
1	A	21	ARG	Sidechain
1	A	229	ARG	Sidechain
1	A	29	ARG	Sidechain
1	A	332	ARG	Sidechain
2	B	8	ARG	Sidechain

## 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	3746	3729	3604	26	0
2	B	103	100	100	3	0
3	A	15	0	0	0	0
4	A	11	15	13	0	0
5	A	8	11	12	0	0
6	A	4	6	6	1	0
7	A	384	0	0	5	0
7	B	12	0	0	0	0
All	All	4283	3861	3735	26	0

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

All (26) 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:333[B]:ASN:OD1	1:A:336:GLU:OE2	1.68	1.10
1:A:249:LEU:H	2:B:3:ACE:H2	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333[B]:ASN:CG	1:A:336:GLU:OE2	2.26	0.78
1:A:151:LYS:HE3	7:A:885:HOH:O	1.84	0.77
1:A:326:ARG:HH11	6:A:606:EDO:H12	1.53	0.72
1:A:322[A]:MET:HE2	1:A:344[A]:THR:HG21	1.77	0.66
1:A:407:PRO:HB2	1:A:549:PRO:HG2	1.80	0.64
1:A:408:GLU:HG3	7:A:724:HOH:O	1.99	0.62
1:A:18:ASP:OD1	1:A:21:ARG:NH1	2.33	0.61
1:A:249:LEU:H	2:B:3:ACE:CH3	2.14	0.59
1:A:448[A]:GLU:HG3	7:A:781:HOH:O	2.02	0.59
1:A:458:VAL:HG13	1:A:550:VAL:HG13	1.86	0.56
1:A:321:TYR:HB2	1:A:344[B]:THR:HG22	1.89	0.55
1:A:437:ALA:HB1	1:A:576:LYS:HG2	1.89	0.54
1:A:333[B]:ASN:ND2	1:A:336:GLU:OE2	2.39	0.54
1:A:44:VAL:HG12	1:A:48:LEU:HD12	1.92	0.51
1:A:112:VAL:HG13	1:A:187:GLY:HA2	1.96	0.47
1:A:458:VAL:CG1	1:A:550:VAL:HG13	2.46	0.46
1:A:450:GLN:HG3	7:A:926:HOH:O	2.18	0.44
1:A:328:HIS:CD2	1:A:336:GLU:HB3	2.53	0.43
1:A:360:ILE:HD12	1:A:360:ILE:HA	1.96	0.42
1:A:35:VAL:HA	1:A:143:LEU:HD12	2.01	0.42
1:A:44:VAL:CG1	1:A:48:LEU:HD12	2.50	0.42
1:A:21:ARG:NH2	7:A:715:HOH:O	2.50	0.40
1:A:249:LEU:N	2:B:3:ACE:H2	2.26	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	484/489 (99%)	470 (97%)	14 (3%)	0	100	100
2	B	12/14 (86%)	12 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	496/503 (99%)	482 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	401/411 (98%)	400 (100%)	1 (0%)	92	85
2	B	9/9 (100%)	8 (89%)	1 (11%)	5	0
All	All	410/420 (98%)	408 (100%)	2 (0%)	86	76

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	429	THR
2	B	15	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
6	EDO	A	606	-	3,3,3	0.16	0	2,2,2	0.11	0
3	SO4	A	602	-	4,4,4	0.31	0	6,6,6	0.34	0
5	PG0	A	605	-	7,7,7	0.29	0	6,6,6	0.14	0
3	SO4	A	601	-	4,4,4	0.34	0	6,6,6	0.12	0
3	SO4	A	603	-	4,4,4	0.24	0	6,6,6	0.05	0
4	1PE	A	604	-	10,10,15	0.37	0	9,9,14	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG0	A	605	-	-	3/5/5/5	-
6	EDO	A	606	-	-	1/1/1/1	-
4	1PE	A	604	-	-	2/8/8/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	605	PG0	O1-C3-C4-O2

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Mol	Chain	Res	Type	Atoms
5	A	605	PG0	OTT-C1-C2-O1
6	A	606	EDO	O1-C1-C2-O2
4	A	604	1PE	OH5-C14-C24-OH4
5	A	605	PG0	C1-C2-O1-C3
4	A	604	1PE	C14-C24-OH4-C13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	606	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	468/489 (95%)	0.14	31 (6%) 26 31	6, 19, 40, 54	10 (2%)
2	B	12/14 (85%)	0.16	0 100 100	13, 24, 43, 51	0
All	All	480/503 (95%)	0.14	31 (6%) 26 32	6, 19, 41, 54	10 (2%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	VAL	6.6
1	A	77	TYR	4.7
1	A	75	LEU	4.2
1	A	53	VAL	4.0
1	A	78	PHE	3.7
1	A	567	ALA	3.7
1	A	581	ALA	3.7
1	A	134	PHE	3.5
1	A	566	VAL	3.4
1	A	188	PRO	3.4
1	A	74	GLY	3.2
1	A	2	GLY	3.2
1	A	187	GLY	3.0
1	A	202	GLY	3.0
1	A	76	THR	2.9
1	A	10	LEU	2.7
1	A	109	GLU	2.7
1	A	203	ASN	2.6
1	A	189	ASN	2.6
1	A	190	GLY	2.5
1	A	458	VAL	2.4
1	A	569	LYS	2.4
1	A	204	GLU	2.3
1	A	251	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	400	GLN	2.3
1	A	401	GLY	2.3
1	A	429	THR	2.3
1	A	201	LYS	2.2
1	A	568	THR	2.2
1	A	250	HIS	2.1
1	A	9	THR	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	603	5/5	0.65	0.15	65,69,76,78	0
3	SO4	A	601	5/5	0.75	0.19	65,79,85,88	0
4	1PE	A	604	11/16	0.78	0.16	38,46,53,54	3
3	SO4	A	602	5/5	0.82	0.14	31,38,44,50	0
5	PG0	A	605	8/8	0.83	0.18	43,49,55,62	3
6	EDO	A	606	4/4	0.84	0.14	45,49,52,52	2

## 6.5 Other polymers [i](#)

There are no such residues in this entry.