



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:51 pm GMT

PDB ID : 5AK6  
Title : ligand complex structure of soluble epoxide hydrolase  
Authors : Oster, L.; Tapani, S.; Xue, Y.; Kack, H.  
Deposited on : 2015-03-02  
Resolution : 2.15 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

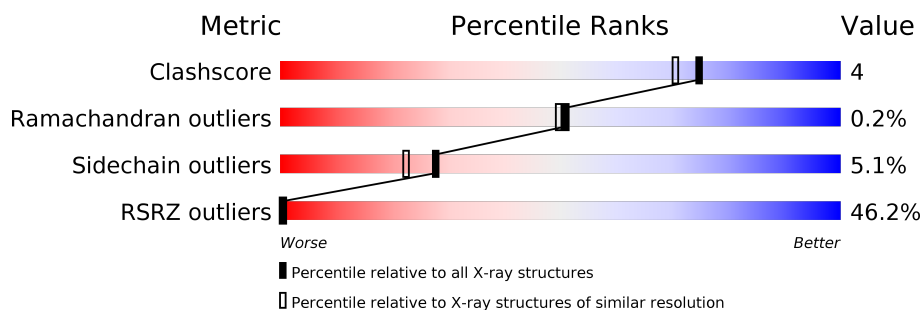
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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	549	<div> <div>46%</div> <div>85%</div> <div>13%</div> <div>..</div> </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
2	SO4	A	1548	-	-	-	X
2	SO4	A	1549	-	-	-	X
3	PEG	A	1550	-	-	-	X
3	PEG	A	1551	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	1552	-	-	-	X
5	YPN	A	1555	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4683 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 BIFUNCTIONAL EPOXIDE HYDROLASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4286	2748	722	780	36			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP P34913

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

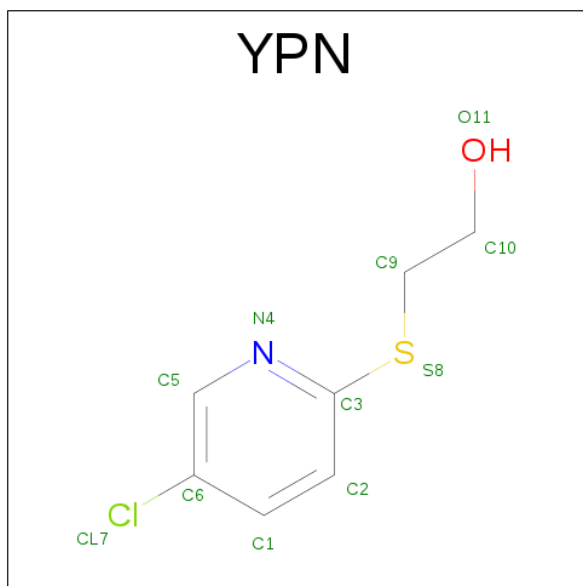
- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is 2-[(5-CHLORO-2-PYRIDYL)SULFANYL]ETHANOL (three-letter code:

YPN) (formula: C<sub>7</sub>H<sub>8</sub>ClNOS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	S	0	0
			11	7	1	1	1	1		
5	A	1	Total	C	Cl	N	O	S	0	0
			11	7	1	1	1	1		
5	A	1	Total	C	Cl	N	O	S	0	0
			11	7	1	1	1	1		

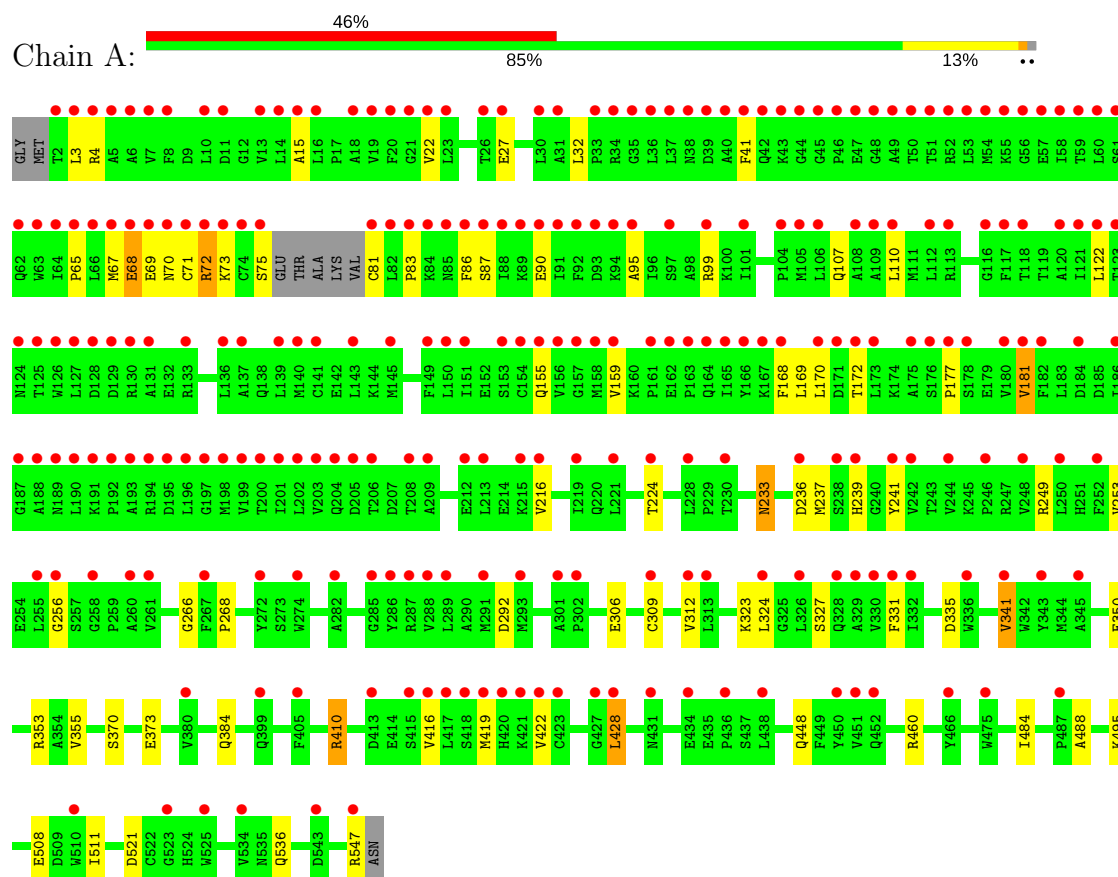
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	334	Total	O	0	0
			334	334		

### 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 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: BIFUNCTIONAL EPOXIDE HYDROLASE 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.74Å 91.74Å 245.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.48 – 2.15 79.45 – 2.12	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.48-2.15) 98.4 (79.45-2.12)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.12Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, $R_{free}$	0.204 , 0.248 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	4683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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: GOL, PEG, YPN, SO4

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	0.55	0/4390	0.73	1/5947 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ASP	N-CA-C	-5.79	95.36	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	4286	0	4288	30	12
2	A	10	0	0	0	0
3	A	14	0	20	3	0
4	A	6	0	8	0	0
5	A	33	0	24	2	0
6	A	334	0	0	4	8
All	All	4683	0	4340	32	15

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 (32) 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:331:PHE:HB3	1:A:341:VAL:HG22	1.52	0.91
1:A:41:PHE:HA	1:A:67:MET:HE1	1.57	0.86
1:A:384:GLN:HE22	5:A:1553:YPN:H5	1.54	0.72
1:A:422:VAL:HG11	1:A:428:LEU:HD22	1.78	0.65
1:A:309:CYS:SG	1:A:312:VAL:HG13	2.41	0.60
1:A:350:GLU:HG3	6:A:2204:HOH:O	2.03	0.57
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.84	0.57
1:A:41:PHE:HA	1:A:67:MET:CE	2.34	0.56
1:A:22:VAL:HG11	1:A:95:ALA:HB2	1.88	0.55
1:A:233:ASN:ND2	6:A:2133:HOH:O	2.40	0.55
3:A:1550:PEG:H31	6:A:2333:HOH:O	2.07	0.54
3:A:1551:PEG:H21	5:A:1555:YPN:N4	2.23	0.53
1:A:341:VAL:HG13	1:A:355:VAL:HG23	1.90	0.51
1:A:27:GLU:HA	1:A:32:LEU:HD12	1.94	0.50
1:A:341:VAL:HG13	1:A:355:VAL:CG2	2.42	0.49
1:A:69:GLU:HG3	1:A:73:LYS:HZ2	1.76	0.49
1:A:3:LEU:HD13	1:A:181:VAL:HG22	1.95	0.48
1:A:495:LYS:HD2	1:A:521:ASP:HA	1.96	0.48
1:A:83:PRO:HG2	1:A:86:PHE:HB2	1.95	0.48
1:A:484:ILE:HB	1:A:511:ILE:HG12	1.97	0.46
1:A:410:ARG:HD2	1:A:416:VAL:HG22	1.98	0.46
1:A:69:GLU:HG3	1:A:73:LYS:NZ	2.31	0.46
1:A:355:VAL:O	1:A:488:ALA:HA	2.16	0.46
1:A:168:PHE:O	1:A:172:THR:HG23	2.17	0.44
1:A:170:LEU:HD13	1:A:177:PRO:HD3	2.00	0.43
1:A:107:GLN:HG2	6:A:2053:HOH:O	2.17	0.43
1:A:122:LEU:HD22	1:A:169:LEU:HD22	2.00	0.42
1:A:15:ALA:HB1	1:A:99:ARG:HG2	2.02	0.42
1:A:370:SER:HB2	1:A:373:GLU:HG3	2.02	0.41
1:A:70:ASN:HA	1:A:73:LYS:HZ3	1.85	0.41
1:A:536:GLN:HB2	3:A:1550:PEG:H41	2.03	0.40
1:A:87:SER:HB3	1:A:90:GLU:HB2	2.03	0.40

All (15) 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)
1:A:68:GLU:OE1	1:A:72:ARG:NH2[8_435]	1.28	0.92
6:A:2093:HOH:O	6:A:2312:HOH:O[8_545]	1.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:SER:OG	6:A:2071:HOH:O[12_544]	1.65	0.55
1:A:239:HIS:O	1:A:241:TYR:N[12_544]	1.69	0.51
1:A:239:HIS:N	1:A:241:TYR:O[12_544]	1.84	0.36
1:A:155:GLN:NE2	6:A:2290:HOH:O[12_544]	1.92	0.28
1:A:327:SER:N	6:A:2151:HOH:O[12_544]	1.94	0.26
1:A:237:MET:O	6:A:2140:HOH:O[12_544]	1.96	0.24
1:A:236:ASP:OD1	1:A:323:LYS:NZ[12_544]	2.04	0.16
1:A:256:GLY:N	1:A:324:LEU:O[12_544]	2.06	0.14
1:A:65:PRO:O	1:A:69:GLU:OE2[8_435]	2.08	0.12
1:A:236:ASP:O	1:A:323:LYS:CD[12_544]	2.10	0.10
6:A:2077:HOH:O	6:A:2205:HOH:O[12_544]	2.12	0.08
6:A:2134:HOH:O	6:A:2196:HOH:O[12_544]	2.15	0.05
1:A:324:LEU:O	6:A:2147:HOH:O[12_544]	2.15	0.05

## 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	537/549 (98%)	523 (97%)	13 (2%)	1 (0%)	51	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	PRO

### 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	468/474 (99%)	444 (95%)	24 (5%)	28	22

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	68	GLU
1	A	71	CYS
1	A	72	ARG
1	A	75	SER
1	A	81	CYS
1	A	110	LEU
1	A	159	VAL
1	A	181	VAL
1	A	216	VAL
1	A	224	THR
1	A	233	ASN
1	A	249	ARG
1	A	253	VAL
1	A	306	GLU
1	A	341	VAL
1	A	353	ARG
1	A	410	ARG
1	A	419	MET
1	A	428	LEU
1	A	448	GLN
1	A	460	ARG
1	A	508	GLU
1	A	547	ARG

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	138	GLN
1	A	233	ASN
1	A	384	GLN
1	A	452	GLN
1	A	513	HIS

### 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 ⓘ

8 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	$\# Z  > 2$
2	SO4	A	1548	-	4,4,4	0.38	0	6,6,6	0.17	0
2	SO4	A	1549	-	4,4,4	0.44	0	6,6,6	0.26	0
3	PEG	A	1550	-	6,6,6	0.71	0	5,5,5	1.07	0
3	PEG	A	1551	-	6,6,6	0.52	0	5,5,5	1.03	0
4	GOL	A	1552	-	5,5,5	0.69	0	5,5,5	0.60	0
5	YPN	A	1553	-	11,11,11	0.50	0	13,13,13	0.89	0
5	YPN	A	1554	-	11,11,11	0.33	0	13,13,13	0.76	0
5	YPN	A	1555	-	11,11,11	0.75	0	13,13,13	0.85	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
2	SO4	A	1548	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1549	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	1550	-	-	0/4/4/4	0/0/0/0
3	PEG	A	1551	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1552	-	-	0/4/4/4	0/0/0/0
5	YPN	A	1553	-	-	0/4/4/4	0/1/1/1
5	YPN	A	1554	-	-	0/4/4/4	0/1/1/1
5	YPN	A	1555	-	-	1/4/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1555	YPN	N4-C3-S8-C9

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1550	PEG	2	0
3	A	1551	PEG	1	0
5	A	1553	YPN	1	0
5	A	1555	YPN	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	541/549 (98%)	2.31	250 (46%) <b>0</b> <b>0</b>	12, 30, 67, 98	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	PHE	11.3
1	A	75	SER	10.6
1	A	47	GLU	9.9
1	A	84	LYS	9.1
1	A	71	CYS	8.6
1	A	44	GLY	8.5
1	A	66	LEU	8.2
1	A	36	LEU	8.0
1	A	74	CYS	7.2
1	A	72	ARG	7.2
1	A	92	PHE	7.0
1	A	40	ALA	7.0
1	A	73	LYS	6.9
1	A	86	PHE	6.9
1	A	37	LEU	6.7
1	A	81	CYS	6.6
1	A	39	ASP	6.4
1	A	154	CYS	6.4
1	A	82	LEU	6.4
1	A	3	LEU	5.8
1	A	136	LEU	5.8
1	A	43	LYS	5.7
1	A	202	LEU	5.6
1	A	139	LEU	5.6
1	A	30	LEU	5.6
1	A	85	ASN	5.5
1	A	63	TRP	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	49	ALA	5.5
1	A	59	THR	5.5
1	A	159	VAL	5.4
1	A	168	PHE	5.4
1	A	26	THR	5.3
1	A	19	VAL	5.2
1	A	91	ILE	5.2
1	A	203	VAL	5.2
1	A	188	ALA	5.1
1	A	151	ILE	5.1
1	A	241	TYR	5.0
1	A	70	ASN	5.0
1	A	51	THR	4.9
1	A	131	ALA	4.9
1	A	167	LYS	4.9
1	A	11	ASP	4.8
1	A	180	VAL	4.8
1	A	201	ILE	4.8
1	A	127	LEU	4.8
1	A	137	ALA	4.7
1	A	15	ALA	4.6
1	A	69	GLU	4.6
1	A	58	ILE	4.6
1	A	126	TRP	4.5
1	A	182	PHE	4.5
1	A	62	GLN	4.5
1	A	14	LEU	4.4
1	A	149	PHE	4.4
1	A	88	ILE	4.4
1	A	7	VAL	4.4
1	A	213	LEU	4.3
1	A	246	PRO	4.3
1	A	21	GLY	4.3
1	A	189	ASN	4.2
1	A	65	PRO	4.2
1	A	48	GLY	4.2
1	A	23	LEU	4.2
1	A	34	ARG	4.2
1	A	54	MET	4.2
1	A	165	ILE	4.2
1	A	416	VAL	4.2
1	A	116	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	209	ALA	4.1
1	A	261	VAL	4.1
1	A	105	MET	4.1
1	A	256	GLY	4.1
1	A	53	LEU	4.1
1	A	124	ASN	4.0
1	A	101	ILE	4.0
1	A	161	PRO	4.0
1	A	192	PRO	4.0
1	A	150	LEU	3.9
1	A	83	PRO	3.9
1	A	67	MET	3.8
1	A	419	MET	3.7
1	A	46	PRO	3.7
1	A	236	ASP	3.6
1	A	255	LEU	3.6
1	A	172	THR	3.6
1	A	125	THR	3.6
1	A	109	ALA	3.5
1	A	163	PRO	3.5
1	A	143	LEU	3.5
1	A	45	GLY	3.5
1	A	198	MET	3.5
1	A	156	VAL	3.5
1	A	186	ILE	3.4
1	A	510	TRP	3.4
1	A	108	ALA	3.4
1	A	199	VAL	3.4
1	A	112	LEU	3.4
1	A	216	VAL	3.4
1	A	10	LEU	3.4
1	A	60	LEU	3.4
1	A	118	THR	3.4
1	A	219	ILE	3.4
1	A	196	LEU	3.4
1	A	145	MET	3.3
1	A	90	GLU	3.3
1	A	5	ALA	3.3
1	A	18	ALA	3.3
1	A	200	THR	3.3
1	A	13	VAL	3.3
1	A	6	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	195	ASP	3.2
1	A	418	SER	3.2
1	A	547	ARG	3.2
1	A	117	PHE	3.2
1	A	421	LYS	3.2
1	A	177	PRO	3.2
1	A	417	LEU	3.2
1	A	525	TRP	3.2
1	A	61	SER	3.2
1	A	175	ALA	3.2
1	A	194	ARG	3.2
1	A	56	GLY	3.1
1	A	162	GLU	3.1
1	A	120	ALA	3.1
1	A	166	TYR	3.1
1	A	170	LEU	3.1
1	A	228	LEU	3.1
1	A	22	VAL	3.1
1	A	123	THR	3.1
1	A	64	ILE	3.1
1	A	2	THR	3.1
1	A	157	GLY	3.0
1	A	16	LEU	3.0
1	A	31	ALA	3.0
1	A	55	LYS	3.0
1	A	27	GLU	3.0
1	A	187	GLY	3.0
1	A	181	VAL	3.0
1	A	155	GLN	2.9
1	A	129	ASP	2.9
1	A	153	SER	2.9
1	A	282	ALA	2.9
1	A	434	GLU	2.9
1	A	35	GLY	2.8
1	A	33	PRO	2.8
1	A	289	LEU	2.8
1	A	191	LYS	2.8
1	A	95	ALA	2.8
1	A	329	ALA	2.8
1	A	50	THR	2.8
1	A	130	ARG	2.8
1	A	324	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	190	LEU	2.7
1	A	413	ASP	2.7
1	A	288	VAL	2.7
1	A	330	VAL	2.7
1	A	423	CYS	2.7
1	A	399	GLN	2.7
1	A	193	ALA	2.6
1	A	206	THR	2.6
1	A	332	ILE	2.6
1	A	87	SER	2.6
1	A	42	GLN	2.6
1	A	99	ARG	2.6
1	A	122	LEU	2.6
1	A	158	MET	2.6
1	A	221	LEU	2.6
1	A	238	SER	2.6
1	A	331	PHE	2.6
1	A	133	ARG	2.5
1	A	171	ASP	2.5
1	A	380	VAL	2.5
1	A	57	GLU	2.5
1	A	436	PRO	2.5
1	A	258	GLY	2.5
1	A	204	GLN	2.5
1	A	93	ASP	2.5
1	A	141	CYS	2.5
1	A	341	VAL	2.5
1	A	104	PRO	2.5
1	A	345	ALA	2.5
1	A	52	ARG	2.5
1	A	466	TYR	2.5
1	A	260	ALA	2.5
1	A	208	THR	2.4
1	A	452	GLN	2.4
1	A	286	TYR	2.4
1	A	8	PHE	2.4
1	A	428	LEU	2.4
1	A	121	ILE	2.4
1	A	94	LYS	2.4
1	A	140	MET	2.4
1	A	215	LYS	2.4
1	A	178	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	291	MET	2.4
1	A	252	PHE	2.4
1	A	302	PRO	2.4
1	A	420	HIS	2.4
1	A	301	ALA	2.4
1	A	328	GLN	2.4
1	A	197	GLY	2.4
1	A	106	LEU	2.3
1	A	176	SER	2.3
1	A	38	ASN	2.3
1	A	272	TYR	2.3
1	A	212	GLU	2.3
1	A	405	PHE	2.3
1	A	224	THR	2.3
1	A	164	GLN	2.3
1	A	110	LEU	2.3
1	A	285	GLY	2.3
1	A	41	PHE	2.3
1	A	242	VAL	2.2
1	A	239	HIS	2.2
1	A	313	LEU	2.2
1	A	4	ARG	2.2
1	A	97	SER	2.2
1	A	68	GLU	2.2
1	A	438	LEU	2.2
1	A	534	VAL	2.2
1	A	184	ASP	2.2
1	A	287	ARG	2.2
1	A	250	LEU	2.2
1	A	205	ASP	2.2
1	A	267	PHE	2.2
1	A	293	MET	2.2
1	A	89	LYS	2.2
1	A	336	TRP	2.1
1	A	343	TYR	2.1
1	A	422	VAL	2.1
1	A	543	ASP	2.1
1	A	427	GLY	2.1
1	A	431	ASN	2.1
1	A	326	LEU	2.1
1	A	274	TRP	2.1
1	A	450	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	128	ASP	2.1
1	A	244	VAL	2.1
1	A	312	VAL	2.1
1	A	487	PRO	2.1
1	A	309	CYS	2.1
1	A	523	GLY	2.1
1	A	230	THR	2.0
1	A	248	VAL	2.0
1	A	451	VAL	2.0
1	A	475	TRP	2.0
1	A	173	LEU	2.0
1	A	415	SER	2.0
1	A	113	ARG	2.0

## 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
3	PEG	A	1551	7/7	0.19	0.44	8.97	65,65,66,66	0
3	PEG	A	1550	7/7	0.56	0.41	7.35	46,47,48,49	0
5	YPN	A	1555	11/11	0.58	0.35	5.96	50,60,69,69	0
2	SO4	A	1548	5/5	0.89	0.33	3.54	77,81,82,83	0
4	GOL	A	1552	6/6	0.28	0.40	3.47	60,62,62,63	0
2	SO4	A	1549	5/5	0.52	0.43	2.95	74,78,79,79	0
5	YPN	A	1553	11/11	0.87	0.18	-0.34	23,27,29,33	0
5	YPN	A	1554	11/11	0.84	0.20	-0.34	34,39,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.