



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:16 PM GMT

PDB ID : 4XWY  
Title : Crystal structure of human sepiapterin reductase in complex with an N-acetylserotonin analogue  
Authors : Johnsson, K.; Hovius, R.; Gorszka, K.I.; Pojer, F.  
Deposited on : 2015-01-29  
Resolution : 2.35 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

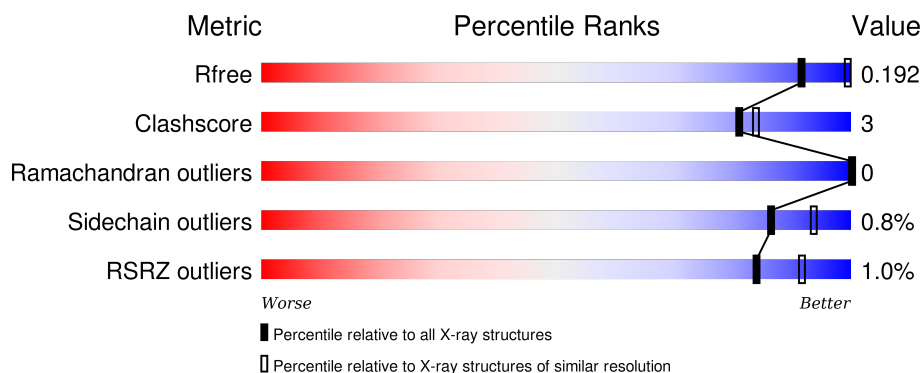
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	275	<div> <div>88%</div> <div>6% 7%</div> </div>
1	B	275	<div> <div>89%</div> <div>• 7%</div> </div>
1	C	275	<div> <div>88%</div> <div>5% 7%</div> </div>
1	D	275	<div> <div>3%</div> <div>81% 12% 7%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8330 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 Sepiapterin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			1942	1224	343	364	11			
1	B	257	Total	C	N	O	S	0	1	0
			1942	1224	343	364	11			
1	C	257	Total	C	N	O	S	0	1	0
			1942	1224	343	364	11			
1	D	257	Total	C	N	O	S	0	1	0
			1942	1224	343	364	11			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP P35270
A	-15	HIS	-	expression tag	UNP P35270
A	-14	HIS	-	expression tag	UNP P35270
A	-13	HIS	-	expression tag	UNP P35270
A	-12	HIS	-	expression tag	UNP P35270
A	-11	HIS	-	expression tag	UNP P35270
A	-10	HIS	-	expression tag	UNP P35270
A	-9	GLU	-	expression tag	UNP P35270
A	-8	ASN	-	expression tag	UNP P35270
A	-7	LEU	-	expression tag	UNP P35270
A	-6	TYR	-	expression tag	UNP P35270
A	-5	PHE	-	expression tag	UNP P35270
A	-4	GLN	-	expression tag	UNP P35270
A	-3	GLY	-	expression tag	UNP P35270
B	-16	MET	-	initiating methionine	UNP P35270
B	-15	HIS	-	expression tag	UNP P35270
B	-14	HIS	-	expression tag	UNP P35270
B	-13	HIS	-	expression tag	UNP P35270
B	-12	HIS	-	expression tag	UNP P35270
B	-11	HIS	-	expression tag	UNP P35270
B	-10	HIS	-	expression tag	UNP P35270

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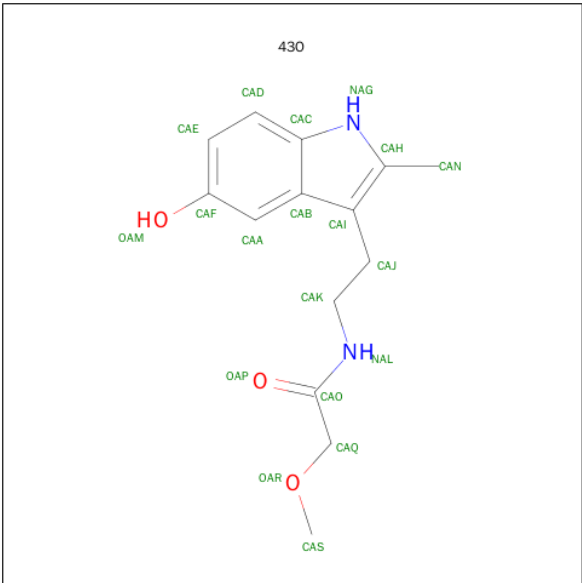
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLU	-	expression tag	UNP P35270
B	-8	ASN	-	expression tag	UNP P35270
B	-7	LEU	-	expression tag	UNP P35270
B	-6	TYR	-	expression tag	UNP P35270
B	-5	PHE	-	expression tag	UNP P35270
B	-4	GLN	-	expression tag	UNP P35270
B	-3	GLY	-	expression tag	UNP P35270
C	-16	MET	-	initiating methionine	UNP P35270
C	-15	HIS	-	expression tag	UNP P35270
C	-14	HIS	-	expression tag	UNP P35270
C	-13	HIS	-	expression tag	UNP P35270
C	-12	HIS	-	expression tag	UNP P35270
C	-11	HIS	-	expression tag	UNP P35270
C	-10	HIS	-	expression tag	UNP P35270
C	-9	GLU	-	expression tag	UNP P35270
C	-8	ASN	-	expression tag	UNP P35270
C	-7	LEU	-	expression tag	UNP P35270
C	-6	TYR	-	expression tag	UNP P35270
C	-5	PHE	-	expression tag	UNP P35270
C	-4	GLN	-	expression tag	UNP P35270
C	-3	GLY	-	expression tag	UNP P35270
D	-16	MET	-	initiating methionine	UNP P35270
D	-15	HIS	-	expression tag	UNP P35270
D	-14	HIS	-	expression tag	UNP P35270
D	-13	HIS	-	expression tag	UNP P35270
D	-12	HIS	-	expression tag	UNP P35270
D	-11	HIS	-	expression tag	UNP P35270
D	-10	HIS	-	expression tag	UNP P35270
D	-9	GLU	-	expression tag	UNP P35270
D	-8	ASN	-	expression tag	UNP P35270
D	-7	LEU	-	expression tag	UNP P35270
D	-6	TYR	-	expression tag	UNP P35270
D	-5	PHE	-	expression tag	UNP P35270
D	-4	GLN	-	expression tag	UNP P35270
D	-3	GLY	-	expression tag	UNP P35270

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is N-[2-(5-hydroxy-2-methyl-1H-indol-3-yl)ethyl]-2-methoxyacetamide (three-letter code: 43O) (formula: C<sub>14</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	14	2	3		
3	B	1	Total	C	N	O	0	0
			19	14	2	3		
3	C	1	Total	C	N	O	0	0
			19	14	2	3		
3	D	1	Total	C	N	O	0	0
			19	14	2	3		

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



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	71	Total	O	0	0
			71	71		
5	C	70	Total	O	0	0
			70	70		
5	D	41	Total	O	0	0
			41	41		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.84Å 144.84Å 180.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	125.44 – 2.35 46.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (125.44-2.35) 99.9 (46.31-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.185 , 0.217 0.193 , 0.192	Depositor DCC
$R_{free}$ test set	4340 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.2	EDS
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 89101 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 43O, SO4, NDP

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	0.44	0/1975	0.60	0/2672
1	B	0.41	0/1975	0.57	0/2672
1	C	0.43	0/1975	0.57	0/2672
1	D	0.37	0/1975	0.53	0/2672
All	All	0.42	0/7900	0.57	0/10688

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1942	0	2013	11	0
1	B	1942	0	2013	7	0
1	C	1942	0	2013	9	0
1	D	1942	0	2013	31	0
2	A	48	0	26	2	0
2	B	48	0	26	0	0
2	C	48	0	26	0	0
2	D	48	0	26	3	0
3	A	19	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	0	18	1	0
3	C	19	0	17	0	0
3	D	19	0	17	0	0
4	A	20	0	0	0	0
4	B	15	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	67	0	0	0	0
5	B	71	0	0	0	0
5	C	70	0	0	0	0
5	D	41	0	0	0	0
All	All	8330	0	8225	53	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 (53) 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:70:GLU:OE2	1:C:114:SER:OG	1.81	0.98
1:D:18:ARG:NH2	1:D:50:GLU:OE1	2.12	0.81
1:D:237:LYS:NZ	1:D:255:PHE:O	2.14	0.81
1:D:18:ARG:NH2	1:D:50:GLU:CD	2.35	0.80
1:D:7[C]:CYS:SG	1:D:24:LEU:HD21	2.21	0.80
1:A:212:ASP:OD1	1:A:213:PRO:HD2	1.83	0.78
1:B:52:GLY:O	1:B:55:ARG:HG2	1.87	0.74
1:A:59:ARG:HH11	1:A:59:ARG:HG3	1.52	0.72
1:D:18:ARG:NH2	1:D:50:GLU:OE2	2.24	0.71
1:B:7[C]:CYS:SG	1:B:24:LEU:HD21	2.31	0.70
1:A:7[C]:CYS:SG	1:A:24:LEU:HD21	2.32	0.69
1:B:202:MET:HG2	3:B:302:43O:H16	1.74	0.69
1:D:85:ARG:NH2	1:D:138:ALA:O	2.25	0.68
1:B:70:GLU:OE2	1:D:114:SER:OG	2.08	0.67
1:D:232:LYS:O	1:D:236:GLN:HG3	1.95	0.67
1:D:18:ARG:HH21	1:D:50:GLU:CD	1.97	0.66
1:D:215:MET:HE2	1:D:219:LEU:HD11	1.79	0.65
1:D:14:ARG:NH1	2:D:301:NDP:O1X	2.31	0.64
1:B:21:ALA:HB3	1:B:22:PRO:HD3	1.81	0.63
1:C:2:LEU:O	1:C:91:ARG:HD2	2.00	0.62
1:D:215:MET:HE2	1:D:219:LEU:CD1	2.35	0.56
1:D:232:LYS:O	1:D:236:GLN:CG	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:O	1:B:80:LEU:HB2	2.06	0.56
1:D:91:ARG:HG2	1:D:146:ASN:HB3	1.87	0.55
1:C:7[B]:CYS:SG	1:C:24:LEU:HD21	2.46	0.55
1:C:7[A]:CYS:SG	1:C:24:LEU:HD21	2.46	0.54
1:D:240:SER:O	1:D:244:LYS:HG3	2.07	0.54
1:D:91:ARG:CG	1:D:146:ASN:HB3	2.39	0.53
1:D:213:PRO:O	1:D:217:LYS:HG2	2.08	0.52
1:C:86:PRO:HG2	1:C:89:LEU:HD13	1.92	0.52
1:D:225:LYS:HG2	1:D:227:LYS:HE2	1.94	0.50
1:A:160:PRO:C	1:A:161:PHE:HD1	2.15	0.50
1:C:230:ASP:HB3	1:C:233:VAL:HG23	1.93	0.49
1:D:153:SER:O	2:D:301:NDP:H6N	2.12	0.49
1:D:225:LYS:O	1:D:225:LYS:HG3	2.14	0.48
1:D:39:ARG:HB2	2:D:301:NDP:O3X	2.14	0.47
1:A:114:SER:OG	1:C:70:GLU:OE1	2.28	0.47
1:D:55:ARG:HG3	1:D:56:SER:N	2.30	0.47
1:D:230:ASP:HB3	1:D:233:VAL:HG23	1.98	0.46
1:A:59:ARG:NH1	1:A:59:ARG:HG3	2.24	0.45
1:D:5:ALA:HA	1:D:91:ARG:O	2.17	0.44
1:B:137:LYS:HD2	1:D:109:VAL:HG12	2.00	0.43
1:D:7[C]:CYS:HA	1:D:93:LEU:O	2.19	0.42
1:D:146:ASN:OD1	1:D:146:ASN:C	2.58	0.42
1:D:232:LYS:HE3	1:D:232:LYS:HB2	1.86	0.42
1:A:183:LEU:HB3	1:C:162:LYS:HG3	2.02	0.41
1:A:153:SER:O	2:A:801:NDP:H6N	2.21	0.41
1:D:104:VAL:O	1:D:211:VAL:HG23	2.21	0.41
1:D:7[A]:CYS:HA	1:D:93:LEU:O	2.20	0.41
1:D:7[B]:CYS:HA	1:D:93:LEU:O	2.20	0.41
1:A:39:ARG:HB2	2:A:801:NDP:O3X	2.20	0.40
1:C:21:ALA:HB3	1:C:22:PRO:CD	2.51	0.40
1:A:146:ASN:OD1	1:A:146:ASN:C	2.60	0.40

There are no symmetry-related clashes.

## 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	257/275 (94%)	252 (98%)	5 (2%)	0	100	100
1	B	257/275 (94%)	255 (99%)	2 (1%)	0	100	100
1	C	257/275 (94%)	253 (98%)	4 (2%)	0	100	100
1	D	257/275 (94%)	251 (98%)	6 (2%)	0	100	100
All	All	1028/1100 (94%)	1011 (98%)	17 (2%)	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	211/225 (94%)	208 (99%)	3 (1%)	74	86
1	B	211/225 (94%)	209 (99%)	2 (1%)	84	92
1	C	211/225 (94%)	209 (99%)	2 (1%)	84	92
1	D	211/225 (94%)	211 (100%)	0	100	100
All	All	844/900 (94%)	837 (99%)	7 (1%)	86	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	175	ASP
1	A	215	MET
1	B	137	LYS
1	B	220	GLN
1	C	75	GLN
1	C	82	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

17 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	NDP	A	801	-	44,52,52	1.10	4 (9%)	55,80,80	1.51	5 (9%)
3	43O	A	802	-	19,20,20	2.11	5 (26%)	20,27,27	1.60	4 (20%)
4	SO4	A	803	-	4,4,4	0.44	0	6,6,6	0.27	0
4	SO4	A	804	-	4,4,4	0.31	0	6,6,6	0.09	0
4	SO4	A	805	-	4,4,4	0.44	0	6,6,6	0.44	0
4	SO4	A	806	-	4,4,4	0.41	0	6,6,6	0.35	0
2	NDP	B	301	-	44,52,52	1.18	3 (6%)	55,80,80	1.54	4 (7%)
3	43O	B	302	-	19,20,20	2.10	6 (31%)	20,27,27	1.16	2 (10%)
4	SO4	B	303	-	4,4,4	0.49	0	6,6,6	0.13	0
4	SO4	B	304	-	4,4,4	0.38	0	6,6,6	0.15	0
4	SO4	B	305	-	4,4,4	1.17	0	6,6,6	0.52	0
2	NDP	C	301	-	44,52,52	1.19	3 (6%)	55,80,80	1.72	9 (16%)
3	43O	C	302	-	19,20,20	2.15	7 (36%)	20,27,27	1.28	2 (10%)
4	SO4	C	303	-	4,4,4	0.31	0	6,6,6	0.13	0
2	NDP	D	301	-	44,52,52	1.19	3 (6%)	55,80,80	1.75	7 (12%)
3	43O	D	302	-	19,20,20	2.10	6 (31%)	20,27,27	1.17	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	D	303	-	4,4,4	0.41	0	6,6,6	0.12	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	NDP	A	801	-	-	0/30/77/77	0/5/5/5
3	43O	A	802	-	-	1/9/9/9	0/2/2/2
4	SO4	A	803	-	-	0/0/0/0	0/0/0/0
4	SO4	A	804	-	-	0/0/0/0	0/0/0/0
4	SO4	A	805	-	-	0/0/0/0	0/0/0/0
4	SO4	A	806	-	-	0/0/0/0	0/0/0/0
2	NDP	B	301	-	-	0/30/77/77	0/5/5/5
3	43O	B	302	-	-	1/9/9/9	0/2/2/2
4	SO4	B	303	-	-	0/0/0/0	0/0/0/0
4	SO4	B	304	-	-	0/0/0/0	0/0/0/0
4	SO4	B	305	-	-	0/0/0/0	0/0/0/0
2	NDP	C	301	-	-	0/30/77/77	0/5/5/5
3	43O	C	302	-	-	1/9/9/9	0/2/2/2
4	SO4	C	303	-	-	0/0/0/0	0/0/0/0
2	NDP	D	301	-	-	0/30/77/77	0/5/5/5
3	43O	D	302	-	-	1/9/9/9	0/2/2/2
4	SO4	D	303	-	-	0/0/0/0	0/0/0/0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	43O	CAI-CAB	-4.84	1.32	1.41
3	B	302	43O	CAD-CAC	-4.74	1.33	1.41
3	A	802	43O	CAD-CAC	-4.72	1.33	1.41
2	D	301	NDP	C4N-C5N	-4.50	1.39	1.49
3	C	302	43O	CAD-CAC	-4.49	1.33	1.41
3	D	302	43O	CAD-CAC	-4.49	1.33	1.41
3	C	302	43O	CAI-CAB	-4.49	1.33	1.41
3	D	302	43O	CAI-CAB	-4.39	1.33	1.41
2	C	301	NDP	C4N-C5N	-4.36	1.39	1.49
3	B	302	43O	CAI-CAB	-4.01	1.34	1.41
3	C	302	43O	CAA-CAB	-4.00	1.34	1.42
3	B	302	43O	CAA-CAB	-3.91	1.34	1.42
3	A	802	43O	CAA-CAB	-3.88	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NDP	C4N-C5N	-3.83	1.40	1.49
3	D	302	43O	CAA-CAB	-3.76	1.34	1.42
2	A	801	NDP	C4N-C5N	-3.57	1.41	1.49
3	D	302	43O	CAI-CAH	-3.08	1.33	1.39
3	B	302	43O	CAI-CAH	-3.05	1.33	1.39
3	A	802	43O	CAI-CAH	-2.97	1.33	1.39
3	C	302	43O	CAB-CAC	-2.91	1.34	1.42
3	C	302	43O	CAI-CAH	-2.89	1.33	1.39
3	D	302	43O	CAB-CAC	-2.88	1.34	1.42
3	B	302	43O	CAB-CAC	-2.75	1.35	1.42
3	A	802	43O	CAB-CAC	-2.41	1.36	1.42
3	C	302	43O	CAD-CAE	2.07	1.40	1.36
3	B	302	43O	CAN-CAH	2.15	1.54	1.50
3	D	302	43O	CAN-CAH	2.21	1.54	1.50
2	A	801	NDP	C2N-C3N	2.22	1.40	1.34
2	A	801	NDP	C5A-C4A	2.28	1.45	1.40
3	C	302	43O	CAN-CAH	2.33	1.55	1.50
2	C	301	NDP	C5A-C4A	2.51	1.46	1.40
2	D	301	NDP	C5A-C4A	2.77	1.46	1.40
2	B	301	NDP	C5A-C4A	2.93	1.47	1.40
2	D	301	NDP	C6N-C5N	3.16	1.39	1.33
2	B	301	NDP	C6N-C5N	3.27	1.39	1.33
2	C	301	NDP	C6N-C5N	3.41	1.39	1.33
2	A	801	NDP	C6N-C5N	3.49	1.39	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NDP	N3A-C2A-N1A	-8.43	122.25	128.87
2	B	301	NDP	N3A-C2A-N1A	-7.68	122.84	128.87
2	A	801	NDP	N3A-C2A-N1A	-7.50	122.98	128.87
2	C	301	NDP	N3A-C2A-N1A	-7.42	123.05	128.87
2	D	301	NDP	C1B-N9A-C4A	-4.67	121.59	126.81
2	C	301	NDP	C1B-N9A-C4A	-3.95	122.40	126.81
2	A	801	NDP	C1B-N9A-C4A	-2.93	123.54	126.81
2	C	301	NDP	O2X-P2B-O2B	-2.85	98.09	106.62
3	B	302	43O	CAS-OAR-CAQ	-2.57	101.99	113.21
3	A	802	43O	CAJ-CAI-CAH	-2.50	124.48	127.20
3	B	302	43O	CAJ-CAI-CAH	-2.47	124.51	127.20
3	A	802	43O	CAJ-CAK-NAL	-2.19	106.46	111.88
2	D	301	NDP	C4N-C5N-C6N	-2.14	119.06	122.58
3	A	802	43O	CAN-CAH-CAI	-2.10	124.77	129.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NDP	C3N-C2N-N1N	-2.08	120.18	123.24
3	D	302	43O	CAJ-CAI-CAH	-2.07	124.95	127.20
3	C	302	43O	CAS-OAR-CAQ	-2.01	104.42	113.21
2	C	301	NDP	C4N-C5N-C6N	-2.00	119.28	122.58
2	C	301	NDP	N6A-C6A-N1A	2.02	121.90	118.52
2	B	301	NDP	O3X-P2B-O2X	2.07	115.03	107.44
2	D	301	NDP	C2A-N1A-C6A	2.09	122.49	118.77
2	C	301	NDP	O2X-P2B-O1X	2.10	117.47	110.63
2	D	301	NDP	N6A-C6A-N1A	2.20	122.20	118.52
2	A	801	NDP	O2N-PN-O1N	2.21	124.07	112.56
2	A	801	NDP	C5N-C4N-C3N	2.28	118.32	112.41
2	B	301	NDP	C5N-C4N-C3N	2.45	118.76	112.41
2	C	301	NDP	O2N-PN-O1N	2.48	125.44	112.56
2	D	301	NDP	C5N-C4N-C3N	2.52	118.93	112.41
2	B	301	NDP	O4B-C1B-N9A	2.69	113.19	108.11
2	C	301	NDP	C5N-C4N-C3N	2.73	119.47	112.41
3	D	302	43O	CAA-CAB-CAC	2.88	121.48	120.34
3	C	302	43O	CAA-CAB-CAC	2.98	121.52	120.34
2	D	301	NDP	O4B-C1B-N9A	3.51	114.74	108.11
2	C	301	NDP	O4B-C1B-N9A	3.74	115.17	108.11
3	A	802	43O	CAA-CAB-CAC	4.55	122.14	120.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	43O	CAQ-CAO-NAL-CAK
3	A	802	43O	CAQ-CAO-NAL-CAK
3	C	302	43O	CAQ-CAO-NAL-CAK
3	D	302	43O	CAQ-CAO-NAL-CAK

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NDP	2	0
3	B	302	43O	1	0
2	D	301	NDP	3	0

## 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 [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	257/275 (93%)	-0.47	1 (0%) 93 97	25, 39, 67, 101	0
1	B	257/275 (93%)	-0.44	0 100 100	28, 42, 71, 103	0
1	C	257/275 (93%)	-0.44	0 100 100	26, 44, 70, 87	0
1	D	257/275 (93%)	-0.06	9 (3%) 48 61	33, 53, 88, 168	0
All	All	1028/1100 (93%)	-0.35	10 (0%) 84 92	25, 45, 76, 168	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	54	GLU	5.2
1	D	53	ALA	3.3
1	D	224	ALA	3.2
1	D	225	LYS	3.0
1	D	227	LYS	2.4
1	D	31	GLY	2.4
1	D	217	LYS	2.3
1	D	220	GLN	2.2
1	A	55	ARG	2.1
1	D	55	ARG	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
3	43O	C	302	19/19	0.95	0.13	1.41	32,38,46,50	0
3	43O	B	302	19/19	0.94	0.12	0.58	33,35,42,47	0
3	43O	A	802	19/19	0.96	0.12	0.19	32,35,39,50	0
3	43O	D	302	19/19	0.96	0.12	0.10	40,46,62,64	0
2	NDP	C	301	48/48	0.98	0.11	-0.04	26,33,40,52	0
2	NDP	A	801	48/48	0.99	0.10	-0.04	21,28,38,46	0
4	SO4	A	803	5/5	0.98	0.10	-0.09	61,62,72,76	0
2	NDP	B	301	48/48	0.99	0.09	-0.61	24,34,39,48	0
2	NDP	D	301	48/48	0.98	0.10	-0.69	37,44,53,63	0
4	SO4	B	303	5/5	0.94	0.11	-	58,66,76,80	0
4	SO4	A	806	5/5	0.95	0.09	-	61,67,82,97	0
4	SO4	B	305	5/5	0.96	0.23	-	44,46,50,50	0
4	SO4	C	303	5/5	0.98	0.09	-	56,65,70,74	0
4	SO4	B	304	5/5	0.96	0.15	-	82,98,100,107	0
4	SO4	D	303	5/5	0.95	0.16	-	76,78,87,92	0
4	SO4	A	804	5/5	0.97	0.12	-	65,74,81,88	0
4	SO4	A	805	5/5	0.95	0.14	-	71,75,88,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.