



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:42 PM GMT

PDB ID : 4J7X  
Title : Crystal structure of human sepiapterin reductase in complex with sulfasalazine  
Authors : Groenlund Pedersen, M.; Pojer, F.; Johnsson, K.  
Deposited on : 2013-02-14  
Resolution : 2.60 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.

---

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

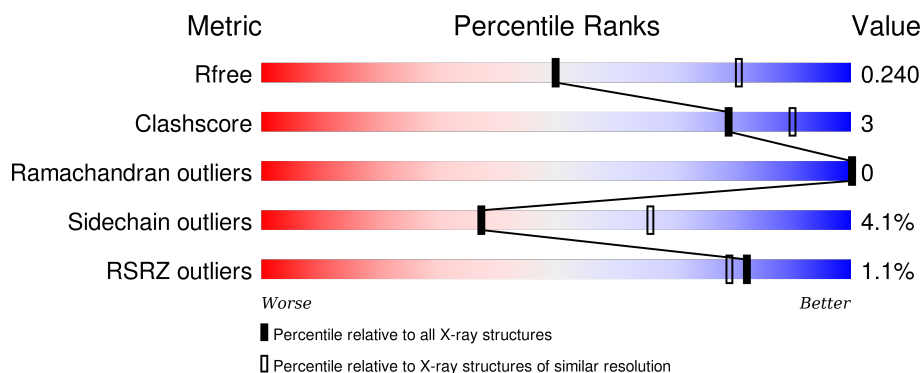
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	288	<div> <div>3%</div> <div>83% 5% • 11%</div> </div>
1	B	288	<div> <div>79% 8% • 11%</div> </div>
1	F	288	<div> <div>79% 9% • 11%</div> </div>
1	J	288	<div> <div>3%</div> <div>80% 8% • 11%</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
5	PEG	B	806	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8267 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	0	0
			1936	1220	343	364	9			
1	B	257	Total	C	N	O	S	0	1	0
			1947	1226	347	365	9			
1	F	257	Total	C	N	O	S	0	0	0
			1936	1220	343	364	9			
1	J	257	Total	C	N	O	S	0	0	0
			1936	1220	343	364	9			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	EXPRESSION TAG	UNP P35270
A	-28	SER	-	EXPRESSION TAG	UNP P35270
A	-27	TYR	-	EXPRESSION TAG	UNP P35270
A	-26	TYR	-	EXPRESSION TAG	UNP P35270
A	-25	HIS	-	EXPRESSION TAG	UNP P35270
A	-24	HIS	-	EXPRESSION TAG	UNP P35270
A	-23	HIS	-	EXPRESSION TAG	UNP P35270
A	-22	HIS	-	EXPRESSION TAG	UNP P35270
A	-21	HIS	-	EXPRESSION TAG	UNP P35270
A	-20	HIS	-	EXPRESSION TAG	UNP P35270
A	-19	LEU	-	EXPRESSION TAG	UNP P35270
A	-18	GLU	-	EXPRESSION TAG	UNP P35270
A	-17	SER	-	EXPRESSION TAG	UNP P35270
A	-16	THR	-	EXPRESSION TAG	UNP P35270
A	-15	SER	-	EXPRESSION TAG	UNP P35270
A	-14	LEU	-	EXPRESSION TAG	UNP P35270
A	-13	TYR	-	EXPRESSION TAG	UNP P35270
A	-12	LYS	-	EXPRESSION TAG	UNP P35270
A	-11	LYS	-	EXPRESSION TAG	UNP P35270
A	-10	ALA	-	EXPRESSION TAG	UNP P35270
A	-9	GLY	-	EXPRESSION TAG	UNP P35270

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	LEU	-	EXPRESSION TAG	UNP P35270
A	-7	GLU	-	EXPRESSION TAG	UNP P35270
A	-6	GLY	-	EXPRESSION TAG	UNP P35270
A	-5	VAL	-	EXPRESSION TAG	UNP P35270
A	-4	ARG	-	EXPRESSION TAG	UNP P35270
A	-3	THR	-	EXPRESSION TAG	UNP P35270
B	-29	MET	-	EXPRESSION TAG	UNP P35270
B	-28	SER	-	EXPRESSION TAG	UNP P35270
B	-27	TYR	-	EXPRESSION TAG	UNP P35270
B	-26	TYR	-	EXPRESSION TAG	UNP P35270
B	-25	HIS	-	EXPRESSION TAG	UNP P35270
B	-24	HIS	-	EXPRESSION TAG	UNP P35270
B	-23	HIS	-	EXPRESSION TAG	UNP P35270
B	-22	HIS	-	EXPRESSION TAG	UNP P35270
B	-21	HIS	-	EXPRESSION TAG	UNP P35270
B	-20	HIS	-	EXPRESSION TAG	UNP P35270
B	-19	LEU	-	EXPRESSION TAG	UNP P35270
B	-18	GLU	-	EXPRESSION TAG	UNP P35270
B	-17	SER	-	EXPRESSION TAG	UNP P35270
B	-16	THR	-	EXPRESSION TAG	UNP P35270
B	-15	SER	-	EXPRESSION TAG	UNP P35270
B	-14	LEU	-	EXPRESSION TAG	UNP P35270
B	-13	TYR	-	EXPRESSION TAG	UNP P35270
B	-12	LYS	-	EXPRESSION TAG	UNP P35270
B	-11	LYS	-	EXPRESSION TAG	UNP P35270
B	-10	ALA	-	EXPRESSION TAG	UNP P35270
B	-9	GLY	-	EXPRESSION TAG	UNP P35270
B	-8	LEU	-	EXPRESSION TAG	UNP P35270
B	-7	GLU	-	EXPRESSION TAG	UNP P35270
B	-6	GLY	-	EXPRESSION TAG	UNP P35270
B	-5	VAL	-	EXPRESSION TAG	UNP P35270
B	-4	ARG	-	EXPRESSION TAG	UNP P35270
B	-3	THR	-	EXPRESSION TAG	UNP P35270
F	-29	MET	-	EXPRESSION TAG	UNP P35270
F	-28	SER	-	EXPRESSION TAG	UNP P35270
F	-27	TYR	-	EXPRESSION TAG	UNP P35270
F	-26	TYR	-	EXPRESSION TAG	UNP P35270
F	-25	HIS	-	EXPRESSION TAG	UNP P35270
F	-24	HIS	-	EXPRESSION TAG	UNP P35270
F	-23	HIS	-	EXPRESSION TAG	UNP P35270
F	-22	HIS	-	EXPRESSION TAG	UNP P35270
F	-21	HIS	-	EXPRESSION TAG	UNP P35270

*Continued on next page...*

*Continued from previous page...*

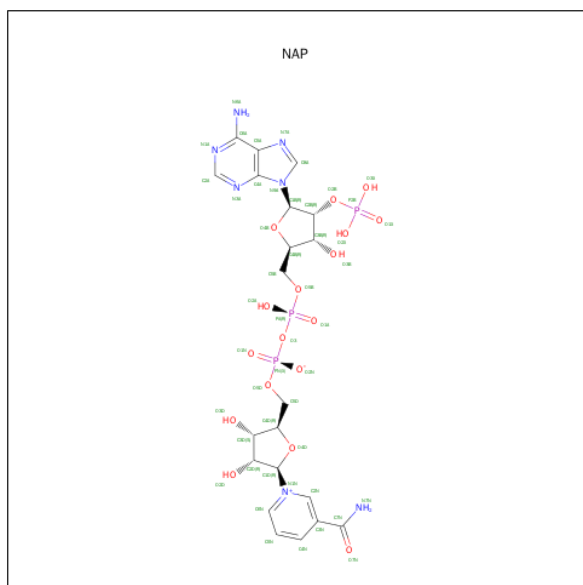
Chain	Residue	Modelled	Actual	Comment	Reference
F	-20	HIS	-	EXPRESSION TAG	UNP P35270
F	-19	LEU	-	EXPRESSION TAG	UNP P35270
F	-18	GLU	-	EXPRESSION TAG	UNP P35270
F	-17	SER	-	EXPRESSION TAG	UNP P35270
F	-16	THR	-	EXPRESSION TAG	UNP P35270
F	-15	SER	-	EXPRESSION TAG	UNP P35270
F	-14	LEU	-	EXPRESSION TAG	UNP P35270
F	-13	TYR	-	EXPRESSION TAG	UNP P35270
F	-12	LYS	-	EXPRESSION TAG	UNP P35270
F	-11	LYS	-	EXPRESSION TAG	UNP P35270
F	-10	ALA	-	EXPRESSION TAG	UNP P35270
F	-9	GLY	-	EXPRESSION TAG	UNP P35270
F	-8	LEU	-	EXPRESSION TAG	UNP P35270
F	-7	GLU	-	EXPRESSION TAG	UNP P35270
F	-6	GLY	-	EXPRESSION TAG	UNP P35270
F	-5	VAL	-	EXPRESSION TAG	UNP P35270
F	-4	ARG	-	EXPRESSION TAG	UNP P35270
F	-3	THR	-	EXPRESSION TAG	UNP P35270
J	-29	MET	-	EXPRESSION TAG	UNP P35270
J	-28	SER	-	EXPRESSION TAG	UNP P35270
J	-27	TYR	-	EXPRESSION TAG	UNP P35270
J	-26	TYR	-	EXPRESSION TAG	UNP P35270
J	-25	HIS	-	EXPRESSION TAG	UNP P35270
J	-24	HIS	-	EXPRESSION TAG	UNP P35270
J	-23	HIS	-	EXPRESSION TAG	UNP P35270
J	-22	HIS	-	EXPRESSION TAG	UNP P35270
J	-21	HIS	-	EXPRESSION TAG	UNP P35270
J	-20	HIS	-	EXPRESSION TAG	UNP P35270
J	-19	LEU	-	EXPRESSION TAG	UNP P35270
J	-18	GLU	-	EXPRESSION TAG	UNP P35270
J	-17	SER	-	EXPRESSION TAG	UNP P35270
J	-16	THR	-	EXPRESSION TAG	UNP P35270
J	-15	SER	-	EXPRESSION TAG	UNP P35270
J	-14	LEU	-	EXPRESSION TAG	UNP P35270
J	-13	TYR	-	EXPRESSION TAG	UNP P35270
J	-12	LYS	-	EXPRESSION TAG	UNP P35270
J	-11	LYS	-	EXPRESSION TAG	UNP P35270
J	-10	ALA	-	EXPRESSION TAG	UNP P35270
J	-9	GLY	-	EXPRESSION TAG	UNP P35270
J	-8	LEU	-	EXPRESSION TAG	UNP P35270
J	-7	GLU	-	EXPRESSION TAG	UNP P35270
J	-6	GLY	-	EXPRESSION TAG	UNP P35270

*Continued on next page...*

Continued from previous page...

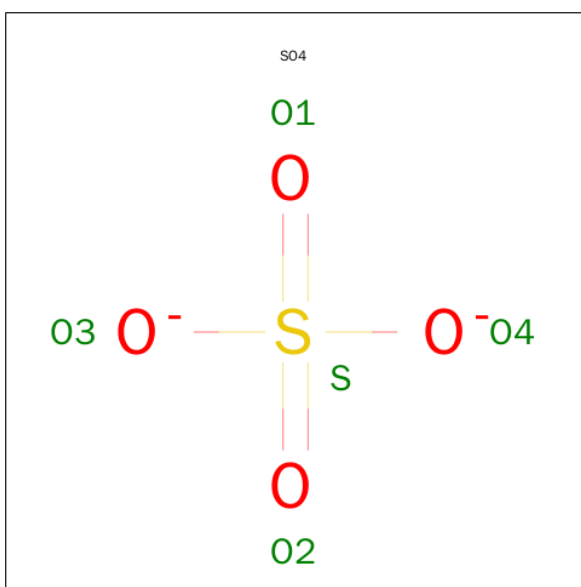
Chain	Residue	Modelled	Actual	Comment	Reference
J	-5	VAL	-	EXPRESSION TAG	UNP P35270
J	-4	ARG	-	EXPRESSION TAG	UNP P35270
J	-3	THR	-	EXPRESSION TAG	UNP P35270

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

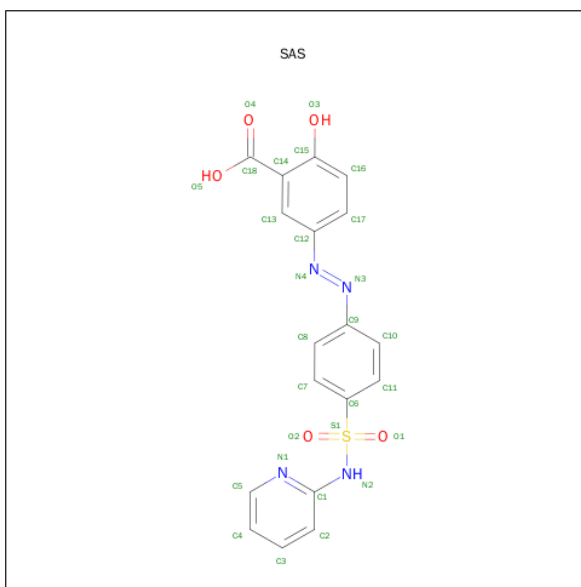
- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		

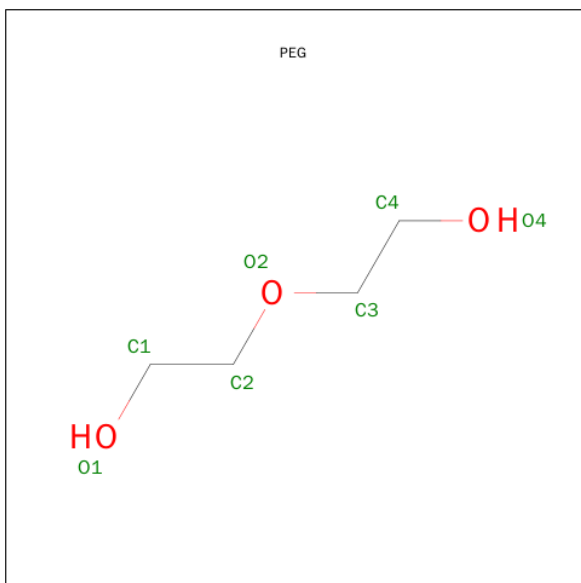
- Molecule 4 is 2-HYDROXY-(5-([4-(2-PYRIDINYLAMINO)SULFONYL]PHENYL)AZO)B ENZOIC ACID (three-letter code: SAS) (formula: C<sub>18</sub>H<sub>14</sub>N<sub>4</sub>O<sub>5</sub>S).





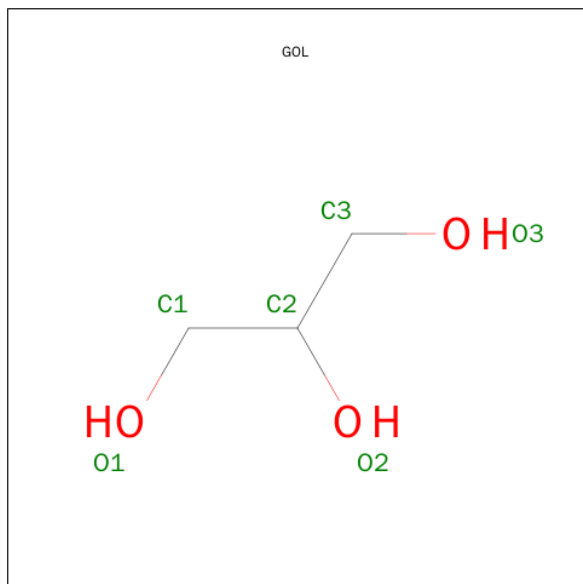
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
4	B	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
4	F	1	Total	C	N	O	S	0	0
			28	18	4	5	1		
4	J	1	Total	C	N	O	S	0	0
			28	18	4	5	1		

- Molecule 5 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
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	J	1	Total C O 7 4 3	0	0
5	J	1	Total C O 7 4 3	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 6 3 3	0	0
6	J	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	33	Total O 33 33	0	0
7	B	31	Total O 31 31	0	0

*Continued on next page...*

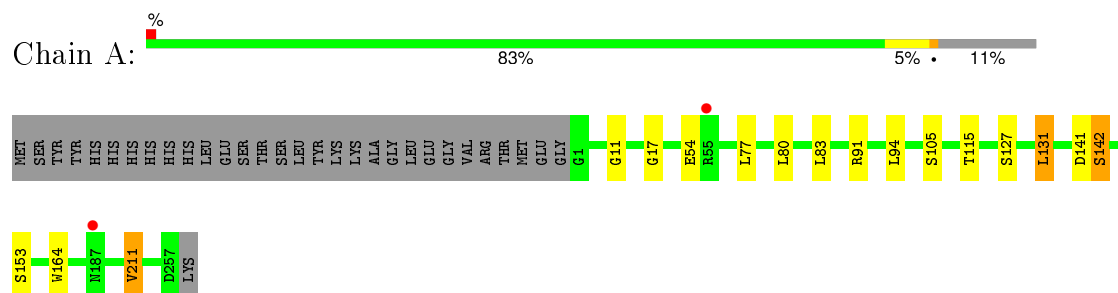
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	25	Total	O	0	0
			25	25		
7	J	15	Total	O	0	0
			15	15		

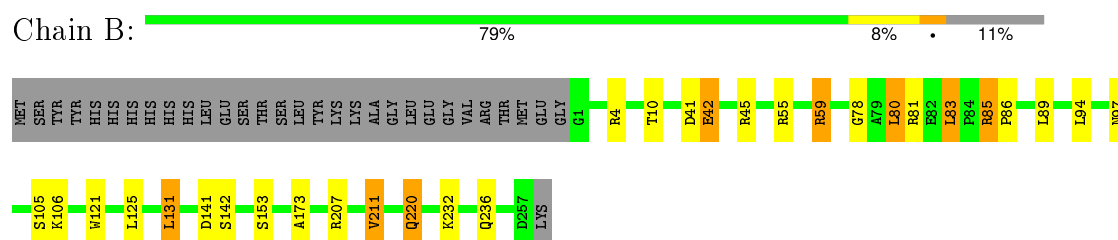
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

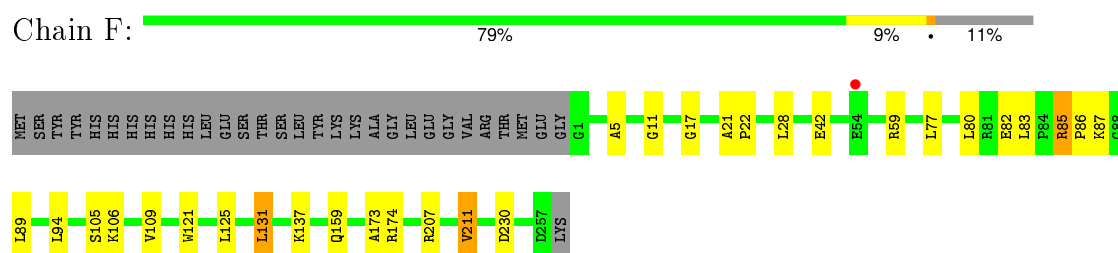
- Molecule 1: Sepiapterin reductase



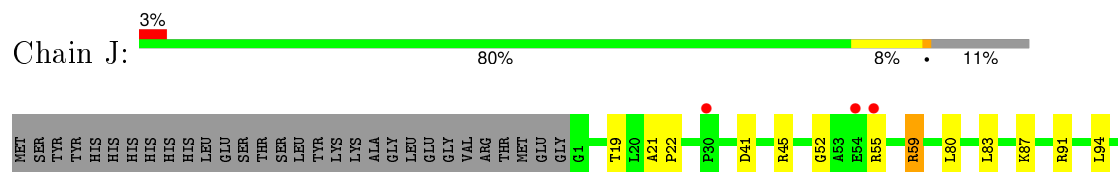
- Molecule 1: Sepiapterin reductase

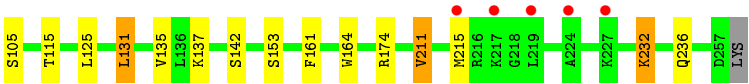


- Molecule 1: Sepiapterin reductase



- Molecule 1: Sepiapterin reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.19Å 149.19Å 180.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.84 – 2.60 48.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.84-2.60) 99.3 (48.84-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.218 , 0.242 0.217 , 0.240	Depositor DCC
$R_{free}$ test set	3514 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.1	EDS
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 69086 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8267	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: SAS, GOL, NAP, PEG, 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	0.42	1/1963 (0.1%)	0.60	0/2656
1	B	0.42	1/1974 (0.1%)	0.60	0/2670
1	F	0.45	3/1963 (0.2%)	0.59	0/2656
1	J	0.42	1/1963 (0.1%)	0.56	0/2656
All	All	0.42	6/7863 (0.1%)	0.59	0/10638

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	82	GLU	CD-OE1	5.54	1.31	1.25
1	F	121	TRP	CD2-CE2	5.27	1.47	1.41
1	J	164	TRP	CD2-CE2	5.13	1.47	1.41
1	B	121	TRP	CD2-CE2	5.12	1.47	1.41
1	F	82	GLU	CD-OE2	5.09	1.31	1.25
1	A	164	TRP	CD2-CE2	5.08	1.47	1.41

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	1936	0	2003	8	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1947	0	2015	17	0
1	F	1936	0	2003	17	0
1	J	1936	0	2003	15	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	F	48	0	25	0	0
2	J	48	0	25	1	0
3	A	20	0	0	0	0
3	B	15	0	0	0	0
3	F	10	0	0	0	0
3	J	5	0	0	0	0
4	A	28	0	12	0	0
4	B	28	0	12	0	0
4	F	28	0	12	0	0
4	J	28	0	12	0	0
5	A	7	0	10	0	0
5	B	7	0	10	0	0
5	F	14	0	20	0	0
5	J	14	0	20	1	0
6	F	6	0	8	0	0
6	J	6	0	8	0	0
7	A	33	0	0	1	0
7	B	31	0	0	0	0
7	F	25	0	0	2	0
7	J	15	0	0	0	0
All	All	8267	0	8248	57	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 (57) 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:J:59:ARG:HG2	1:J:59:ARG:HH11	1.19	1.03
1:F:85:ARG:HH11	1:F:85:ARG:HG2	1.28	0.96
1:A:91:ARG:HD2	7:A:901:HOH:O	1.72	0.89
1:B:105:SER:O	1:B:211:VAL:HG13	1.79	0.82
1:B:59[A]:ARG:HG2	1:B:59[A]:ARG:HH21	1.47	0.80
1:J:59:ARG:HG2	1:J:59:ARG:NH1	1.93	0.74
1:F:85:ARG:HG2	1:F:85:ARG:NH1	2.01	0.68
1:B:59[A]:ARG:HG2	1:B:59[A]:ARG:NH2	2.08	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:105:SER:O	1:J:211:VAL:HG13	2.00	0.62
1:B:42:GLU:HG3	1:B:42:GLU:O	1.96	0.61
1:A:105:SER:O	1:A:211:VAL:HG13	2.06	0.56
1:J:21:ALA:HB3	1:J:22:PRO:HD3	1.88	0.56
1:B:86:PRO:HG2	1:B:89:LEU:HD13	1.91	0.53
1:J:232:LYS:O	1:J:236:GLN:HG3	2.09	0.52
1:F:21:ALA:HB3	1:F:22:PRO:HD3	1.90	0.52
1:A:94:LEU:HD11	1:A:131:LEU:HD13	1.90	0.52
1:B:59[A]:ARG:HH21	1:B:59[A]:ARG:CG	2.21	0.51
1:F:77:LEU:O	1:F:80:LEU:HB2	2.11	0.51
1:F:94:LEU:HD11	1:F:131:LEU:CD1	2.41	0.50
1:B:153:SER:O	2:B:801:NAP:H6N	2.12	0.50
1:F:105:SER:O	1:F:211:VAL:HG13	2.12	0.49
1:A:11:GLY:O	1:A:17:GLY:HA3	2.13	0.49
1:J:19:THR:HG21	1:J:232:LYS:HE2	1.94	0.48
1:J:161:PHE:HB3	1:J:215:MET:HE1	1.95	0.48
1:F:159:GLN:NE2	7:F:923:HOH:O	2.46	0.48
1:B:207:ARG:HG2	1:B:220:GLN:HE21	1.79	0.48
1:F:125:LEU:HD21	1:F:173:ALA:HB3	1.96	0.47
1:J:125:LEU:HD23	1:J:174:ARG:HG3	1.96	0.47
1:B:94:LEU:HD11	1:B:131:LEU:CD1	2.44	0.47
1:A:127:SER:O	1:A:131:LEU:HB2	2.15	0.47
1:J:153:SER:O	2:J:801:NAP:H6N	2.15	0.47
1:F:42:GLU:O	1:F:42:GLU:HG2	2.14	0.46
1:A:153:SER:O	2:A:801:NAP:H6N	2.16	0.46
1:A:77:LEU:O	1:A:80:LEU:HB2	2.15	0.46
1:J:52:GLY:HA3	1:J:55:ARG:HH11	1.81	0.45
1:J:80:LEU:HD11	1:J:135:VAL:HG22	1.98	0.45
1:F:86:PRO:HG2	1:F:89:LEU:HD13	1.99	0.44
5:J:805:PEG:H11	5:J:806:PEG:H42	1.98	0.44
1:F:5:ALA:HB3	1:F:28:LEU:HD22	2.00	0.44
1:J:94:LEU:HD11	1:J:131:LEU:CD1	2.48	0.44
1:F:109:VAL:HG12	1:J:137:LYS:HD2	1.98	0.44
1:B:125:LEU:HD21	1:B:173:ALA:HB3	2.00	0.44
1:F:85:ARG:NH1	1:F:85:ARG:CG	2.77	0.44
1:B:141:ASP:OD1	1:B:142:SER:N	2.51	0.43
1:F:106:LYS:HB2	1:F:106:LYS:HE3	1.89	0.43
1:J:59:ARG:HD3	1:J:59:ARG:N	2.34	0.42
1:F:125:LEU:HD23	1:F:174:ARG:HG3	2.02	0.42
1:J:41:ASP:O	1:J:45:ARG:HG3	2.19	0.42
1:B:85:ARG:HA	1:B:86:PRO:HD2	1.87	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:ARG:HD3	7:F:908:HOH:O	2.20	0.41
1:B:80:LEU:HD23	1:B:83:LEU:HD22	2.02	0.41
1:B:10:THR:O	1:B:97:ASN:HB3	2.20	0.41
1:B:78:GLY:HA2	1:B:81:ARG:NH1	2.35	0.41
1:B:232:LYS:O	1:B:236:GLN:HG2	2.21	0.41
1:F:11:GLY:O	1:F:17:GLY:HA3	2.20	0.41
1:B:41:ASP:O	1:B:45:ARG:HG3	2.21	0.40
1:A:141:ASP:OD1	1:A:142:SER:N	2.54	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	255/288 (88%)	253 (99%)	2 (1%)	0	100	100
1	B	256/288 (89%)	253 (99%)	3 (1%)	0	100	100
1	F	255/288 (88%)	252 (99%)	3 (1%)	0	100	100
1	J	255/288 (88%)	252 (99%)	3 (1%)	0	100	100
All	All	1021/1152 (89%)	1010 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	209/236 (89%)	203 (97%)	6 (3%)	50	77
1	B	210/236 (89%)	198 (94%)	12 (6%)	25	49
1	F	209/236 (89%)	201 (96%)	8 (4%)	40	68
1	J	209/236 (89%)	200 (96%)	9 (4%)	35	64
All	All	837/944 (89%)	802 (96%)	35 (4%)	37	65

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	83	LEU
1	A	115	THR
1	A	131	LEU
1	A	142	SER
1	A	211	VAL
1	B	4	ARG
1	B	42	GLU
1	B	55	ARG
1	B	59[A]	ARG
1	B	59[B]	ARG
1	B	80	LEU
1	B	83	LEU
1	B	85	ARG
1	B	106	LYS
1	B	131	LEU
1	B	211	VAL
1	B	220	GLN
1	F	59	ARG
1	F	83	LEU
1	F	85	ARG
1	F	87	LYS
1	F	131	LEU
1	F	137	LYS
1	F	211	VAL
1	F	230	ASP
1	J	59	ARG
1	J	83	LEU
1	J	87	LYS
1	J	91	ARG
1	J	115	THR
1	J	131	LEU
1	J	142	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	211	VAL
1	J	232	LYS

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	46	GLN
1	B	46	GLN
1	B	204	GLN
1	B	220	GLN
1	F	159	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

26 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	NAP	A	801	-	42,52,52	1.40	5 (11%)	54,80,80	1.72	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	802	-	4,4,4	0.32	0	6,6,6	0.12	0
3	SO4	A	803	-	4,4,4	0.38	0	6,6,6	0.13	0
3	SO4	A	804	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	A	805	-	4,4,4	0.39	0	6,6,6	0.21	0
4	SAS	A	806	-	27,30,30	1.40	3 (11%)	38,42,42	1.96	7 (18%)
5	PEG	A	807	-	6,6,6	0.44	0	5,5,5	0.33	0
2	NAP	B	801	-	42,52,52	1.54	6 (14%)	54,80,80	1.72	7 (12%)
3	SO4	B	802	-	4,4,4	0.37	0	6,6,6	0.10	0
3	SO4	B	803	-	4,4,4	0.40	0	6,6,6	0.16	0
4	SAS	B	804	-	27,30,30	1.47	3 (11%)	38,42,42	1.95	7 (18%)
3	SO4	B	805	-	4,4,4	0.38	0	6,6,6	0.06	0
5	PEG	B	806	-	6,6,6	0.52	0	5,5,5	0.18	0
2	NAP	F	801	-	42,52,52	1.54	5 (11%)	54,80,80	1.68	4 (7%)
3	SO4	F	802	-	4,4,4	0.37	0	6,6,6	0.12	0
3	SO4	F	803	-	4,4,4	0.41	0	6,6,6	0.10	0
6	GOL	F	804	-	5,5,5	0.42	0	5,5,5	0.40	0
4	SAS	F	805	-	27,30,30	1.40	3 (11%)	38,42,42	1.92	6 (15%)
5	PEG	F	806	-	6,6,6	0.56	0	5,5,5	0.19	0
5	PEG	F	807	-	6,6,6	0.51	0	5,5,5	0.29	0
2	NAP	J	801	-	42,52,52	1.41	5 (11%)	54,80,80	1.67	5 (9%)
3	SO4	J	802	-	4,4,4	0.39	0	6,6,6	0.13	0
6	GOL	J	803	-	5,5,5	0.38	0	5,5,5	0.34	0
4	SAS	J	804	-	27,30,30	1.41	3 (11%)	38,42,42	1.99	7 (18%)
5	PEG	J	805	-	6,6,6	0.96	0	5,5,5	0.58	0
5	PEG	J	806	-	6,6,6	0.54	0	5,5,5	0.28	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	NAP	A	801	-	-	0/27/67/67	0/5/5/5
3	SO4	A	802	-	-	0/0/0/0	0/0/0/0
3	SO4	A	803	-	-	0/0/0/0	0/0/0/0
3	SO4	A	804	-	-	0/0/0/0	0/0/0/0
3	SO4	A	805	-	-	0/0/0/0	0/0/0/0
4	SAS	A	806	-	-	0/16/20/20	0/3/3/3
5	PEG	A	807	-	-	0/4/4/4	0/0/0/0
2	NAP	B	801	-	-	0/27/67/67	0/5/5/5
3	SO4	B	802	-	-	0/0/0/0	0/0/0/0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	803	-	-	0/0/0/0	0/0/0/0
4	SAS	B	804	-	-	0/16/20/20	0/3/3/3
3	SO4	B	805	-	-	0/0/0/0	0/0/0/0
5	PEG	B	806	-	-	0/4/4/4	0/0/0/0
2	NAP	F	801	-	-	0/27/67/67	0/5/5/5
3	SO4	F	802	-	-	0/0/0/0	0/0/0/0
3	SO4	F	803	-	-	0/0/0/0	0/0/0/0
6	GOL	F	804	-	-	0/4/4/4	0/0/0/0
4	SAS	F	805	-	-	0/16/20/20	0/3/3/3
5	PEG	F	806	-	-	0/4/4/4	0/0/0/0
5	PEG	F	807	-	-	0/4/4/4	0/0/0/0
2	NAP	J	801	-	-	0/27/67/67	0/5/5/5
3	SO4	J	802	-	-	0/0/0/0	0/0/0/0
6	GOL	J	803	-	-	0/4/4/4	0/0/0/0
4	SAS	J	804	-	-	0/16/20/20	0/3/3/3
5	PEG	J	805	-	-	0/4/4/4	0/0/0/0
5	PEG	J	806	-	-	0/4/4/4	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	805	SAS	C12-N4	-2.63	1.33	1.44
4	B	804	SAS	C12-N4	-2.62	1.33	1.44
4	F	805	SAS	C9-N3	-2.54	1.33	1.44
4	J	804	SAS	C12-N4	-2.54	1.33	1.44
4	B	804	SAS	C9-N3	-2.49	1.34	1.44
4	J	804	SAS	C9-N3	-2.48	1.34	1.44
4	A	806	SAS	C12-N4	-2.47	1.34	1.44
4	A	806	SAS	C9-N3	-2.33	1.34	1.44
2	A	801	NAP	P2B-O2X	2.00	1.61	1.54
2	J	801	NAP	C6N-N1N	2.01	1.40	1.35
2	J	801	NAP	C3N-C7N	2.07	1.53	1.50
2	F	801	NAP	P2B-O2X	2.08	1.62	1.54
2	B	801	NAP	C6N-N1N	2.10	1.41	1.35
2	B	801	NAP	C3N-C7N	2.14	1.53	1.50
2	B	801	NAP	O4B-C1B	2.15	1.43	1.41
2	F	801	NAP	O4B-C1B	2.29	1.44	1.41
2	A	801	NAP	O4B-C1B	2.57	1.44	1.41
2	A	801	NAP	P2B-O1X	3.03	1.61	1.51
2	J	801	NAP	O4D-C1D	3.04	1.45	1.41
2	F	801	NAP	P2B-O1X	3.16	1.61	1.51
2	J	801	NAP	P2B-O1X	3.17	1.61	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAP	O4D-C1D	3.19	1.45	1.41
2	B	801	NAP	P2B-O1X	3.25	1.61	1.51
2	B	801	NAP	O4D-C1D	4.59	1.47	1.41
2	F	801	NAP	O4D-C1D	4.77	1.47	1.41
2	A	801	NAP	O7N-C7N	5.25	1.35	1.24
2	J	801	NAP	O7N-C7N	5.54	1.36	1.24
2	F	801	NAP	O7N-C7N	5.55	1.36	1.24
2	B	801	NAP	O7N-C7N	5.62	1.36	1.24
4	F	805	SAS	O1-S1	5.67	1.49	1.43
4	A	806	SAS	O1-S1	5.68	1.49	1.43
4	J	804	SAS	O1-S1	5.78	1.49	1.43
4	B	804	SAS	O1-S1	5.83	1.49	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	NAP	N3A-C2A-N1A	-9.75	121.43	128.89
2	F	801	NAP	N3A-C2A-N1A	-9.60	121.54	128.89
2	A	801	NAP	N3A-C2A-N1A	-9.48	121.63	128.89
2	J	801	NAP	N3A-C2A-N1A	-9.15	121.89	128.89
4	J	804	SAS	O2-S1-O1	-8.67	108.03	119.54
4	B	804	SAS	O2-S1-O1	-8.66	108.05	119.54
4	A	806	SAS	O2-S1-O1	-8.40	108.40	119.54
4	F	805	SAS	O2-S1-O1	-7.61	109.44	119.54
2	J	801	NAP	PN-O3-PA	-3.80	122.07	132.73
2	A	801	NAP	PN-O3-PA	-2.99	124.33	132.73
2	F	801	NAP	PN-O3-PA	-2.93	124.51	132.73
2	A	801	NAP	C4D-O4D-C1D	-2.65	106.80	109.72
2	B	801	NAP	PN-O3-PA	-2.55	125.57	132.73
2	J	801	NAP	O4D-C1D-N1N	-2.50	105.39	108.13
2	B	801	NAP	C5B-C4B-C3B	-2.48	105.38	115.21
2	F	801	NAP	O3-PN-O5D	-2.46	96.41	102.94
2	A	801	NAP	C5B-C4B-C3B	-2.35	105.89	115.21
2	A	801	NAP	O4D-C1D-N1N	-2.34	105.56	108.13
4	J	804	SAS	C2-C1-N1	-2.24	118.84	122.49
4	F	805	SAS	C15-C14-C18	-2.22	119.33	121.60
2	J	801	NAP	C4A-C5A-N7A	-2.20	107.45	109.48
2	B	801	NAP	O3-PN-O5D	-2.11	97.33	102.94
2	A	801	NAP	O3-PN-O5D	-2.07	97.45	102.94
4	B	804	SAS	C15-C14-C18	-2.05	119.50	121.60
2	J	801	NAP	C5B-C4B-C3B	-2.03	107.14	115.21
2	B	801	NAP	C4A-C5A-N7A	-2.03	107.62	109.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	SAS	C12-N4-N3	2.02	123.05	113.28
2	B	801	NAP	O7N-C7N-C3N	2.07	121.85	119.59
4	J	804	SAS	C12-N4-N3	2.15	123.66	113.28
4	J	804	SAS	O2-S1-N2	2.16	112.16	106.69
2	F	801	NAP	O4B-C1B-N9A	2.24	112.78	108.10
4	F	805	SAS	C6-S1-N2	2.36	109.91	106.87
4	J	804	SAS	C6-S1-N2	2.42	109.98	106.87
4	A	806	SAS	C13-C14-C15	2.42	120.64	117.49
4	A	806	SAS	C12-N4-N3	2.46	125.17	113.28
4	B	804	SAS	C13-C14-C15	2.48	120.71	117.49
4	F	805	SAS	C13-C14-C15	2.59	120.86	117.49
4	A	806	SAS	C6-S1-N2	2.64	110.27	106.87
2	B	801	NAP	O4B-C1B-N9A	2.66	113.66	108.10
4	B	804	SAS	C5-N1-C1	2.91	121.29	117.28
4	A	806	SAS	O1-S1-C6	2.96	111.71	107.96
4	B	804	SAS	C6-S1-N2	3.03	110.77	106.87
4	A	806	SAS	C5-N1-C1	3.42	121.99	117.28
4	F	805	SAS	C5-N1-C1	3.68	122.36	117.28
4	B	804	SAS	N2-C1-N1	3.71	118.08	114.27
4	A	806	SAS	N2-C1-N1	3.89	118.26	114.27
4	J	804	SAS	C5-N1-C1	4.09	122.91	117.28
4	F	805	SAS	N2-C1-N1	4.36	118.74	114.27
4	J	804	SAS	N2-C1-N1	4.54	118.92	114.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAP	1	0
2	B	801	NAP	1	0
2	J	801	NAP	1	0
5	J	805	PEG	1	0
5	J	806	PEG	1	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 ⓘ

### 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	257/288 (89%)	-0.34	2 (0%) 87 85	22, 36, 54, 85	0
1	B	257/288 (89%)	-0.31	0 100 100	23, 39, 62, 76	0
1	F	257/288 (89%)	-0.23	1 (0%) 93 91	27, 39, 65, 107	0
1	J	257/288 (89%)	0.06	8 (3%) 52 45	30, 48, 85, 104	0
All	All	1028/1152 (89%)	-0.20	11 (1%) 82 79	22, 40, 68, 107	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	55	ARG	3.7
1	F	54	GLU	3.6
1	J	224	ALA	3.0
1	J	227	LYS	2.9
1	J	54	GLU	2.8
1	J	215	MET	2.4
1	J	219	LEU	2.3
1	J	30	PRO	2.2
1	A	187	ASN	2.2
1	A	55	ARG	2.2
1	J	217	LYS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [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
5	PEG	B	806	7/7	0.75	0.21	3.39	68,75,80,81	0
4	SAS	F	805	28/28	0.97	0.16	1.07	26,40,53,55	0
6	GOL	F	804	6/6	0.80	0.23	1.00	47,50,51,55	0
4	SAS	A	806	28/28	0.97	0.15	0.85	26,37,49,49	0
4	SAS	B	804	28/28	0.97	0.17	0.85	33,43,61,62	0
3	SO4	A	804	5/5	0.89	0.24	0.39	85,86,88,88	0
4	SAS	J	804	28/28	0.93	0.22	0.18	45,65,88,88	0
2	NAP	A	801	48/48	0.99	0.14	0.11	24,29,32,33	0
3	SO4	A	805	5/5	0.93	0.17	-0.01	69,70,72,77	0
2	NAP	B	801	48/48	0.98	0.14	-0.03	27,30,35,37	0
2	NAP	F	801	48/48	0.98	0.15	-0.17	25,31,35,36	0
2	NAP	J	801	48/48	0.97	0.14	-0.60	42,47,52,54	0
3	SO4	B	803	5/5	0.93	0.17	-	78,79,83,84	0
5	PEG	F	806	7/7	0.66	0.35	-	67,73,78,79	0
3	SO4	A	802	5/5	0.98	0.11	-	59,59,60,60	0
3	SO4	F	803	5/5	0.81	0.24	-	95,101,102,104	0
3	SO4	B	805	5/5	0.77	0.31	-	139,141,142,144	0
6	GOL	J	803	6/6	0.93	0.14	-	60,62,63,63	0
3	SO4	F	802	5/5	0.92	0.13	-	68,69,69,73	0
5	PEG	J	805	7/7	0.66	0.27	-	86,90,91,93	0
5	PEG	J	806	7/7	0.47	0.45	-	106,111,115,116	0
5	PEG	F	807	7/7	0.55	0.34	-	86,89,92,93	0
3	SO4	J	802	5/5	0.89	0.20	-	91,92,94,96	0
3	SO4	A	803	5/5	0.89	0.32	-	78,78,81,81	0
5	PEG	A	807	7/7	0.76	0.22	-	75,77,77,78	0
3	SO4	B	802	5/5	0.96	0.10	-	73,74,76,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.