



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:50 AM GMT

PDB ID : 4HWK  
Title : Crystal structure of human sepiapterin reductase in complex with sulfapyridine  
Authors : Groenlund Pedersen, M.; Pojer, F.; Johnsson, K.  
Deposited on : 2012-11-08  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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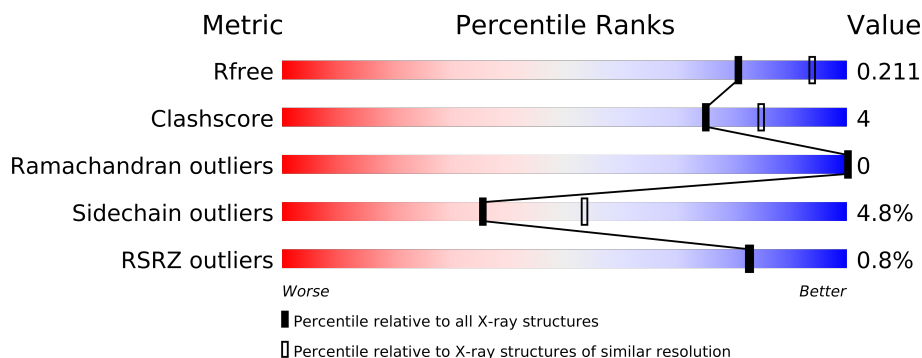
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	288	
1	B	288	
1	C	288	
1	D	288	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	802	-	X
3	SO4	B	802	-	X
3	SO4	B	804	-	X
3	SO4	B	805	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	D	802	-	X
4	GOL	A	804	-	X
4	GOL	A	806	-	X
4	GOL	A	809	-	X
4	GOL	B	803	-	X
4	GOL	B	807	-	X
6	PEG	A	810	-	X
6	PEG	C	805	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8479 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1223	344	365	10			
1	B	257	Total	C	N	O	S	0	1	0
			1945	1225	345	366	9			
1	C	257	Total	C	N	O	S	0	1	0
			1942	1223	344	365	10			
1	D	257	Total	C	N	O	S	0	2	0
			1951	1228	346	367	10			

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

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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
C	-29	MET	-	EXPRESSION TAG	UNP P35270
C	-28	SER	-	EXPRESSION TAG	UNP P35270
C	-27	TYR	-	EXPRESSION TAG	UNP P35270
C	-26	TYR	-	EXPRESSION TAG	UNP P35270
C	-25	HIS	-	EXPRESSION TAG	UNP P35270
C	-24	HIS	-	EXPRESSION TAG	UNP P35270
C	-23	HIS	-	EXPRESSION TAG	UNP P35270
C	-22	HIS	-	EXPRESSION TAG	UNP P35270
C	-21	HIS	-	EXPRESSION TAG	UNP P35270

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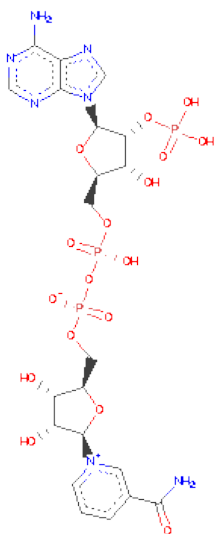
Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	EXPRESSION TAG	UNP P35270
C	-19	LEU	-	EXPRESSION TAG	UNP P35270
C	-18	GLU	-	EXPRESSION TAG	UNP P35270
C	-17	SER	-	EXPRESSION TAG	UNP P35270
C	-16	THR	-	EXPRESSION TAG	UNP P35270
C	-15	SER	-	EXPRESSION TAG	UNP P35270
C	-14	LEU	-	EXPRESSION TAG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

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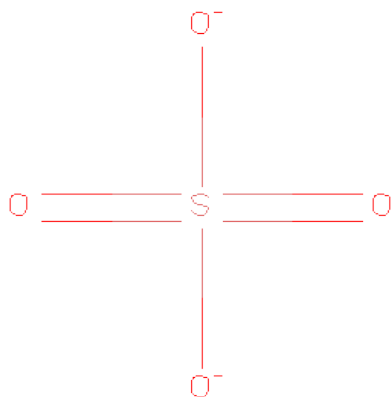
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	VAL	-	EXPRESSION TAG	UNP P35270
D	-4	ARG	-	EXPRESSION TAG	UNP P35270
D	-3	THR	-	EXPRESSION TAG	UNP P35270

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (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	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		

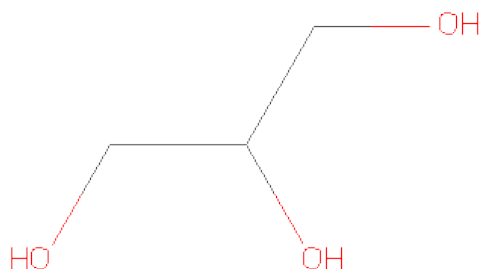
- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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	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	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

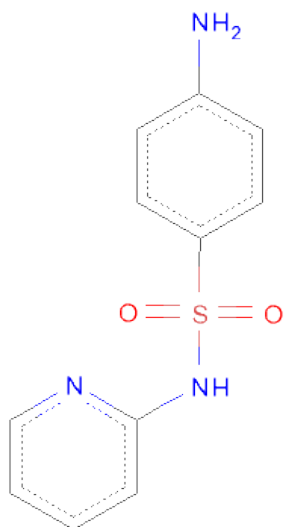
- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





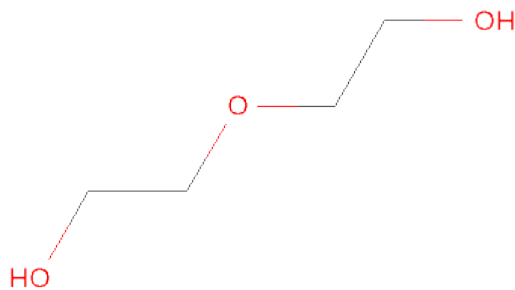
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 4-AMINO-N-(PYRIDIN-2-YL)BENZENESULFONAMIDE (three-letter code: SFY) (formula:  $C_{11}H_{11}N_3O_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			17	11	3	2	1		
5	B	1	Total	C	N	O	S	0	0
			17	11	3	2	1		
5	C	1	Total	C	N	O	S	0	0
			17	11	3	2	1		
5	D	1	Total	C	N	O	S	0	0
			17	11	3	2	1		

- Molecule 6 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
6	A	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

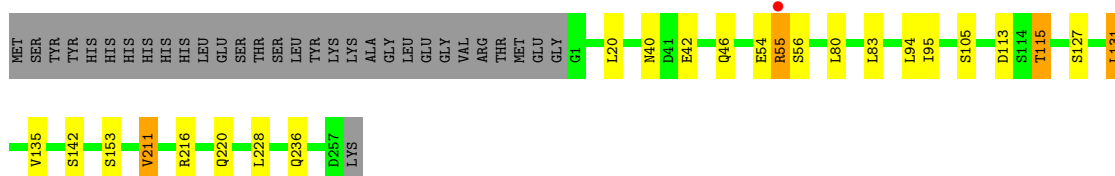
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	104	Total	O	0	0
			104	104		
7	B	101	Total	O	0	0
			101	101		
7	C	85	Total	O	0	0
			85	85		
7	D	48	Total	O	0	0
			48	48		

### 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.

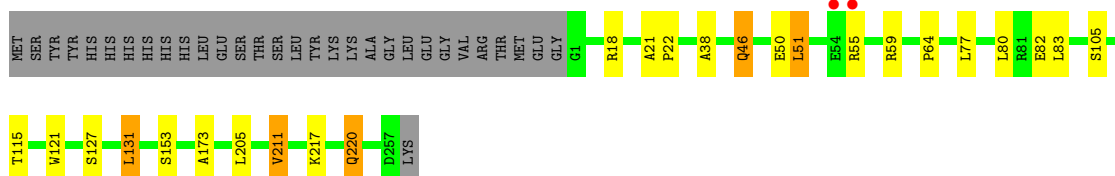
- Molecule 1: Sepiapterin reductase

Chain A:



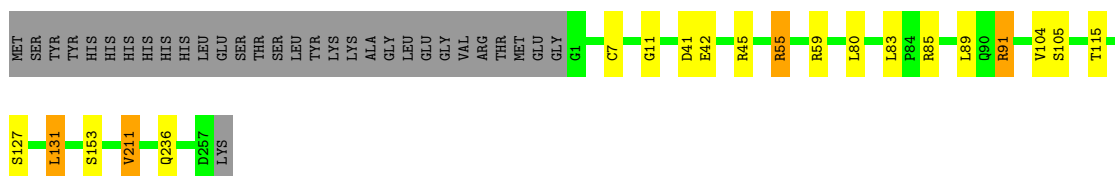
- Molecule 1: Sepiapterin reductase

Chain B:



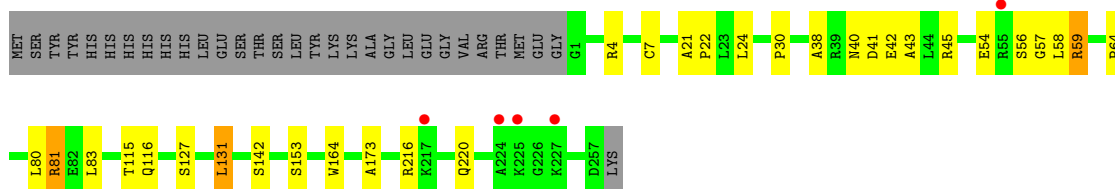
- Molecule 1: Sepiapterin reductase

Chain C:



- Molecule 1: Sepiapterin reductase

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.45Å 148.45Å 179.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.91 – 2.40 46.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.91-2.40) 99.7 (46.91-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.194 , 0.211 0.194 , 0.211	Depositor DCC
$R_{free}$ test set	4377 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 19.8	EDS
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 87279 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8479	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAP, PEG, SO4, SFY

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	0.39	0/1969	0.53	0/2664
1	B	0.39	1/1972 (0.1%)	0.54	0/2668
1	C	0.39	0/1969	0.55	0/2664
1	D	0.40	1/1978 (0.1%)	0.55	0/2676
All	All	0.39	2/7888 (0.0%)	0.54	0/10672

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	164	TRP	CD2-CE2	5.14	1.47	1.41
1	B	121	TRP	CD2-CE2	5.13	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1942	0	2007	19	0
1	B	1945	0	2010	17	0
1	C	1942	0	2007	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1951	0	2014	24	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	2	0
2	D	48	0	25	1	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	24	0	32	1	0
4	B	12	0	16	1	0
4	C	6	0	8	0	0
5	A	17	0	11	0	0
5	B	17	0	11	1	0
5	C	17	0	11	0	0
5	D	17	0	11	0	0
6	A	7	0	10	0	0
6	C	7	0	10	0	0
7	A	104	0	0	2	0
7	B	101	0	0	1	0
7	C	85	0	0	1	0
7	D	48	0	0	0	0
All	All	8479	0	8258	66	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (66) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:216:ARG:O	1:A:220:GLN:HG3	1.66	0.94
1:D:216:ARG:O	1:D:220:GLN:HG3	1.76	0.85
1:C:91:ARG:HH11	1:C:91:ARG:HG2	1.44	0.82
1:D:30:PRO:HA	1:D:57:GLY:HA3	1.66	0.76
1:A:46:GLN:HE21	1:B:59:ARG:HH11	1.35	0.74
1:D:81:ARG:NH1	1:D:81:ARG:HG3	2.03	0.73
1:D:40:ASN:ND2	1:D:43:ALA:CB	2.54	0.70
1:D:81:ARG:HH11	1:D:81:ARG:HG3	1.57	0.69
1:B:220:GLN:NE2	7:B:973:HOH:O	2.25	0.68
1:A:115:THR:HG22	7:A:966:HOH:O	1.93	0.68
1:A:54:GLU:HG3	1:B:55:ARG:O	1.94	0.67
5:B:806:SFY:H4	4:B:807:GOL:H12	1.60	0.65
1:D:40:ASN:ND2	1:D:43:ALA:HB2	2.13	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:91:ARG:HH11	1:C:91:ARG:CG	2.10	0.63
1:A:228:LEU:HB2	4:A:806:GOL:H11	1.82	0.61
1:C:105:SER:O	1:C:211:VAL:HG13	2.03	0.58
1:A:153:SER:O	2:A:801:NAP:H6N	2.03	0.58
1:C:153:SER:O	2:C:801:NAP:H6N	2.04	0.58
1:D:7[B]:CYS:SG	1:D:24:LEU:HD21	2.45	0.56
1:D:153:SER:O	2:D:801:NAP:H6N	2.06	0.55
1:A:46:GLN:HE21	1:B:59:ARG:NH1	2.03	0.55
1:B:153:SER:O	2:B:801:NAP:H6N	2.07	0.55
1:B:21:ALA:HB3	1:B:22:PRO:HD3	1.88	0.55
1:D:40:ASN:HD21	1:D:43:ALA:HB2	1.72	0.54
1:B:105:SER:O	1:B:211:VAL:HG13	2.08	0.53
1:A:46:GLN:NE2	1:B:59:ARG:HH11	2.05	0.52
1:D:40:ASN:ND2	1:D:43:ALA:HB3	2.24	0.52
1:D:81:ARG:CG	1:D:81:ARG:HH11	2.18	0.50
1:D:40:ASN:HD22	1:D:43:ALA:HB3	1.78	0.48
1:D:56:SER:O	1:D:58:LEU:N	2.44	0.48
1:D:21:ALA:HB3	1:D:22:PRO:HD3	1.94	0.48
1:A:55:ARG:HG2	1:A:56:SER:N	2.28	0.48
1:C:91:ARG:NH1	1:C:91:ARG:CG	2.75	0.48
1:A:113:ASP:OD1	1:A:115:THR:HG23	2.14	0.47
1:A:105:SER:O	1:A:211:VAL:HG13	2.14	0.47
1:A:127:SER:O	1:A:131:LEU:HB2	2.14	0.47
1:D:40:ASN:HD22	1:D:43:ALA:CB	2.27	0.47
1:A:40:ASN:OD1	1:A:42:GLU:HB3	2.15	0.47
1:D:30:PRO:CA	1:D:57:GLY:HA3	2.40	0.46
1:B:50:GLU:O	1:B:50:GLU:CG	2.62	0.46
1:D:30:PRO:HA	1:D:57:GLY:CA	2.40	0.46
1:D:40:ASN:OD1	1:D:42:GLU:HB3	2.15	0.46
1:D:41:ASP:O	1:D:45:ARG:HG3	2.16	0.45
1:C:127:SER:O	1:C:131:LEU:HB2	2.17	0.45
1:A:220:GLN:NE2	7:A:970:HOH:O	2.30	0.45
1:D:40:ASN:ND2	1:D:43:ALA:H	2.14	0.45
1:B:38:ALA:O	1:B:64:PRO:HA	2.18	0.44
1:D:38:ALA:O	1:D:64:PRO:HA	2.18	0.44
1:A:94:LEU:HD11	1:A:131:LEU:HD13	2.00	0.43
1:C:55:ARG:HD3	7:C:960:HOH:O	2.19	0.43
1:D:59:ARG:HB2	1:D:59:ARG:HE	1.45	0.43
1:A:80:LEU:HD21	1:A:135:VAL:HG22	2.00	0.43
1:C:41:ASP:O	1:C:45:ARG:HG3	2.19	0.43
1:B:127:SER:O	1:B:131:LEU:HB2	2.19	0.42
1:B:77:LEU:O	1:B:80:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:127:SER:O	1:D:131:LEU:HB2	2.19	0.42
1:B:51:LEU:HD12	1:B:51:LEU:HA	1.91	0.42
1:B:50:GLU:HG2	1:B:50:GLU:O	2.19	0.42
1:C:104:VAL:O	1:C:211:VAL:HG22	2.19	0.42
1:B:18:ARG:HH22	1:B:46:GLN:HG3	1.86	0.41
1:A:20:LEU:HD21	1:A:95:ILE:HD13	2.02	0.41
1:A:216:ARG:O	1:A:220:GLN:CG	2.54	0.41
1:B:173:ALA:HB2	1:D:173:ALA:HB2	2.03	0.41
1:C:11:GLY:HA2	2:C:801:NAP:H1B	2.02	0.40
1:B:18:ARG:HH22	1:B:46:GLN:CG	2.34	0.40
1:A:55:ARG:HH11	1:A:55:ARG:HD3	1.77	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	256/288 (89%)	252 (98%)	4 (2%)	0	100	100
1	B	256/288 (89%)	252 (98%)	4 (2%)	0	100	100
1	C	256/288 (89%)	251 (98%)	5 (2%)	0	100	100
1	D	257/288 (89%)	253 (98%)	4 (2%)	0	100	100
All	All	1025/1152 (89%)	1008 (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	210/236 (89%)	203 (97%)	7 (3%)	50	71
1	B	210/236 (89%)	200 (95%)	10 (5%)	35	53
1	C	210/236 (89%)	196 (93%)	14 (7%)	23	35
1	D	211/236 (89%)	200 (95%)	11 (5%)	32	49
All	All	841/944 (89%)	799 (95%)	42 (5%)	35	51

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	83	LEU
1	A	115	THR
1	A	131	LEU
1	A	142	SER
1	A	211	VAL
1	A	236	GLN
1	B	46	GLN
1	B	51	LEU
1	B	82	GLU
1	B	83	LEU
1	B	115	THR
1	B	131	LEU
1	B	205	LEU
1	B	211	VAL
1	B	217	LYS
1	B	220	GLN
1	C	7[A]	CYS
1	C	7[B]	CYS
1	C	42	GLU
1	C	55	ARG
1	C	59	ARG
1	C	80	LEU
1	C	83	LEU
1	C	85	ARG
1	C	89	LEU
1	C	91	ARG
1	C	115	THR
1	C	131	LEU
1	C	211	VAL
1	C	236	GLN
1	D	4	ARG
1	D	54	GLU

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Mol	Chain	Res	Type
1	D	59	ARG
1	D	80	LEU
1	D	81	ARG
1	D	83	LEU
1	D	115	THR
1	D	116[A]	GLN
1	D	116[B]	GLN
1	D	131	LEU
1	D	142	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	D	40	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	-	52,52,52	1.33	5 (9%)	80,80,80	1.63	9 (11%)
3	SO4	A	802	-	4,4,4	0.34	0	6,6,6	0.12	0
4	GOL	A	803	-	5,5,5	0.33	0	5,5,5	0.26	0
4	GOL	A	804	-	5,5,5	0.33	0	5,5,5	0.24	0
3	SO4	A	805	-	4,4,4	0.41	0	6,6,6	0.08	0
4	GOL	A	806	-	5,5,5	0.34	0	5,5,5	0.63	0
5	SFY	A	807	-	18,18,18	3.02	4 (22%)	25,25,25	2.05	4 (16%)
3	SO4	A	808	-	4,4,4	0.43	0	6,6,6	0.08	0
4	GOL	A	809	-	5,5,5	0.38	0	5,5,5	0.17	0
6	PEG	A	810	-	6,6,6	0.43	0	5,5,5	0.34	0
2	NAP	B	801	-	52,52,52	1.35	4 (7%)	80,80,80	1.51	8 (10%)
3	SO4	B	802	-	4,4,4	0.35	0	6,6,6	0.10	0
4	GOL	B	803	-	5,5,5	0.39	0	5,5,5	0.30	0
3	SO4	B	804	-	4,4,4	0.44	0	6,6,6	0.12	0
3	SO4	B	805	-	4,4,4	0.40	0	6,6,6	0.08	0
5	SFY	B	806	-	18,18,18	3.05	4 (22%)	25,25,25	2.10	4 (16%)
4	GOL	B	807	-	5,5,5	0.32	0	5,5,5	0.27	0
2	NAP	C	801	-	52,52,52	1.36	5 (9%)	80,80,80	1.62	10 (12%)
3	SO4	C	802	-	4,4,4	0.39	0	6,6,6	0.07	0
4	GOL	C	803	-	5,5,5	0.32	0	5,5,5	0.21	0
5	SFY	C	804	-	18,18,18	3.05	4 (22%)	25,25,25	2.04	4 (16%)
6	PEG	C	805	-	6,6,6	0.45	0	5,5,5	0.27	0
2	NAP	D	801	-	52,52,52	1.37	5 (9%)	80,80,80	1.49	7 (8%)
3	SO4	D	802	-	4,4,4	0.39	0	6,6,6	0.07	0
5	SFY	D	803	-	18,18,18	3.03	4 (22%)	25,25,25	2.16	4 (16%)
3	SO4	D	804	-	4,4,4	0.42	0	6,6,6	0.09	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	-	-	0/35/67/67	0/3/5/5
3	SO4	A	802	-	-	0/0/0/0	0/0/0/0
4	GOL	A	803	-	-	0/4/4/4	0/0/0/0
4	GOL	A	804	-	-	0/4/4/4	0/0/0/0
3	SO4	A	805	-	-	0/0/0/0	0/0/0/0
4	GOL	A	806	-	-	0/4/4/4	0/0/0/0
5	SFY	A	807	-	-	0/11/11/11	0/2/2/2
3	SO4	A	808	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	809	-	-	0/4/4/4	0/0/0/0
6	PEG	A	810	-	-	0/4/4/4	0/0/0/0
2	NAP	B	801	-	-	0/35/67/67	0/3/5/5
3	SO4	B	802	-	-	0/0/0/0	0/0/0/0
4	GOL	B	803	-	-	0/4/4/4	0/0/0/0
3	SO4	B	804	-	-	0/0/0/0	0/0/0/0
3	SO4	B	805	-	-	0/0/0/0	0/0/0/0
5	SFY	B	806	-	-	0/11/11/11	0/2/2/2
4	GOL	B	807	-	-	0/4/4/4	0/0/0/0
2	NAP	C	801	-	-	0/35/67/67	0/3/5/5
3	SO4	C	802	-	-	0/0/0/0	0/0/0/0
4	GOL	C	803	-	-	0/4/4/4	0/0/0/0
5	SFY	C	804	-	-	0/11/11/11	0/2/2/2
6	PEG	C	805	-	-	0/4/4/4	0/0/0/0
2	NAP	D	801	-	-	0/35/67/67	0/3/5/5
3	SO4	D	802	-	-	0/0/0/0	0/0/0/0
5	SFY	D	803	-	-	0/11/11/11	0/2/2/2
3	SO4	D	804	-	-	0/0/0/0	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	804	SFY	CAP-SAQ	-10.55	1.60	1.76
5	B	806	SFY	CAP-SAQ	-10.54	1.60	1.76
5	D	803	SFY	CAP-SAQ	-10.44	1.61	1.76
5	A	807	SFY	CAP-SAQ	-10.39	1.61	1.76
2	D	801	NAP	O7N-C7N	4.97	1.35	1.24
2	B	801	NAP	O7N-C7N	4.95	1.35	1.24
2	A	801	NAP	O7N-C7N	4.94	1.35	1.24
2	C	801	NAP	O7N-C7N	4.91	1.35	1.24
2	D	801	NAP	C2N-N1N	4.83	1.41	1.35
5	C	804	SFY	OAB-SAQ	4.66	1.48	1.43
5	D	803	SFY	OAC-SAQ	4.62	1.48	1.43
5	B	806	SFY	OAB-SAQ	4.60	1.48	1.43
5	A	807	SFY	OAB-SAQ	4.56	1.48	1.43
5	A	807	SFY	OAC-SAQ	4.53	1.48	1.43
2	B	801	NAP	C2N-N1N	4.50	1.41	1.35
2	A	801	NAP	C2N-N1N	4.47	1.41	1.35
5	B	806	SFY	OAC-SAQ	4.47	1.48	1.43
2	C	801	NAP	C2N-N1N	4.36	1.40	1.35
5	D	803	SFY	OAB-SAQ	4.35	1.48	1.43
5	C	804	SFY	OAC-SAQ	4.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	NAP	C4A-N9A	-3.16	1.33	1.37
2	A	801	NAP	C4A-N9A	-3.08	1.33	1.37
2	D	801	NAP	C4A-N9A	-3.03	1.33	1.37
2	B	801	NAP	O4D-C1D	2.96	1.45	1.41
2	C	801	NAP	C4A-N9A	-2.96	1.33	1.37
2	C	801	NAP	O4D-C1D	2.94	1.45	1.41
5	A	807	SFY	CAN-NAA	2.90	1.49	1.38
5	C	804	SFY	CAN-NAA	2.88	1.49	1.38
5	B	806	SFY	CAN-NAA	2.86	1.49	1.38
5	D	803	SFY	CAN-NAA	2.83	1.49	1.38
2	D	801	NAP	O4D-C1D	2.29	1.44	1.41
2	C	801	NAP	O4B-C1B	2.21	1.44	1.41
2	A	801	NAP	O4D-C1D	2.17	1.44	1.41
2	A	801	NAP	O4B-C1B	2.09	1.44	1.41
2	D	801	NAP	P2B-O3X	2.02	1.62	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	NAP	N3A-C2A-N1A	-8.88	121.28	128.71
2	D	801	NAP	N3A-C2A-N1A	-8.51	121.59	128.71
2	A	801	NAP	N3A-C2A-N1A	-8.46	121.64	128.71
2	B	801	NAP	N3A-C2A-N1A	-8.29	121.78	128.71
5	D	803	SFY	OAC-SAQ-OAB	-7.87	108.96	119.55
5	A	807	SFY	OAC-SAQ-OAB	-7.69	109.20	119.55
5	B	806	SFY	OAC-SAQ-OAB	-7.62	109.30	119.55
5	C	804	SFY	OAC-SAQ-OAB	-7.25	109.80	119.55
2	A	801	NAP	O4B-C1B-N9A	5.62	113.66	108.44
2	C	801	NAP	O4B-C1B-N9A	5.36	113.42	108.44
2	C	801	NAP	N3A-C4A-N9A	4.35	133.30	125.43
2	B	801	NAP	N3A-C4A-N9A	4.33	133.25	125.43
2	D	801	NAP	N3A-C4A-N9A	4.29	133.18	125.43
2	A	801	NAP	N3A-C4A-N9A	4.19	132.99	125.43
5	C	804	SFY	NAM-CAO-NAL	4.01	118.37	114.32
5	B	806	SFY	NAM-CAO-NAL	4.00	118.36	114.32
2	B	801	NAP	O4B-C1B-N9A	3.96	112.13	108.44
5	D	803	SFY	NAM-CAO-NAL	3.95	118.31	114.32
5	A	807	SFY	NAM-CAO-NAL	3.91	118.27	114.32
5	D	803	SFY	CAP-SAQ-NAM	3.50	110.96	106.81
5	D	803	SFY	CAF-NAL-CAO	3.24	122.04	117.26
5	C	804	SFY	CAP-SAQ-NAM	3.23	110.64	106.81
5	B	806	SFY	CAF-NAL-CAO	2.99	121.67	117.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	804	SFY	CAF-NAL-CAO	2.98	121.66	117.26
5	B	806	SFY	CAP-SAQ-NAM	2.89	110.23	106.81
2	C	801	NAP	C5A-C4A-N3A	-2.86	119.47	125.70
2	C	801	NAP	O2B-P2B-O1X	2.86	114.78	106.79
2	A	801	NAP	O2B-P2B-O1X	2.84	114.72	106.79
5	A	807	SFY	CAF-NAL-CAO	2.83	121.44	117.26
2	A	801	NAP	C5A-C4A-N3A	-2.82	119.55	125.70
2	D	801	NAP	C5A-C4A-N3A	-2.81	119.58	125.70
2	B	801	NAP	C5A-C4A-N3A	-2.78	119.64	125.70
2	B	801	NAP	O2B-P2B-O1X	2.72	114.39	106.79
2	D	801	NAP	O4D-C1D-N1N	-2.72	105.17	107.95
2	A	801	NAP	O4D-C1D-N1N	-2.66	105.23	107.95
2	A	801	NAP	C4A-C5A-N7A	-2.45	107.42	109.52
2	D	801	NAP	C4A-C5A-N7A	-2.44	107.43	109.52
2	B	801	NAP	PN-O3-PA	-2.42	122.56	132.95
2	C	801	NAP	C2A-N3A-C4A	2.35	120.69	114.01
2	C	801	NAP	C4A-C5A-N7A	-2.35	107.51	109.52
2	D	801	NAP	C2A-N3A-C4A	2.24	120.39	114.01
5	A	807	SFY	CAP-SAQ-NAM	2.22	109.44	106.81
2	D	801	NAP	PN-O3-PA	-2.22	123.43	132.95
2	B	801	NAP	C4A-C5A-N7A	-2.21	107.63	109.52
2	B	801	NAP	C2A-N3A-C4A	2.20	120.27	114.01
2	A	801	NAP	C2A-N3A-C4A	2.19	120.25	114.01
2	C	801	NAP	PN-O3-PA	-2.18	123.58	132.95
2	A	801	NAP	C4D-O4D-C1D	-2.07	107.50	109.75
2	C	801	NAP	O4D-C1D-C2D	-2.01	103.68	106.77
2	C	801	NAP	C2B-C1B-N9A	-2.00	106.14	113.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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%)	-0.54	1 (0%) 90 90	18, 30, 46, 68	0
1	B	257/288 (89%)	-0.50	2 (0%) 83 82	21, 32, 51, 86	0
1	C	257/288 (89%)	-0.45	0 100 100	19, 33, 52, 67	0
1	D	257/288 (89%)	-0.18	5 (1%) 64 61	23, 40, 68, 92	0
All	All	1028/1152 (89%)	-0.42	8 (0%) 83 82	18, 33, 56, 92	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	224	ALA	4.4
1	B	54	GLU	3.1
1	D	217	LYS	2.9
1	D	55	ARG	2.7
1	D	227	LYS	2.7
1	D	225	LYS	2.2
1	A	55	ARG	2.1
1	B	55	ARG	2.0

### 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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	B	807	6/6	0.36	9.25	58,62,62,63	0
4	GOL	A	806	6/6	0.34	9.14	51,53,54,55	0
6	PEG	A	810	7/7	0.24	6.40	61,62,64,64	0
3	SO4	B	802	5/5	0.12	6.11	58,58,60,60	0
4	GOL	A	809	6/6	0.22	5.33	50,51,52,53	0
3	SO4	B	804	5/5	0.21	4.92	73,74,75,76	0
3	SO4	D	802	5/5	0.15	4.41	73,73,73,74	0
6	PEG	C	805	7/7	0.29	3.73	71,73,75,75	0
4	GOL	A	804	6/6	0.17	3.36	51,54,54,55	0
3	SO4	B	805	5/5	0.19	3.04	95,95,97,99	0
3	SO4	A	802	5/5	0.12	2.83	53,54,55,55	0
4	GOL	B	803	6/6	0.19	2.75	47,49,50,53	0
4	GOL	C	803	6/6	0.12	1.26	55,57,58,58	0
5	SFY	B	806	17/17	0.11	1.10	19,22,25,26	0
4	GOL	A	803	6/6	0.17	1.02	54,55,56,56	0
5	SFY	D	803	17/17	0.15	0.64	38,39,45,45	0
2	NAP	D	801	48/48	0.12	0.05	34,37,41,42	0
2	NAP	C	801	48/48	0.10	0.02	23,26,28,29	0
3	SO4	A	805	5/5	0.22	-0.12	97,98,99,99	0
2	NAP	B	801	48/48	0.09	-0.14	18,23,27,27	0
2	NAP	A	801	48/48	0.09	-0.45	19,21,23,23	0
3	SO4	D	804	5/5	0.22	-0.56	105,105,107,108	0
5	SFY	A	807	17/17	0.09	-0.74	20,22,25,25	0
5	SFY	C	804	17/17	0.10	-0.91	26,28,32,33	0
3	SO4	C	802	5/5	0.08	-2.57	56,57,57,58	0
3	SO4	A	808	5/5	0.35	-	117,118,119,120	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.