



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 11:15 pm GMT

PDB ID : 2O2Q  
Title : Crystal structure of the C-terminal domain of rat 10'formyltetrahydrofolate dehydrogenase in complex with NADP  
Authors : Tsybovsky, Y.; Donato, H.; Krupenko, N.I.; Davies, C.; Krupenko, S.A.  
Deposited on : 2006-11-30  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

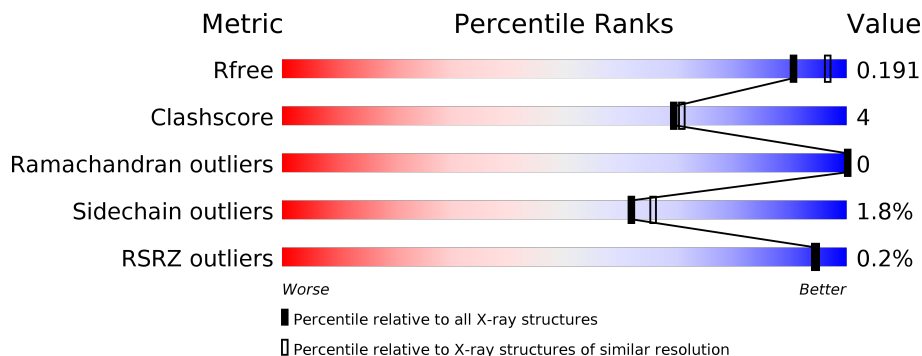
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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	517	
1	B	517	
1	C	517	
1	D	517	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17833 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 Formyltetrahydrofolate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	2	20	0
			3919	2487	674	737	21			
1	B	498	Total	C	N	O	S	1	19	0
			3908	2479	674	734	21			
1	C	498	Total	C	N	O	S	1	17	0
			3896	2472	675	728	21			
1	D	498	Total	C	N	O	S	2	19	0
			3906	2478	671	736	21			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	INITIATING METHIONINE	UNP Q5HQB2
A	387	ARG	-	CLONING ARTIFACT	UNP Q5HQB2
A	388	GLY	-	CLONING ARTIFACT	UNP Q5HQB2
A	389	SER	-	CLONING ARTIFACT	UNP Q5HQB2
A	390	HIS	-	EXPRESSION TAG	UNP Q5HQB2
A	391	HIS	-	EXPRESSION TAG	UNP Q5HQB2
A	392	HIS	-	EXPRESSION TAG	UNP Q5HQB2
A	393	HIS	-	EXPRESSION TAG	UNP Q5HQB2
A	394	HIS	-	EXPRESSION TAG	UNP Q5HQB2
A	395	THR	-	CLONING ARTIFACT	UNP Q5HQB2
A	396	THR	-	CLONING ARTIFACT	UNP Q5HQB2
B	386	MET	-	INITIATING METHIONINE	UNP Q5HQB2
B	387	ARG	-	CLONING ARTIFACT	UNP Q5HQB2
B	388	GLY	-	CLONING ARTIFACT	UNP Q5HQB2
B	389	SER	-	CLONING ARTIFACT	UNP Q5HQB2
B	390	HIS	-	EXPRESSION TAG	UNP Q5HQB2
B	391	HIS	-	EXPRESSION TAG	UNP Q5HQB2
B	392	HIS	-	EXPRESSION TAG	UNP Q5HQB2
B	393	HIS	-	EXPRESSION TAG	UNP Q5HQB2
B	394	HIS	-	EXPRESSION TAG	UNP Q5HQB2
B	395	THR	-	CLONING ARTIFACT	UNP Q5HQB2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	396	THR	-	CLONING ARTIFACT	UNP Q5HQB2
C	386	MET	-	INITIATING METHIONINE	UNP Q5HQB2
C	387	ARG	-	CLONING ARTIFACT	UNP Q5HQB2
C	388	GLY	-	CLONING ARTIFACT	UNP Q5HQB2
C	389	SER	-	CLONING ARTIFACT	UNP Q5HQB2
C	390	HIS	-	EXPRESSION TAG	UNP Q5HQB2
C	391	HIS	-	EXPRESSION TAG	UNP Q5HQB2
C	392	HIS	-	EXPRESSION TAG	UNP Q5HQB2
C	393	HIS	-	EXPRESSION TAG	UNP Q5HQB2
C	394	HIS	-	EXPRESSION TAG	UNP Q5HQB2
C	395	THR	-	CLONING ARTIFACT	UNP Q5HQB2
C	396	THR	-	CLONING ARTIFACT	UNP Q5HQB2
D	386	MET	-	INITIATING METHIONINE	UNP Q5HQB2
D	387	ARG	-	CLONING ARTIFACT	UNP Q5HQB2
D	388	GLY	-	CLONING ARTIFACT	UNP Q5HQB2
D	389	SER	-	CLONING ARTIFACT	UNP Q5HQB2
D	390	HIS	-	EXPRESSION TAG	UNP Q5HQB2
D	391	HIS	-	EXPRESSION TAG	UNP Q5HQB2
D	392	HIS	-	EXPRESSION TAG	UNP Q5HQB2
D	393	HIS	-	EXPRESSION TAG	UNP Q5HQB2
D	394	HIS	-	EXPRESSION TAG	UNP Q5HQB2
D	395	THR	-	CLONING ARTIFACT	UNP Q5HQB2
D	396	THR	-	CLONING ARTIFACT	UNP Q5HQB2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



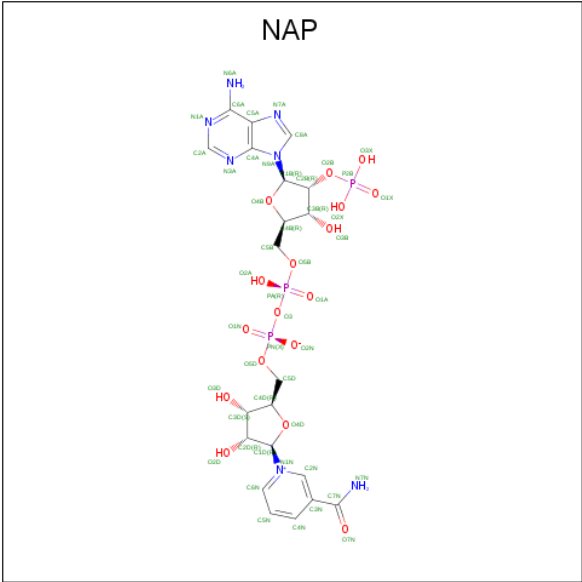
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total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

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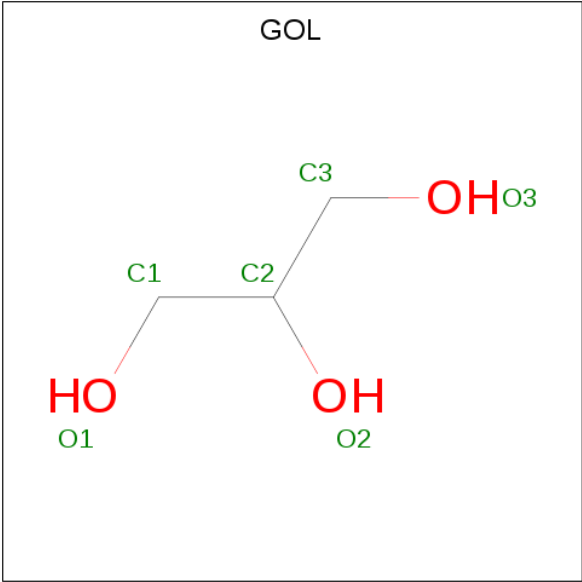
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	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 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
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 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
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

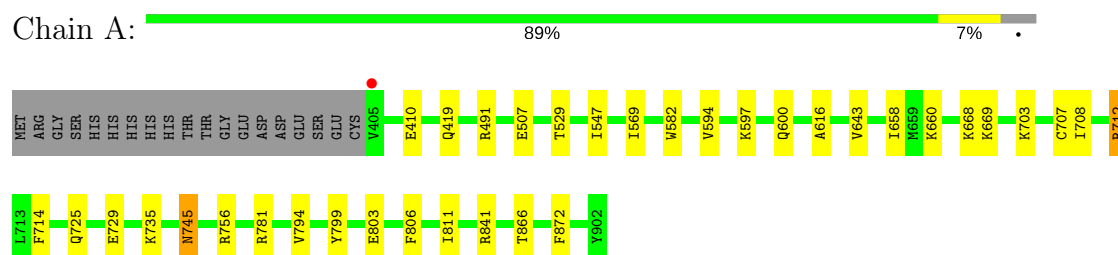
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	460	Total	O	0	4
			460	460		
6	B	429	Total	O	0	3
			429	429		
6	C	484	Total	O	0	3
			484	484		
6	D	471	Total	O	0	4
			471	471		

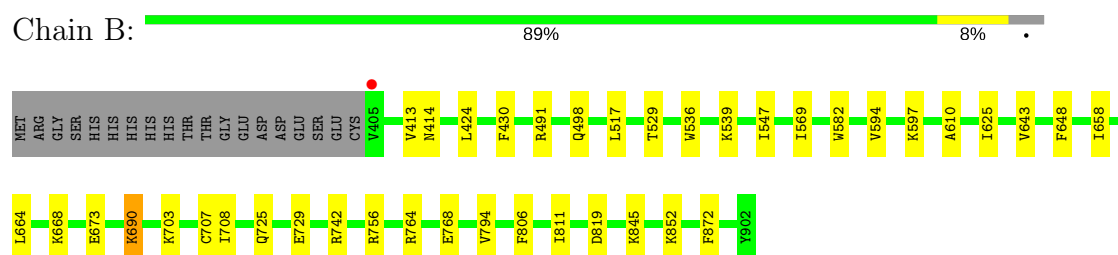
### 3 Residue-property plots

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.

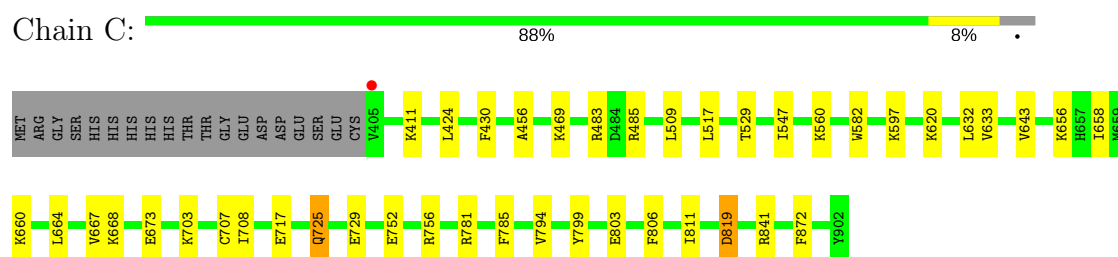
- Molecule 1: Formyltetrahydrofolate dehydrogenase



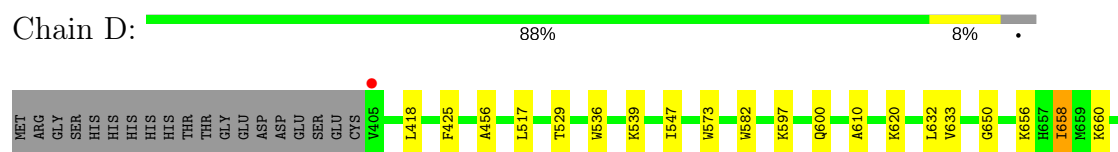
- Molecule 1: Formyltetrahydrofolate dehydrogenase



- Molecule 1: Formyltetrahydrofolate dehydrogenase



- Molecule 1: Formyltetrahydrofolate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.40Å 194.50Å 97.30Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 49.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (50.00-2.00) 97.0 (49.00-2.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.168 , 0.190 0.171 , 0.191	Depositor DCC
$R_{free}$ test set	14997 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, NAP, 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	0.56	0/4077	0.61	1/5510 (0.0%)
1	B	0.53	0/4071	0.60	0/5502
1	C	0.83	2/4051 (0.0%)	0.66	3/5475 (0.1%)
1	D	0.58	2/4066 (0.0%)	0.60	0/5496
All	All	0.64	4/16265 (0.0%)	0.62	4/21983 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	620[A]	LYS	CE-NZ	25.59	2.13	1.49
1	C	620[B]	LYS	CE-NZ	25.59	2.13	1.49
1	D	620[A]	LYS	CD-CE	-7.24	1.33	1.51
1	D	620[B]	LYS	CD-CE	-7.24	1.33	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	620[A]	LYS	CD-CE-NZ	-11.04	86.31	111.70
1	C	620[B]	LYS	CD-CE-NZ	-11.04	86.31	111.70
1	A	712	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	C	485	ARG	NE-CZ-NH2	-5.25	117.68	120.30

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	3919	0	3942	28	0
1	B	3908	0	3927	35	0
1	C	3896	0	3918	37	0
1	D	3906	0	3920	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	45	0	0	1	0
3	B	30	0	0	1	0
3	C	35	0	0	0	0
3	D	30	0	0	0	0
4	A	48	0	24	6	0
4	B	48	0	24	10	0
4	C	48	0	24	9	0
4	D	48	0	24	10	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	460	0	0	6	0
6	B	429	0	0	6	0
6	C	484	0	0	1	0
6	D	471	0	0	3	0
All	All	17833	0	15835	129	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 4.

All (129) 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:C:841[B]:ARG:HH11	1:C:841[B]:ARG:HG2	1.16	1.09
1:A:708:ILE:HG21	1:A:872:PHE:HE1	1.37	0.86
1:B:707[A]:CYS:SG	4:B:903:NAP:C4N	2.68	0.81
1:D:707[A]:CYS:SG	4:D:903:NAP:C4N	2.68	0.80
1:C:799:TYR:CE2	1:C:803[A]:GLU:HG3	2.18	0.79
1:A:707[A]:CYS:SG	4:A:903:NAP:C4N	2.72	0.78
1:C:841[B]:ARG:NH1	1:C:841[B]:ARG:HG2	1.96	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:708:ILE:HG21	1:D:872:PHE:HE1	1.48	0.77
1:C:707[A]:CYS:SG	4:C:903:NAP:C4N	2.72	0.76
1:D:708:ILE:CG2	1:D:872:PHE:HE1	2.01	0.73
1:D:799:TYR:CE2	1:D:803[A]:GLU:HG3	2.23	0.73
1:B:768[B]:GLU:HG3	6:B:3280:HOH:O	1.90	0.69
1:C:708:ILE:HG21	1:C:872:PHE:HE1	1.58	0.69
1:A:708:ILE:HG21	1:A:872:PHE:CE1	2.26	0.68
1:C:752:GLU:OE2	1:C:756[B]:ARG:NH2	2.27	0.67
1:A:410:GLU:OE1	1:A:419[B]:GLN:NE2	2.25	0.66
1:D:707[A]:CYS:HB3	4:D:903:NAP:C4N	2.24	0.66
1:B:708:ILE:CG2	1:B:872:PHE:HE1	2.10	0.65
1:A:756[A]:ARG:NH2	6:A:3344:HOH:O	2.30	0.64
1:B:756[A]:ARG:NH2	6:B:3363:HOH:O	2.30	0.64
1:A:491[A]:ARG:NH2	6:A:3483:HOH:O	2.31	0.63
1:A:707[A]:CYS:HB3	4:A:903:NAP:C4N	2.28	0.63
1:C:707[A]:CYS:HB3	4:C:903:NAP:C4N	2.29	0.62
1:A:708:ILE:CG2	1:A:872:PHE:HE1	2.11	0.60
1:A:660:LYS:HD3	1:B:664:LEU:HD21	1.83	0.60
1:C:664:LEU:HD21	1:D:660:LYS:HE3	1.83	0.59
1:C:707[A]:CYS:HB3	4:C:903:NAP:C5N	2.33	0.59
1:B:491[B]:ARG:HH12	1:B:498:GLN:HE22	1.52	0.58
1:D:708:ILE:CG2	1:D:872:PHE:CE1	2.84	0.58
1:A:708:ILE:CG2	1:A:872:PHE:CE1	2.86	0.58
1:B:707[A]:CYS:HB3	4:B:903:NAP:C4N	2.32	0.57
1:A:707[A]:CYS:HB3	4:A:903:NAP:C3N	2.34	0.57
1:C:725[A]:GLN:OE1	1:C:729:GLU:OE2	2.21	0.57
1:D:707[A]:CYS:HB3	4:D:903:NAP:C5N	2.34	0.57
1:B:707[A]:CYS:HB3	4:B:903:NAP:C5N	2.36	0.55
1:B:708:ILE:HG21	1:B:872:PHE:HE1	1.71	0.55
1:A:735:LYS:H	1:A:745:ASN:HD21	1.53	0.55
1:D:806:PHE:CE1	4:D:903:NAP:H2D	2.41	0.54
1:C:708:ILE:HG21	1:C:872:PHE:CE1	2.41	0.54
1:B:872:PHE:HE2	4:B:903:NAP:O7N	1.91	0.54
1:B:708:ILE:CG2	1:B:872:PHE:CE1	2.92	0.53
1:D:708:ILE:HG21	1:D:872:PHE:CE1	2.36	0.52
1:D:673:GLU:HB3	4:D:903:NAP:N7N	2.25	0.52
1:A:569:ILE:HD12	1:A:594:VAL:HG21	1.92	0.52
1:B:725[A]:GLN:NE2	1:B:729:GLU:OE2	2.43	0.52
1:A:725[A]:GLN:NE2	1:A:729:GLU:OE2	2.36	0.51
1:D:658:ILE:HD11	4:D:903:NAP:C2A	2.40	0.51
1:D:707[A]:CYS:HB3	4:D:903:NAP:C3N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:872:PHE:HE2	4:C:903:NAP:O7N	1.93	0.51
1:A:600:GLN:NE2	6:A:3200:HOH:O	2.42	0.51
1:D:573:TRP:NE1	4:D:903:NAP:O2N	2.44	0.50
1:D:781[B]:ARG:HD2	1:D:785:PHE:CD2	2.46	0.50
1:A:658:ILE:HD11	4:A:903:NAP:C2A	2.42	0.50
1:A:712:ARG:HG3	6:A:3066:HOH:O	2.12	0.50
1:B:806:PHE:CE1	4:B:903:NAP:H2D	2.47	0.50
1:D:517:LEU:HD11	1:D:701:PHE:CZ	2.47	0.50
1:D:725[A]:GLN:NE2	1:D:729:GLU:OE2	2.43	0.50
1:A:841[B]:ARG:NH2	6:A:3377:HOH:O	2.44	0.49
1:C:781[B]:ARG:HD2	1:C:785:PHE:CD2	2.47	0.49
1:D:872:PHE:HE2	4:D:903:NAP:O7N	1.96	0.49
1:C:643:VAL:O	1:C:668:LYS:HE3	2.11	0.49
1:C:667:VAL:HG13	1:D:656:LYS:HG2	1.95	0.49
1:D:529:THR:HG21	1:D:582:TRP:HA	1.95	0.49
1:B:529:THR:HG21	1:B:582:TRP:HA	1.95	0.49
1:D:738:ASN:HB3	1:D:741[A]:GLU:HG3	1.95	0.49
1:C:469:LYS:HE2	6:C:3246:HOH:O	2.12	0.49
1:C:708:ILE:CG2	1:C:872:PHE:CE1	2.96	0.48
1:A:799:TYR:CE2	1:A:803[A]:GLU:HG3	2.49	0.48
1:D:797:HIS:HD2	6:D:3333:HOH:O	1.96	0.48
1:C:708:ILE:CG2	1:C:872:PHE:HE1	2.25	0.48
1:D:692:VAL:O	1:D:696:MET:HG2	2.12	0.48
1:B:610:ALA:HB2	1:B:625:ILE:HD12	1.96	0.47
1:B:536:TRP:CE2	1:D:539:LYS:HD3	2.51	0.46
1:C:529:THR:HG21	1:C:582:TRP:HA	1.98	0.46
1:B:756[B]:ARG:NH2	6:B:3424:HOH:O	2.47	0.46
1:B:707[B]:CYS:HB3	4:B:903:NAP:C2N	2.46	0.46
1:B:673:GLU:HB3	4:B:903:NAP:N7N	2.31	0.46
1:C:411:LYS:HD3	1:C:509:LEU:HD21	1.98	0.46
1:A:707[A]:CYS:HB3	4:A:903:NAP:C5N	2.45	0.45
1:B:690:LYS:HD3	6:B:3413:HOH:O	2.15	0.45
1:D:735:LYS:H	1:D:745:ASN:HD21	1.64	0.45
1:D:794:VAL:HG21	1:D:811:ILE:HG23	1.98	0.45
1:D:707[B]:CYS:HB3	4:D:903:NAP:C2N	2.45	0.45
1:C:819:ASP:OD2	1:C:819:ASP:C	2.54	0.45
1:D:632:LEU:HD23	1:D:632:LEU:C	2.37	0.45
1:C:707[A]:CYS:HB3	4:C:903:NAP:C3N	2.47	0.45
1:B:708:ILE:HG21	1:B:872:PHE:CE1	2.52	0.44
1:A:794:VAL:HG21	1:A:811:ILE:HG23	1.99	0.44
1:B:648:PHE:CD1	1:B:658:ILE:CD1	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768[B]:GLU:CG	6:B:3280:HOH:O	2.56	0.44
1:D:456:ALA:HB3	1:D:633:VAL:HG21	1.99	0.44
1:B:707[A]:CYS:HB3	4:B:903:NAP:C3N	2.46	0.43
1:B:764:ARG:O	1:B:768[B]:GLU:HG2	2.18	0.43
1:B:794:VAL:HG21	1:B:811:ILE:HG23	1.99	0.43
1:D:735:LYS:N	1:D:745:ASN:HD21	2.16	0.43
1:A:643:VAL:O	1:A:668:LYS:HE3	2.19	0.42
1:B:673:GLU:HG2	6:B:3397:HOH:O	2.19	0.42
1:C:560[A]:LYS:HD3	6:D:3456:HOH:O	2.19	0.42
1:D:600:GLN:NE2	6:D:3114:HOH:O	2.53	0.42
1:A:707[B]:CYS:HB3	4:A:903:NAP:C2N	2.48	0.42
1:A:529:THR:HG21	1:A:582:TRP:HA	2.01	0.42
1:B:424:LEU:O	1:B:430:PHE:HA	2.20	0.42
1:C:656:LYS:HG2	1:D:667:VAL:HG13	2.02	0.42
1:C:632:LEU:C	1:C:632:LEU:HD23	2.40	0.42
1:C:707[A]:CYS:HB3	4:C:903:NAP:C6N	2.50	0.42
1:C:707[B]:CYS:HB3	4:C:903:NAP:C2N	2.50	0.42
1:B:569:ILE:HD12	1:B:594:VAL:HG21	2.01	0.41
1:B:643:VAL:O	1:B:668:LYS:HE3	2.20	0.41
1:B:673:GLU:HB3	4:B:903:NAP:C7N	2.51	0.41
1:C:794:VAL:HG21	1:C:811:ILE:HG23	2.02	0.41
1:D:425:PHE:CD2	1:D:610:ALA:HB1	2.55	0.41
1:D:650:GLY:O	1:D:674:LEU:HA	2.21	0.41
1:B:539:LYS:HD3	1:D:536:TRP:CE2	2.56	0.41
1:C:660:LYS:HG3	1:D:660:LYS:HG3	2.03	0.41
1:C:806:PHE:CE1	4:C:903:NAP:H2D	2.56	0.41
1:A:712:ARG:HG2	1:A:714:PHE:CE1	2.56	0.41
1:C:673:GLU:HB3	4:C:903:NAP:N7N	2.36	0.41
1:B:852:LYS:NZ	3:B:3004:SO4:O1	2.43	0.40
1:B:414:ASN:OD1	1:B:742:ARG:NH2	2.43	0.40
1:C:424:LEU:O	1:C:430:PHE:HA	2.22	0.40
1:C:456:ALA:HB3	1:C:633:VAL:HG21	2.03	0.40
1:C:781[B]:ARG:HD2	1:C:785:PHE:CE2	2.56	0.40
1:A:866:THR:HG21	5:A:1:GOL:H31	2.03	0.40
1:B:707[A]:CYS:HB3	4:B:903:NAP:C6N	2.52	0.40
6:A:3039:HOH:O	1:C:483:ARG:HD3	2.22	0.40
1:A:669:LYS:NZ	3:A:3015:SO4:O4	2.41	0.40
1:A:491[A]:ARG:HD2	1:A:616:ALA:O	2.22	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	516/517 (100%)	502 (97%)	14 (3%)	0	100	100
1	B	515/517 (100%)	503 (98%)	12 (2%)	0	100	100
1	C	513/517 (99%)	497 (97%)	16 (3%)	0	100	100
1	D	515/517 (100%)	500 (97%)	15 (3%)	0	100	100
All	All	2059/2068 (100%)	2002 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/426 (101%)	421 (98%)	8 (2%)	60	64
1	B	428/426 (100%)	420 (98%)	8 (2%)	60	64
1	C	426/426 (100%)	417 (98%)	9 (2%)	56	60
1	D	428/426 (100%)	422 (99%)	6 (1%)	69	74
All	All	1711/1704 (100%)	1680 (98%)	31 (2%)	62	66

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	507	GLU
1	A	547	ILE

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Mol	Chain	Res	Type
1	A	597	LYS
1	A	703	LYS
1	A	745	ASN
1	A	781[A]	ARG
1	A	781[B]	ARG
1	A	806	PHE
1	B	413	VAL
1	B	517	LEU
1	B	547	ILE
1	B	597	LYS
1	B	690	LYS
1	B	703	LYS
1	B	819	ASP
1	B	845	LYS
1	C	517	LEU
1	C	547	ILE
1	C	597	LYS
1	C	658	ILE
1	C	703	LYS
1	C	717	GLU
1	C	725[A]	GLN
1	C	725[B]	GLN
1	C	819	ASP
1	D	418	LEU
1	D	547	ILE
1	D	597	LYS
1	D	658	ILE
1	D	703	LYS
1	D	745	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	GLN
1	A	706	ASN
1	A	745	ASN
1	A	777	ASN
1	A	797	HIS
1	B	600	GLN
1	B	706	ASN
1	B	797	HIS
1	C	600	GLN

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Mol	Chain	Res	Type
1	C	706	ASN
1	C	797	HIS
1	D	407	ASN
1	D	600	GLN
1	D	706	ASN
1	D	745	ASN
1	D	797	HIS

### 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](#)

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 for Mogul analysis.

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	$\# Z  > 2$
5	GOL	A	1	-	5,5,5	0.35	0	5,5,5	0.44	0
3	SO4	A	3001	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	A	3002	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	A	3006	-	4,4,4	0.17	0	6,6,6	0.31	0
3	SO4	A	3011	-	4,4,4	0.16	0	6,6,6	0.13	0
3	SO4	A	3014	-	4,4,4	0.29	0	6,6,6	0.30	0
3	SO4	A	3015	-	4,4,4	0.28	0	6,6,6	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	3018	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	A	3021	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	A	3024	-	4,4,4	0.20	0	6,6,6	0.18	0
4	NAP	A	903	1,2	44,52,52	1.61	4 (9%)	53,80,80	1.51	3 (5%)
5	GOL	B	2	-	5,5,5	0.33	0	5,5,5	0.35	0
3	SO4	B	3004	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	B	3005	-	4,4,4	0.21	0	6,6,6	0.32	0
3	SO4	B	3009	-	4,4,4	0.18	0	6,6,6	0.07	0
3	SO4	B	3019	-	4,4,4	0.22	0	6,6,6	0.14	0
3	SO4	B	3022	-	4,4,4	0.19	0	6,6,6	0.28	0
3	SO4	B	3025	-	4,4,4	0.16	0	6,6,6	0.18	0
4	NAP	B	903	1,2	44,52,52	1.61	3 (6%)	53,80,80	1.65	3 (5%)
5	GOL	C	3	-	5,5,5	0.38	0	5,5,5	0.36	0
3	SO4	C	3007	-	4,4,4	0.19	0	6,6,6	0.39	0
3	SO4	C	3010	-	4,4,4	0.16	0	6,6,6	0.16	0
3	SO4	C	3013	-	4,4,4	0.25	0	6,6,6	0.47	0
3	SO4	C	3017	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	C	3023	-	4,4,4	0.19	0	6,6,6	0.20	0
3	SO4	C	3026	-	4,4,4	0.19	0	6,6,6	0.31	0
3	SO4	C	3028	-	4,4,4	0.24	0	6,6,6	0.30	0
4	NAP	C	903	1,2	44,52,52	1.60	3 (6%)	53,80,80	1.62	2 (3%)
3	SO4	D	3003	-	4,4,4	0.20	0	6,6,6	0.18	0
3	SO4	D	3008	-	4,4,4	0.15	0	6,6,6	0.27	0
3	SO4	D	3012	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	D	3016	-	4,4,4	0.26	0	6,6,6	0.40	0
3	SO4	D	3020	-	4,4,4	0.21	0	6,6,6	0.15	0
3	SO4	D	3027	-	4,4,4	0.17	0	6,6,6	0.16	0
5	GOL	D	4	-	5,5,5	0.32	0	5,5,5	0.21	0
4	NAP	D	903	1,2	44,52,52	1.53	4 (9%)	53,80,80	1.62	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1	-	-	0/4/4/4	0/0/0/0
3	SO4	A	3001	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3002	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3006	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3011	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3014	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	3015	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3018	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3021	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3024	-	-	0/0/0/0	0/0/0/0
4	NAP	A	903	1,2	-	0/27/67/67	0/5/5/5
5	GOL	B	2	-	-	0/4/4/4	0/0/0/0
3	SO4	B	3004	-	-	0/0/0/0	0/0/0/0
3	SO4	B	3005	-	-	0/0/0/0	0/0/0/0
3	SO4	B	3009	-	-	0/0/0/0	0/0/0/0
3	SO4	B	3019	-	-	0/0/0/0	0/0/0/0
3	SO4	B	3022	-	-	0/0/0/0	0/0/0/0
3	SO4	B	3025	-	-	0/0/0/0	0/0/0/0
4	NAP	B	903	1,2	-	0/27/67/67	0/5/5/5
5	GOL	C	3	-	-	0/4/4/4	0/0/0/0
3	SO4	C	3007	-	-	0/0/0/0	0/0/0/0
3	SO4	C	3010	-	-	0/0/0/0	0/0/0/0
3	SO4	C	3013	-	-	0/0/0/0	0/0/0/0
3	SO4	C	3017	-	-	0/0/0/0	0/0/0/0
3	SO4	C	3023	-	-	0/0/0/0	0/0/0/0
3	SO4	C	3026	-	-	0/0/0/0	0/0/0/0
3	SO4	C	3028	-	-	0/0/0/0	0/0/0/0
4	NAP	C	903	1,2	-	0/27/67/67	0/5/5/5
3	SO4	D	3003	-	-	0/0/0/0	0/0/0/0
3	SO4	D	3008	-	-	0/0/0/0	0/0/0/0
3	SO4	D	3012	-	-	0/0/0/0	0/0/0/0
3	SO4	D	3016	-	-	0/0/0/0	0/0/0/0
3	SO4	D	3020	-	-	0/0/0/0	0/0/0/0
3	SO4	D	3027	-	-	0/0/0/0	0/0/0/0
5	GOL	D	4	-	-	0/4/4/4	0/0/0/0
4	NAP	D	903	1,2	-	0/27/67/67	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	903	NAP	C8A-N9A	2.12	1.39	1.36
4	D	903	NAP	C2A-N1A	2.21	1.38	1.33
4	A	903	NAP	P2B-O2B	2.30	1.63	1.59
4	C	903	NAP	C2A-N1A	2.37	1.38	1.33
4	A	903	NAP	C2A-N1A	2.45	1.38	1.33
4	B	903	NAP	C2A-N1A	2.52	1.38	1.33
4	D	903	NAP	C2A-N3A	3.31	1.37	1.32
4	C	903	NAP	C2A-N3A	3.62	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	903	NAP	C2A-N3A	3.85	1.38	1.32
4	A	903	NAP	C2A-N3A	3.91	1.38	1.32
4	D	903	NAP	O7N-C7N	7.83	1.40	1.24
4	C	903	NAP	O7N-C7N	8.14	1.40	1.24
4	A	903	NAP	O7N-C7N	8.16	1.40	1.24
4	B	903	NAP	O7N-C7N	8.32	1.41	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	903	NAP	N3A-C2A-N1A	-10.09	120.22	128.86
4	C	903	NAP	N3A-C2A-N1A	-9.99	120.31	128.86
4	D	903	NAP	N3A-C2A-N1A	-9.87	120.42	128.86
4	A	903	NAP	N3A-C2A-N1A	-9.02	121.14	128.86
4	A	903	NAP	O4B-C1B-C2B	-2.62	102.04	106.60
4	C	903	NAP	O4B-C1B-C2B	-2.29	102.61	106.60
4	B	903	NAP	C1B-N9A-C4A	-2.14	122.94	126.64
4	D	903	NAP	O4B-C1B-C2B	-2.11	102.94	106.60
4	B	903	NAP	O4B-C1B-C2B	-2.09	102.96	106.60
4	A	903	NAP	C3N-C7N-N7N	2.24	120.36	117.76
4	D	903	NAP	C3N-C7N-N7N	2.36	120.50	117.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	GOL	1	0
3	A	3015	SO4	1	0
4	A	903	NAP	6	0
3	B	3004	SO4	1	0
4	B	903	NAP	10	0
4	C	903	NAP	9	0
4	D	903	NAP	10	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	498/517 (96%)	-0.64	1 (0%) 94 94	8, 17, 26, 37	12 (2%)
1	B	498/517 (96%)	-0.62	1 (0%) 94 94	9, 19, 28, 41	11 (2%)
1	C	498/517 (96%)	-0.73	1 (0%) 94 94	8, 15, 23, 39	11 (2%)
1	D	498/517 (96%)	-0.71	1 (0%) 94 94	7, 18, 28, 38	13 (2%)
All	All	1992/2068 (96%)	-0.68	4 (0%) 94 94	7, 17, 26, 41	47 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	VAL	4.8
1	C	405	VAL	4.4
1	B	405	VAL	4.3
1	D	405	VAL	3.8

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	D	4	6/6	0.70	0.24	58,58,58,59	0
5	GOL	C	3	6/6	0.75	0.27	64,66,66,66	0
3	SO4	A	3011	5/5	0.80	0.23	47,47,48,48	5
5	GOL	A	1	6/6	0.83	0.18	52,52,53,53	0
3	SO4	D	3020	5/5	0.85	0.15	42,42,43,44	5
3	SO4	B	3022	5/5	0.86	0.20	32,34,34,35	5
3	SO4	B	3009	5/5	0.86	0.14	48,48,49,49	5
2	MG	A	2001	1/1	0.88	0.13	55,55,55,55	0
3	SO4	C	3017	5/5	0.88	0.18	41,41,42,43	5
2	MG	D	2004	1/1	0.88	0.08	54,54,54,54	0
5	GOL	B	2	6/6	0.88	0.18	52,53,53,53	0
2	MG	B	2002	1/1	0.88	0.08	64,64,64,64	0
3	SO4	C	3023	5/5	0.89	0.17	36,37,38,38	5
2	MG	C	2003	1/1	0.89	0.12	48,48,48,48	0
3	SO4	A	3024	5/5	0.90	0.19	39,40,40,40	5
3	SO4	B	3019	5/5	0.90	0.14	41,41,42,43	5
3	SO4	C	3010	5/5	0.90	0.13	43,43,44,44	5
3	SO4	D	3012	5/5	0.90	0.14	46,46,47,47	5
3	SO4	D	3027	5/5	0.90	0.16	41,41,42,42	5
3	SO4	A	3021	5/5	0.90	0.20	41,43,43,43	5
3	SO4	C	3026	5/5	0.91	0.18	35,35,36,36	5
3	SO4	B	3005	5/5	0.93	0.14	37,37,39,39	5
3	SO4	B	3025	5/5	0.93	0.13	39,39,39,39	5
3	SO4	C	3028	5/5	0.94	0.09	27,31,31,32	5
4	NAP	A	903	48/48	0.95	0.10	16,23,33,36	0
4	NAP	D	903	48/48	0.95	0.10	18,22,32,34	0
3	SO4	A	3018	5/5	0.95	0.11	37,38,39,39	5
4	NAP	C	903	48/48	0.95	0.10	17,19,30,35	0
3	SO4	C	3007	5/5	0.95	0.10	29,29,31,31	5
3	SO4	A	3006	5/5	0.96	0.12	28,29,32,32	5
4	NAP	B	903	48/48	0.96	0.08	19,23,32,35	0
3	SO4	D	3008	5/5	0.96	0.10	28,30,31,31	5
3	SO4	A	3001	5/5	0.96	0.09	40,41,42,42	5
3	SO4	A	3002	5/5	0.96	0.10	28,29,29,31	5
3	SO4	A	3014	5/5	0.97	0.12	28,33,33,34	0
3	SO4	A	3015	5/5	0.97	0.11	22,28,29,29	0
3	SO4	D	3016	5/5	0.98	0.13	25,28,29,30	0
3	SO4	C	3013	5/5	0.98	0.10	22,25,27,27	0
3	SO4	B	3004	5/5	0.98	0.08	27,28,29,29	5
3	SO4	D	3003	5/5	0.98	0.12	18,19,19,20	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.