



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:25 am GMT

PDB ID : 4WZ9  
Title : APN1 from Anopheles gambiae  
Authors : Atkinson, S.C.; Armistead, J.S.; Mathias, D.K.; Sandeu, M.M.; Tao, D.;  
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Deposited on : 2014-11-19  
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

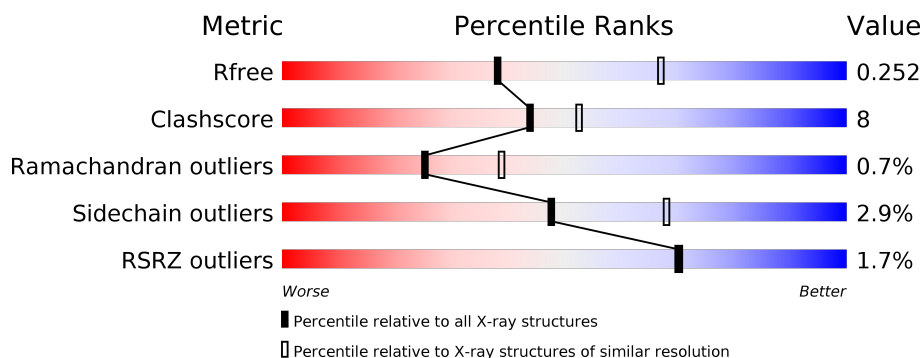
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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	957	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 75%, yellow 15%, orange 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>75%</span> <span>15%</span> <span>8%</span> </div> </div>
1	B	957	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 78%, yellow 14%, orange 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>78%</span> <span>14%</span> <span>7%</span> </div> </div>
2	M	5	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 40%, yellow 40%, orange 20%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>40%</span> <span>40%</span> <span>20%</span> </div> </div>
3	N	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 67%, yellow 33%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>67%</span> <span>33%</span> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	1002	-	-	-	X
5	GOL	B	1003	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14305 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 AGAP004809-PA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	882	Total	C	N	O	S	0	0	0
			7017	4460	1193	1334	30			
1	B	887	Total	C	N	O	S	0	0	0
			7048	4478	1198	1342	30			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ARG	-	expression tag	UNP Q7Q2T8
A	19	SER	-	expression tag	UNP Q7Q2T8
A	20	PRO	-	expression tag	UNP Q7Q2T8
A	21	TRP	-	expression tag	UNP Q7Q2T8
A	943	ALA	PHE	conflict	UNP Q7Q2T8
A	946	ARG	-	expression tag	UNP Q7Q2T8
A	947	GLY	-	expression tag	UNP Q7Q2T8
A	948	HIS	-	expression tag	UNP Q7Q2T8
A	949	PRO	-	expression tag	UNP Q7Q2T8
A	950	PHE	-	expression tag	UNP Q7Q2T8
A	951	GLU	-	expression tag	UNP Q7Q2T8
A	952	GLY	-	expression tag	UNP Q7Q2T8
A	953	LYS	-	expression tag	UNP Q7Q2T8
A	954	PRO	-	expression tag	UNP Q7Q2T8
A	955	ILE	-	expression tag	UNP Q7Q2T8
A	956	PRO	-	expression tag	UNP Q7Q2T8
A	957	ASN	-	expression tag	UNP Q7Q2T8
A	958	PRO	-	expression tag	UNP Q7Q2T8
A	959	LEU	-	expression tag	UNP Q7Q2T8
A	960	LEU	-	expression tag	UNP Q7Q2T8
A	961	GLY	-	expression tag	UNP Q7Q2T8
A	962	LEU	-	expression tag	UNP Q7Q2T8
A	963	ASP	-	expression tag	UNP Q7Q2T8
A	964	SER	-	expression tag	UNP Q7Q2T8
A	965	THR	-	expression tag	UNP Q7Q2T8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	966	ARG	-	expression tag	UNP Q7Q2T8
A	967	THR	-	expression tag	UNP Q7Q2T8
A	968	GLY	-	expression tag	UNP Q7Q2T8
A	969	HIS	-	expression tag	UNP Q7Q2T8
A	970	HIS	-	expression tag	UNP Q7Q2T8
A	971	HIS	-	expression tag	UNP Q7Q2T8
A	972	HIS	-	expression tag	UNP Q7Q2T8
A	973	HIS	-	expression tag	UNP Q7Q2T8
A	974	HIS	-	expression tag	UNP Q7Q2T8
B	18	ARG	-	expression tag	UNP Q7Q2T8
B	19	SER	-	expression tag	UNP Q7Q2T8
B	20	PRO	-	expression tag	UNP Q7Q2T8
B	21	TRP	-	expression tag	UNP Q7Q2T8
B	943	ALA	PHE	conflict	UNP Q7Q2T8
B	946	ARG	-	expression tag	UNP Q7Q2T8
B	947	GLY	-	expression tag	UNP Q7Q2T8
B	948	HIS	-	expression tag	UNP Q7Q2T8
B	949	PRO	-	expression tag	UNP Q7Q2T8
B	950	PHE	-	expression tag	UNP Q7Q2T8
B	951	GLU	-	expression tag	UNP Q7Q2T8
B	952	GLY	-	expression tag	UNP Q7Q2T8
B	953	LYS	-	expression tag	UNP Q7Q2T8
B	954	PRO	-	expression tag	UNP Q7Q2T8
B	955	ILE	-	expression tag	UNP Q7Q2T8
B	956	PRO	-	expression tag	UNP Q7Q2T8
B	957	ASN	-	expression tag	UNP Q7Q2T8
B	958	PRO	-	expression tag	UNP Q7Q2T8
B	959	LEU	-	expression tag	UNP Q7Q2T8
B	960	LEU	-	expression tag	UNP Q7Q2T8
B	961	GLY	-	expression tag	UNP Q7Q2T8
B	962	LEU	-	expression tag	UNP Q7Q2T8
B	963	ASP	-	expression tag	UNP Q7Q2T8
B	964	SER	-	expression tag	UNP Q7Q2T8
B	965	THR	-	expression tag	UNP Q7Q2T8
B	966	ARG	-	expression tag	UNP Q7Q2T8
B	967	THR	-	expression tag	UNP Q7Q2T8
B	968	GLY	-	expression tag	UNP Q7Q2T8
B	969	HIS	-	expression tag	UNP Q7Q2T8
B	970	HIS	-	expression tag	UNP Q7Q2T8
B	971	HIS	-	expression tag	UNP Q7Q2T8
B	972	HIS	-	expression tag	UNP Q7Q2T8
B	973	HIS	-	expression tag	UNP Q7Q2T8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	974	HIS	-	expression tag	UNP Q7Q2T8

- Molecule 2 is a protein called ALA-ALA-ALA-LYS-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	5	Total	C	N	O	0	0	0
			29	18	6	5			

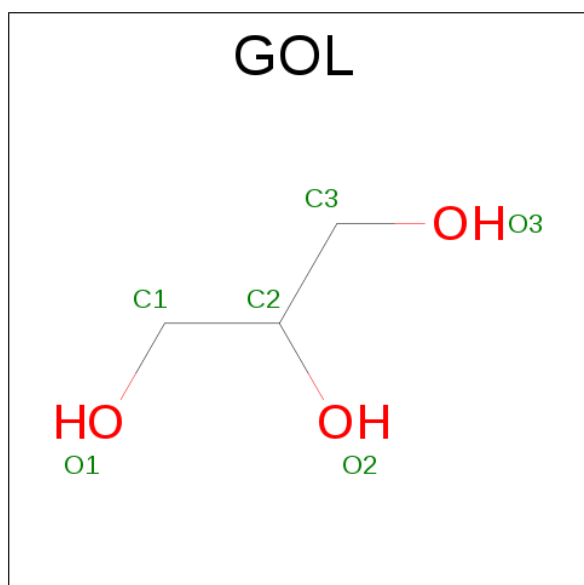
- Molecule 3 is a protein called ALA-ALA-LYS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	N	3	Total	C	N	O	0	0	0
			19	12	4	3			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

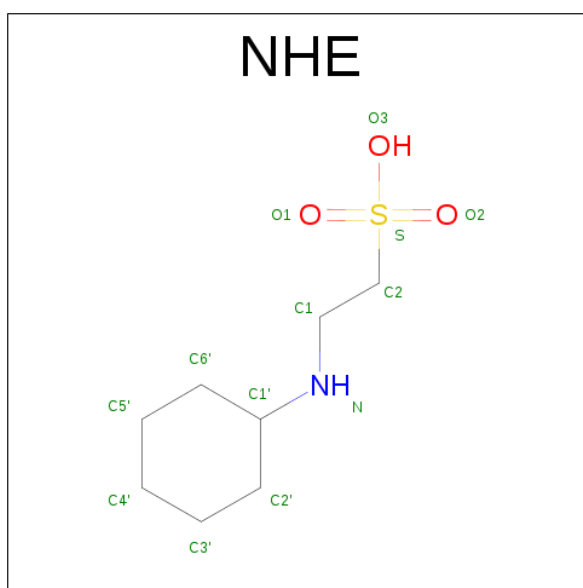
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

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

- Molecule 6 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 13 8 1 3 1	0	0

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

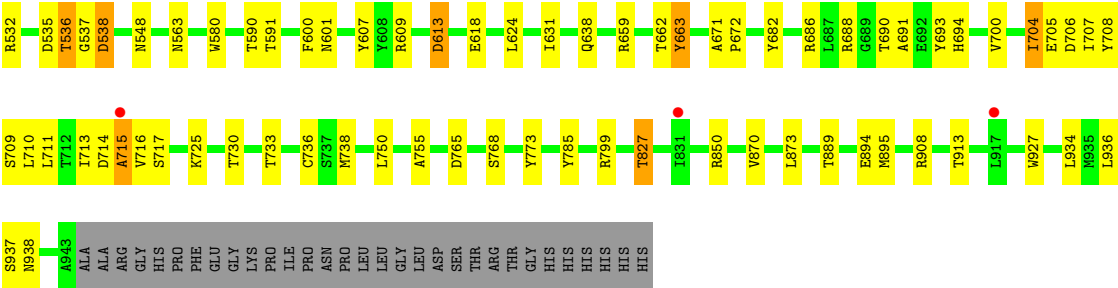
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Cu 1 1	0	0

- Molecule 8 is water.

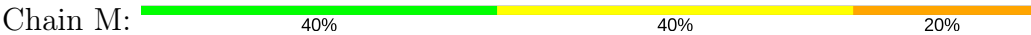
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	73	Total 73	O 73	0	0
8	B	73	Total 73	O 73	0	0







• Molecule 2: ALA-ALA-ALA-LYS-ALA



• Molecule 3: ALA-ALA-LYS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.48Å 132.90Å 146.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 61.40 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.65) 99.3 (61.40-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.200 , 0.254 0.205 , 0.252	Depositor DCC
$R_{free}$ test set	3256 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.0	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: NHE, GOL, ZN, CU

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	0.63	0/7181	0.79	5/9779 (0.1%)
1	B	0.62	0/7213	0.76	6/9824 (0.1%)
2	M	0.71	0/28	0.94	0/36
3	N	0.51	0/18	0.76	0/22
All	All	0.62	0/14440	0.78	11/19661 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	LEU	CB-CG-CD1	8.59	125.59	111.00
1	B	227	LEU	CB-CG-CD2	7.83	124.31	111.00
1	A	176	ASP	C-N-CA	-5.60	110.53	122.30
1	B	61	GLU	N-CA-C	5.50	125.84	111.00
1	B	704	ILE	CB-CA-C	-5.40	100.80	111.60
1	B	227	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	538	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	61	GLU	N-CA-C	5.19	125.01	111.00
1	A	799	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	773	TYR	N-CA-C	-5.14	97.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	ASP	C-N-CA	-5.06	111.68	122.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	GLY	Peptide
1	A	199	GLU	Peptide
1	A	548	ASN	Peptide
1	B	177	GLY	Peptide
1	B	199	GLU	Peptide
1	B	509	GLY	Peptide
1	B	548	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7017	0	6809	128	0
1	B	7048	0	6839	86	0
2	M	29	0	35	7	0
3	N	19	0	25	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	16	0	0
5	B	18	0	24	0	0
6	A	13	0	17	1	0
7	B	1	0	0	0	0
8	A	73	0	0	3	0
8	B	73	0	0	2	1
All	All	14305	0	13765	213	1

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 8.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:MET:CE	1:A:786:LEU:HD12	1.19	1.55
1:A:775:MET:CE	1:A:786:LEU:CD1	1.88	1.50
1:A:775:MET:HE1	1:A:786:LEU:CD1	1.35	1.48
1:A:535:ASP:O	1:A:536:THR:HG23	1.20	1.32
1:A:532:ARG:HG3	1:A:534:TYR:CE1	1.87	1.09
1:A:535:ASP:O	1:A:536:THR:CG2	2.03	1.05
1:A:775:MET:HE2	1:A:786:LEU:CD1	1.90	0.97
1:A:532:ARG:HG3	1:A:534:TYR:CD1	1.99	0.96
1:A:535:ASP:OD1	1:A:594:ALA:CB	2.24	0.86
1:A:714:ASP:O	1:A:716:VAL:N	2.11	0.84
1:A:775:MET:CE	1:A:786:LEU:HD13	2.05	0.84
1:A:60:ASP:O	1:A:61:GLU:HG2	1.77	0.83
1:B:60:ASP:O	1:B:61:GLU:HG2	1.78	0.82
1:A:507:PRO:O	1:A:510:VAL:HG12	1.80	0.82
1:A:535:ASP:OD1	1:A:594:ALA:HB2	1.80	0.81
1:A:532:ARG:HG3	1:A:534:TYR:HE1	1.46	0.78
1:B:714:ASP:O	1:B:716:VAL:N	2.17	0.78
1:A:613:ASP:OD1	1:A:615:HIS:HB2	1.84	0.78
1:A:332:MET:CE	2:M:1:ALA:HB2	2.15	0.77
1:A:535:ASP:C	1:A:536:THR:HG23	2.06	0.76
1:B:713:ILE:O	1:B:750:LEU:HD11	1.86	0.74
1:A:713:ILE:O	1:A:750:LEU:HD11	1.89	0.73
1:A:751:LEU:HD11	1:A:786:LEU:HD21	1.71	0.70
1:A:200:SER:HB2	8:A:1140:HOH:O	1.92	0.69
8:B:1165:HOH:O	3:N:2:LYS:HD2	1.96	0.65
1:A:751:LEU:CD1	1:A:786:LEU:HD21	2.28	0.64
1:A:725:LYS:HE3	1:A:765:ASP:OD2	1.98	0.64
1:A:332:MET:HE1	2:M:1:ALA:HB2	1.78	0.64
1:B:725:LYS:HE3	1:B:765:ASP:OD2	1.98	0.64
1:B:507:PRO:O	1:B:510:VAL:HG12	1.98	0.63
1:A:470:ASN:HD22	1:A:500:ILE:HG22	1.64	0.63
1:B:137:VAL:HG11	1:B:150:PHE:HB3	1.80	0.62
1:A:534:TYR:O	1:A:536:THR:N	2.32	0.62
1:A:241:THR:HG22	1:A:251:PHE:HE1	1.65	0.61
1:B:227:LEU:CD1	1:B:247:MET:O	2.49	0.61
1:A:186:ASP:HB2	6:A:1004:NHE:O3	2.01	0.60
1:A:700:VAL:HG12	1:A:738:MET:HE1	1.84	0.60
1:A:157:GLN:O	1:A:161:TYR:OH	2.13	0.59
1:B:142:ASP:HA	8:B:1129:HOH:O	2.02	0.59
1:A:751:LEU:HD21	1:A:786:LEU:HD11	1.84	0.59
1:B:241:THR:HG22	1:B:251:PHE:HE1	1.66	0.59
1:A:532:ARG:CG	1:A:534:TYR:CE1	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:GLU:HA	1:B:493:TYR:CD2	2.39	0.58
1:B:730:THR:O	1:B:733:THR:HG22	2.03	0.58
1:B:157:GLN:O	1:B:161:TYR:OH	2.15	0.57
1:A:533:SER:OG	1:A:538:ASP:HB2	2.05	0.57
1:B:688:ARG:HA	1:B:693:TYR:CE1	2.40	0.57
1:A:566:HIS:ND1	1:A:596:GLU:OE1	2.33	0.57
1:A:534:TYR:CE2	1:A:615:HIS:CG	2.88	0.56
1:B:704:ILE:O	1:B:706:ASP:N	2.39	0.56
1:B:709:SER:OG	1:B:709:SER:O	2.22	0.56
1:A:489:ASP:OD1	1:A:493:TYR:OH	2.18	0.56
1:B:120:VAL:HG23	1:B:137:VAL:HG21	1.87	0.55
1:B:535:ASP:OD1	1:B:536:THR:N	2.40	0.55
1:A:532:ARG:CG	1:A:534:TYR:HE1	2.17	0.55
1:B:700:VAL:HG12	1:B:738:MET:HE1	1.88	0.55
1:B:125:ASN:HB3	1:B:129:GLY:HA3	1.88	0.55
1:A:489:ASP:OD1	1:A:493:TYR:CZ	2.60	0.55
1:A:775:MET:HE3	1:A:786:LEU:CD1	2.19	0.54
1:B:686:ARG:HD3	1:B:927:TRP:CE2	2.42	0.54
1:B:227:LEU:HD12	1:B:247:MET:C	2.28	0.54
1:A:711:LEU:N	1:A:711:LEU:HD12	2.23	0.53
1:B:256:PRO:CD	1:B:316:MET:CE	2.85	0.53
1:A:274:LEU:C	1:A:274:LEU:HD12	2.29	0.53
1:B:936:LEU:O	1:B:937:SER:OG	2.24	0.53
1:B:690:THR:HG22	1:B:691:ALA:N	2.23	0.53
1:A:867:ASN:OD1	1:A:908:ARG:NH2	2.41	0.52
1:A:590:THR:OG1	1:A:591:THR:N	2.40	0.52
1:A:775:MET:HE2	1:A:786:LEU:HD11	1.83	0.52
1:B:590:THR:OG1	1:B:591:THR:N	2.39	0.52
1:A:256:PRO:CD	1:A:316:MET:CE	2.88	0.52
1:A:934:LEU:O	1:A:938:ASN:HB2	2.10	0.51
1:B:274:LEU:HB3	1:B:279:ARG:HG2	1.93	0.51
1:B:711:LEU:N	1:B:711:LEU:HD12	2.24	0.51
1:A:525:TYR:OH	1:A:609:ARG:NE	2.43	0.51
1:A:58:ALA:HB1	8:A:1116:HOH:O	2.10	0.51
1:A:824:GLY:O	1:A:825:SER:HB3	2.10	0.50
1:B:434:ASN:ND2	1:B:520:THR:CG2	2.74	0.50
1:B:104:ASP:HB3	1:B:155:ILE:HG12	1.93	0.50
1:B:934:LEU:O	1:B:938:ASN:HB2	2.11	0.50
1:A:751:LEU:HD11	1:A:786:LEU:HD11	1.92	0.50
1:A:686:ARG:HD3	1:A:927:TRP:CE2	2.47	0.50
1:B:272:LEU:HD22	1:B:279:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HB3	1:A:126:GLY:O	2.12	0.49
1:A:120:VAL:HG23	1:A:137:VAL:HG11	1.93	0.49
1:A:256:PRO:HG2	1:A:316:MET:HE3	1.94	0.49
1:A:420:TYR:CE2	1:A:449:ARG:HD3	2.47	0.49
1:B:236:PRO:HG2	1:B:317:PRO:HG2	1.92	0.49
1:B:536:THR:N	1:B:537:GLY:HA2	2.27	0.49
1:A:707:ILE:O	1:A:707:ILE:HG13	2.12	0.49
1:B:272:LEU:HD13	1:B:279:ARG:HD3	1.95	0.49
1:A:688:ARG:NH2	1:A:894:GLU:OE2	2.46	0.49
1:A:671:ALA:HB3	1:A:672:PRO:HD3	1.94	0.48
1:B:525:TYR:OH	1:B:609:ARG:NE	2.46	0.48
1:B:563:ASN:O	1:B:600:PHE:O	2.32	0.48
1:A:534:TYR:OH	1:A:613:ASP:OD1	2.27	0.48
1:A:123:LEU:HD11	1:A:162:LEU:HB2	1.94	0.48
1:B:227:LEU:HD13	1:B:247:MET:N	2.29	0.48
1:B:454:LYS:HD2	1:B:607:TYR:CE2	2.48	0.48
1:A:532:ARG:HG2	1:A:613:ASP:OD2	2.14	0.48
1:A:511:THR:HB	1:A:514:GLN:H	1.78	0.48
1:A:532:ARG:NH2	1:A:598:ILE:HD12	2.28	0.48
1:A:709:SER:O	1:A:709:SER:OG	2.28	0.48
1:A:736:CYS:HB3	1:A:773:TYR:CD1	2.49	0.48
1:B:256:PRO:CD	1:B:316:MET:HE1	2.44	0.48
1:B:256:PRO:HG2	1:B:316:MET:HE3	1.95	0.48
1:B:280:VAL:HG21	1:B:290:ALA:HB1	1.95	0.48
1:B:659:ARG:O	1:B:662:THR:OG1	2.31	0.48
1:A:332:MET:HE1	2:M:1:ALA:CB	2.43	0.48
1:B:671:ALA:HB3	1:B:672:PRO:HD3	1.96	0.47
1:A:532:ARG:CG	1:A:534:TYR:CD1	2.86	0.47
1:A:563:ASN:O	1:A:600:PHE:O	2.32	0.47
1:A:58:ALA:CB	8:A:1116:HOH:O	2.62	0.47
1:A:532:ARG:HH21	1:A:598:ILE:HD12	1.79	0.47
1:B:274:LEU:C	1:B:274:LEU:HD12	2.35	0.47
1:A:434:ASN:ND2	1:A:520:THR:CG2	2.78	0.47
1:B:688:ARG:NH2	1:B:894:GLU:OE2	2.47	0.47
1:B:123:LEU:HB3	1:B:126:GLY:O	2.14	0.47
1:B:334:ASN:HB2	1:B:337:LEU:O	2.15	0.47
1:A:227:LEU:HD21	1:A:242:ASP:CG	2.36	0.47
1:A:454:LYS:HD2	1:A:607:TYR:CE2	2.50	0.47
1:B:682:TYR:CZ	1:B:686:ARG:HD2	2.50	0.47
1:B:700:VAL:CG1	1:B:738:MET:HE1	2.45	0.47
1:A:601:ASN:HB3	1:A:638:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PRO:HG2	1:A:317:PRO:HG2	1.97	0.46
1:A:227:LEU:HD21	1:A:242:ASP:OD1	2.14	0.46
1:B:736:CYS:HB3	1:B:773:TYR:CD1	2.50	0.46
1:A:371:GLN:HA	1:A:375:ASN:OD1	2.16	0.46
1:A:736:CYS:HB3	1:A:773:TYR:CG	2.50	0.46
1:A:272:LEU:HD13	1:A:279:ARG:HD3	1.98	0.46
1:A:870:VAL:O	1:A:873:LEU:O	2.33	0.46
1:B:176:ASP:OD2	1:B:205:MET:HE1	2.15	0.46
1:B:707:ILE:C	1:B:709:SER:H	2.16	0.46
1:B:532:ARG:HB2	1:B:613:ASP:OD2	2.15	0.46
1:B:850:ARG:HH22	1:B:889:THR:HG22	1.81	0.46
1:A:256:PRO:CD	1:A:316:MET:HE1	2.46	0.45
1:A:663:TYR:CD1	1:A:663:TYR:C	2.89	0.45
1:B:156:LEU:HD22	1:B:161:TYR:CE2	2.52	0.45
1:B:536:THR:HG23	1:B:538:ASP:N	2.31	0.45
1:A:332:MET:HE1	2:M:1:ALA:CA	2.46	0.45
1:B:704:ILE:O	1:B:707:ILE:HG22	2.16	0.45
1:A:272:LEU:HD22	1:A:279:ARG:NH1	2.32	0.45
1:A:682:TYR:CZ	1:A:686:ARG:HD2	2.51	0.45
1:B:227:LEU:CD1	1:B:247:MET:C	2.85	0.45
1:A:532:ARG:NE	1:A:534:TYR:CE1	2.85	0.45
1:B:663:TYR:CD1	1:B:663:TYR:C	2.88	0.45
1:A:227:LEU:CD2	1:A:242:ASP:OD1	2.65	0.44
1:A:334:ASN:HB2	1:A:337:LEU:O	2.17	0.44
1:A:274:LEU:HB3	1:A:279:ARG:HG2	1.98	0.44
1:B:227:LEU:HD13	1:B:246:ASP:C	2.38	0.44
1:B:755:ALA:HB2	1:B:785:TYR:CD2	2.52	0.44
1:A:534:TYR:O	1:A:537:GLY:N	2.46	0.44
1:A:450:VAL:HA	1:A:454:LYS:HB3	2.00	0.44
1:B:506:LEU:HB3	1:B:510:VAL:HG13	2.00	0.44
1:B:870:VAL:O	1:B:873:LEU:O	2.35	0.44
1:A:333:GLU:HG3	1:A:370:HIS:HB3	1.99	0.44
1:A:332:MET:HB2	1:A:332:MET:HE2	1.85	0.44
1:A:755:ALA:HB2	1:A:785:TYR:CD2	2.53	0.43
1:A:176:ASP:OD2	1:A:205:MET:HE1	2.19	0.43
1:A:175:ASP:HA	1:A:179:TYR:CD1	2.54	0.43
1:A:408:GLU:HB2	1:A:723:LEU:HD22	2.00	0.43
1:A:714:ASP:C	1:A:716:VAL:H	2.20	0.43
1:A:173:THR:OG1	1:B:186:ASP:OD1	2.29	0.43
1:B:511:THR:HB	1:B:514:GLN:H	1.84	0.43
1:B:450:VAL:HA	1:B:454:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH2	1:B:269:ASP:OD2	2.52	0.43
1:A:624:LEU:HD21	1:A:631:ILE:HD12	2.01	0.43
1:A:775:MET:CE	1:A:786:LEU:HD11	2.21	0.43
1:B:176:ASP:OD2	1:B:205:MET:CE	2.67	0.43
1:A:345:LEU:HA	1:A:360:VAL:HG13	2.01	0.42
1:B:280:VAL:O	1:B:280:VAL:HG23	2.19	0.42
1:A:576:ASP:N	1:A:576:ASP:OD1	2.52	0.42
1:A:688:ARG:HA	1:A:693:TYR:CE1	2.54	0.42
1:A:367:GLU:OE1	2:M:2:ALA:HB2	2.19	0.42
1:A:341:ARG:NH2	2:M:4:LYS:HG3	2.33	0.42
1:A:770:THR:O	1:A:773:TYR:O	2.37	0.42
1:B:601:ASN:HB3	1:B:638:GLN:HE22	1.84	0.42
1:A:532:ARG:HH11	1:A:619:LEU:CD1	2.32	0.42
1:B:272:LEU:HD22	1:B:279:ARG:HH11	1.85	0.42
1:B:736:CYS:HB3	1:B:773:TYR:CG	2.55	0.42
1:A:515:ILE:HD13	1:A:580:TRP:CH2	2.55	0.42
1:B:750:LEU:HA	1:B:750:LEU:HD23	1.90	0.42
1:B:338:VAL:HG12	1:B:340:TYR:CE1	2.54	0.42
1:A:233:SER:OG	1:A:234:ASN:N	2.53	0.42
1:A:333:GLU:O	1:A:334:ASN:C	2.58	0.42
1:A:506:LEU:HB3	1:A:510:VAL:HG13	2.02	0.42
1:A:511:THR:HG22	1:A:513:ALA:H	1.84	0.42
1:A:700:VAL:CG1	1:A:738:MET:HE1	2.47	0.42
1:B:711:LEU:O	1:B:715:ALA:HB2	2.21	0.41
1:B:175:ASP:HA	1:B:179:TYR:CD1	2.55	0.41
1:B:333:GLU:HG3	1:B:370:HIS:HB3	2.01	0.41
1:A:305:ASP:OD1	1:A:311:PRO:HA	2.20	0.41
1:A:154:THR:HG22	1:A:155:ILE:N	2.36	0.41
1:B:61:GLU:HB2	1:B:438:ALA:CB	2.51	0.41
1:B:157:GLN:HG3	1:B:158:PRO:HD2	2.01	0.41
1:A:66:PRO:HG2	1:A:107:VAL:HG21	2.02	0.41
1:A:704:ILE:O	1:A:707:ILE:HG22	2.20	0.41
1:A:156:LEU:HD22	1:A:161:TYR:CE2	2.56	0.41
1:A:199:GLU:HA	1:A:261:TYR:HB2	2.03	0.41
1:A:532:ARG:HB3	1:A:539:VAL:HG22	2.03	0.41
1:B:624:LEU:HD21	1:B:631:ILE:HD12	2.03	0.41
1:A:341:ARG:HD3	2:M:4:LYS:HE3	2.03	0.41
1:B:233:SER:OG	1:B:234:ASN:N	2.53	0.41
1:A:71:PRO:HB3	1:A:210:TYR:CD1	2.56	0.41
1:A:715:ALA:HB3	1:A:766:ILE:HG13	2.02	0.41
1:B:176:ASP:O	1:B:197:GLN:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ASP:OD1	1:B:311:PRO:HA	2.21	0.41
1:A:103:THR:OG1	1:A:104:ASP:N	2.54	0.40
1:B:71:PRO:HB3	1:B:210:TYR:CD1	2.56	0.40
1:A:529:ASN:O	1:A:541:ILE:HA	2.21	0.40
1:A:910:ASN:HD21	1:B:827:THR:HB	1.87	0.40
1:B:515:ILE:HD13	1:B:580:TRP:CH2	2.56	0.40
1:A:707:ILE:O	1:A:709:SER:N	2.44	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1102:HOH:O	8:B:1104:HOH:O[2_544]	1.97	0.23

## 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	878/957 (92%)	822 (94%)	48 (6%)	8 (1%)	20	31
1	B	885/957 (92%)	833 (94%)	47 (5%)	5 (1%)	28	43
2	M	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
3	N	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1767/1922 (92%)	1658 (94%)	96 (5%)	13 (1%)	25	39

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	GLY
1	A	534	TYR
1	A	536	THR

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Mol	Chain	Res	Type
1	A	715	ALA
1	B	715	ALA
1	A	535	ASP
1	A	158	PRO
1	B	158	PRO
1	B	705	GLU
1	B	708	TYR
1	A	708	TYR
1	B	507	PRO
1	A	507	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	744/802 (93%)	721 (97%)	23 (3%)	45	66
1	B	747/802 (93%)	727 (97%)	20 (3%)	50	71
2	M	1/1 (100%)	0	1 (100%)	0	0
3	N	1/1 (100%)	1 (100%)	0	100	100
All	All	1493/1606 (93%)	1449 (97%)	44 (3%)	48	68

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ILE
1	A	88	THR
1	A	90	THR
1	A	147	HIS
1	A	265	PHE
1	A	302	LYS
1	A	318	LYS
1	A	454	LYS
1	A	458	VAL
1	A	530	VAL
1	A	532	ARG

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Mol	Chain	Res	Type
1	A	555	THR
1	A	663	TYR
1	A	670	TYR
1	A	707	ILE
1	A	710	LEU
1	A	713	ILE
1	A	717	SER
1	A	719	ASP
1	A	723	LEU
1	A	768	SER
1	A	790	MET
1	A	938	ASN
1	B	70	ILE
1	B	302	LYS
1	B	318	LYS
1	B	411	GLU
1	B	454	LYS
1	B	458	VAL
1	B	530	VAL
1	B	536	THR
1	B	613	ASP
1	B	618	GLU
1	B	663	TYR
1	B	694	HIS
1	B	710	LEU
1	B	717	SER
1	B	768	SER
1	B	799	ARG
1	B	827	THR
1	B	895	MET
1	B	908	ARG
1	B	913	THR
2	M	4	LYS

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	147	HIS
1	A	784	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	1002	-	5,5,5	0.52	0	5,5,5	0.75	0
5	GOL	A	1003	-	5,5,5	0.41	0	5,5,5	0.41	0
6	NHE	A	1004	-	13,13,13	2.13	2 (15%)	15,17,17	2.07	3 (20%)
5	GOL	B	1002	-	5,5,5	0.48	0	5,5,5	0.30	0
5	GOL	B	1003	-	5,5,5	0.42	0	5,5,5	0.36	0
5	GOL	B	1004	-	5,5,5	0.94	0	5,5,5	1.00	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
5	GOL	A	1002	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1003	-	-	0/4/4/4	0/0/0/0
6	NHE	A	1004	-	-	0/7/15/15	0/1/1/1
5	GOL	B	1002	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1003	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1004	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1004	NHE	C2-S	-6.28	1.68	1.77
6	A	1004	NHE	O3-S	3.95	1.60	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1004	NHE	O3-S-O2	-2.09	106.58	111.37
6	A	1004	NHE	O1-S-C2	2.18	108.66	106.79
6	A	1004	NHE	O3-S-C2	6.80	114.42	106.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1004	NHE	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	882/957 (92%)	0.02	11 (1%) 79 79	31, 54, 96, 133	0
1	B	887/957 (92%)	-0.04	20 (2%) 61 59	32, 56, 91, 134	0
2	M	5/5 (100%)	0.38	0 100 100	66, 75, 83, 89	0
3	N	3/3 (100%)	0.10	0 100 100	81, 81, 83, 93	0
All	All	1777/1922 (92%)	-0.01	31 (1%) 70 70	31, 55, 94, 134	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	GLY	5.0
1	B	831	ILE	4.9
1	B	127	VAL	4.8
1	B	124	PRO	4.4
1	A	715	ALA	4.0
1	B	715	ALA	3.7
1	A	496	LEU	3.6
1	B	102	ALA	3.0
1	A	57	GLN	2.9
1	B	125	ASN	2.9
1	B	130	ALA	2.8
1	B	106	LEU	2.7
1	A	580	TRP	2.7
1	B	159	GLY	2.7
1	A	126	GLY	2.6
1	B	68	THR	2.6
1	B	57	GLN	2.6
1	B	128	THR	2.6
1	A	824	GLY	2.6
1	A	588	ILE	2.5
1	A	615	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	98	GLN	2.4
1	B	917	LEU	2.3
1	A	515	ILE	2.3
1	A	508	ASN	2.2
1	B	160	THR	2.2
1	B	120	VAL	2.2
1	B	103	THR	2.2
1	B	123	LEU	2.1
1	A	540	ILE	2.1
1	B	131	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	B	1002	6/6	0.70	0.25	8.01	86,94,98,104	0
5	GOL	B	1003	6/6	0.64	0.28	2.85	79,95,99,108	0
5	GOL	B	1004	6/6	0.81	0.26	1.73	48,56,65,68	0
6	NHE	A	1004	13/13	0.98	0.20	1.11	37,44,51,55	0
5	GOL	A	1003	6/6	0.86	0.16	-0.21	68,72,80,81	0
4	ZN	A	1001	1/1	0.98	0.15	-0.24	50,50,50,50	0
4	ZN	B	1001	1/1	1.00	0.15	-0.37	44,44,44,44	0
5	GOL	A	1002	6/6	0.86	0.14	-	61,69,72,73	0
7	CU	B	1005	1/1	0.77	0.16	-	126,126,126,126	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.