



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:27 PM UTC

PDB ID : 4WZ9 / pdb_00004wz9
Title : APN1 from Anopheles gambiae
Authors : Atkinson, S.C.; Armistead, J.S.; Mathias, D.K.; Sandeu, M.M.; Tao, D.;
Borhani-Dizaji, N.; Morlais, I.; Dinglasan, R.R.; Borg, N.A.
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

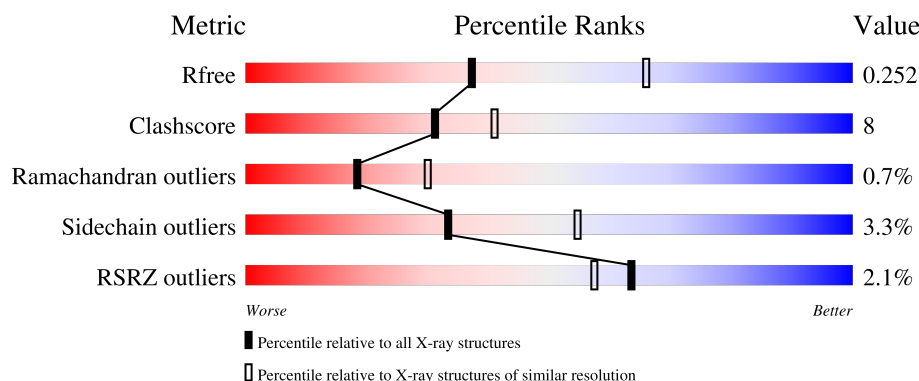
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

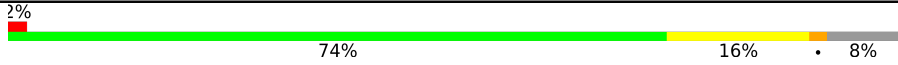
The reported resolution of this entry is 2.65 Å.

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	B	957	
2	M	5	
3	N	3	

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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			

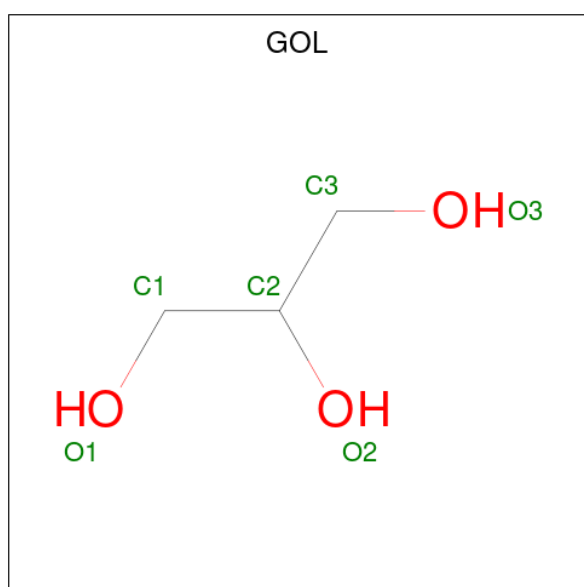
- Molecule 3 is a protein called ALA-ALA-LYS.

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 (CCD ID: ZN) (formula: Zn).

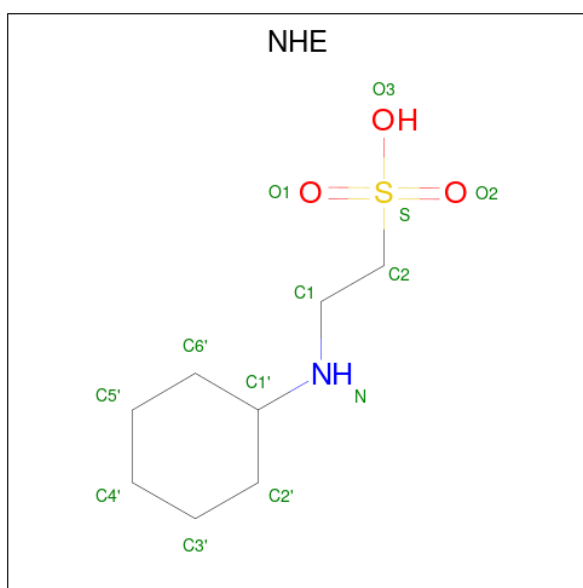
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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 (CCD ID: NHE) (formula: $C_8H_{17}NO_3S$).



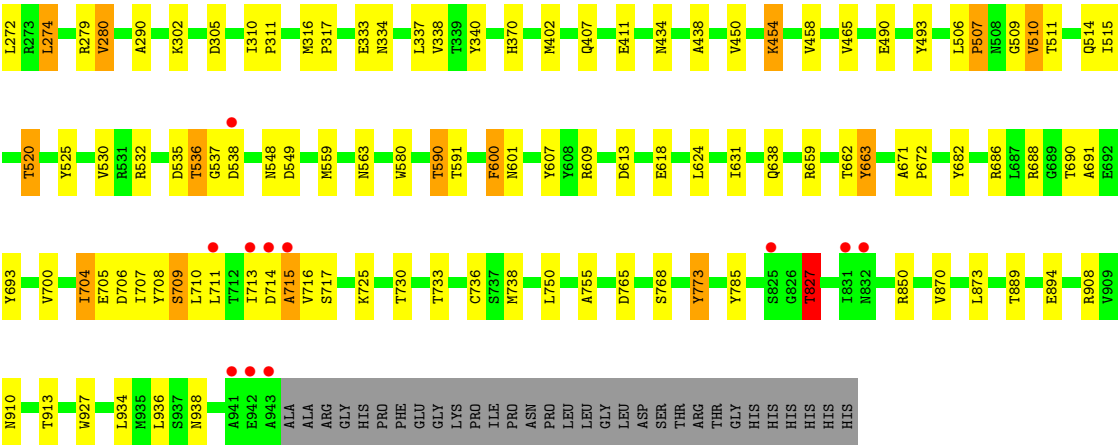
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 13 8 1 3 1	0	0

- Molecule 7 is COPPER (II) ION (CCD ID: 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, α , β , γ	113.48Å 132.90Å 146.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.65) 99.3 (50.00-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL, NHE, 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	0.85	0/7181	1.02	16/9779 (0.2%)
1	B	0.83	0/7213	0.98	16/9824 (0.2%)
2	M	1.02	0/28	1.35	1/36 (2.8%)
3	N	0.57	0/18	0.79	0/22
All	All	0.84	0/14440	1.00	33/19661 (0.2%)

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 (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	GLU	N-CA-C	12.15	125.01	107.88
1	A	773	TYR	N-CA-C	-8.27	97.13	110.20
1	B	274	LEU	N-CA-C	7.16	119.63	108.96
1	B	407	GLN	N-CA-C	-7.16	99.22	109.96
1	B	61	GLU	N-CA-C	7.06	125.84	110.80
1	B	510	VAL	N-CA-C	6.71	117.69	107.77
1	A	274	LEU	N-CA-C	6.56	118.73	108.96
1	A	713	ILE	CB-CA-C	-6.54	103.19	112.22
1	A	407	GLN	N-CA-C	-6.46	100.09	109.59
1	B	704	ILE	CB-CA-C	-6.39	100.80	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	THR	N-CA-C	-6.34	101.09	110.48
1	B	590	THR	N-CA-C	6.26	116.83	108.38
1	B	936	LEU	N-CA-C	-6.20	102.54	110.53
1	A	936	LEU	N-CA-C	6.11	117.73	111.14
1	B	773	TYR	N-CA-C	6.09	117.72	111.14
1	B	549	ASP	N-CA-CB	-6.06	102.31	111.15
1	B	827	THR	N-CA-C	5.82	117.77	108.41
1	A	549	ASP	N-CA-CB	-5.64	102.92	111.15
1	A	176	ASP	CA-C-N	-5.55	110.53	121.41
1	A	176	ASP	C-N-CA	-5.55	110.53	121.41
1	B	600	PHE	N-CA-C	5.48	119.93	112.04
1	B	240	THR	N-CA-C	-5.40	102.05	110.42
1	B	709	SER	N-CA-C	-5.38	102.37	110.06
1	A	832	ASN	N-CA-C	5.37	118.91	111.71
1	B	310	ILE	CA-C-N	-5.27	114.53	119.85
1	B	310	ILE	C-N-CA	-5.27	114.53	119.85
1	A	351	VAL	CB-CA-C	-5.26	105.69	110.63
1	A	709	SER	N-CA-C	-5.26	102.54	110.06
1	A	310	ILE	CA-C-N	-5.18	114.62	119.85
1	A	310	ILE	C-N-CA	-5.18	114.62	119.85
1	A	104	ASP	N-CA-CB	-5.12	102.90	110.53
1	B	280	VAL	N-CA-CB	5.12	118.30	111.64
2	M	4	LYS	N-CA-C	5.10	117.07	110.65

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	138	0
1	B	7048	0	6839	92	0
2	M	29	0	35	6	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	3	1
All	All	14305	0	13765	229	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 (229) 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:HE1	1:A:786:LEU:CD1	1.32	1.58
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	1.36
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:532:ARG:HG3	1:A:534:TYR:CD1	1.99	0.96
1:A:775:MET:HE2	1:A:786:LEU:CD1	1.97	0.92
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:535:ASP:C	1:A:536:THR:HG23	2.06	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:775:MET:HE3	1:A:786:LEU:HD12	1.60	0.78
1:A:613:ASP:OD1	1:A:615:HIS:HB2	1.84	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:CE	2:M:1:ALA:HB2	2.15	0.77
1:B:713:ILE:O	1:B:750:LEU:HD11	1.86	0.74
1:A:775:MET:HE3	1:A:786:LEU:CD1	2.14	0.73
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
1:A:199:GLU:OE1	1:A:332:MET:HE1	1.92	0.68
8:B:1165:HOH:O	3:N:2:LYS:HD2	1.96	0.65
1:A:725:LYS:HE3	1:A:765:ASP:OD2	1.98	0.64
1:A:751:LEU:CD1	1:A:786:LEU:HD21	2.28	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:B:176:ASP:OD2	1:B:205:MET:HE1	2.01	0.61
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: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:176:ASP:OD2	1:A:205:MET:HE1	2.02	0.59
1:B:227:LEU:HD12	1:B:247:MET:C	2.28	0.59
1:A:111:ARG:HH11	1:A:205:MET:HE2	1.68	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
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:A:274:LEU:HD12	1:A:274:LEU:C	2.29	0.57
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:O	1:B:709:SER:OG	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:VAL:HG12	1:A:738:MET:HE1	1.89	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:B:686:ARG:HD3	1:B:927:TRP:CE2	2.42	0.54
1:A:775:MET:CE	1:A:786:LEU:HD11	2.21	0.54
1:A:711:LEU:HD12	1:A:711:LEU:N	2.23	0.53
1:B:256:PRO:CD	1:B:316:MET:CE	2.85	0.53
1:B:707:ILE:C	1:B:709:SER:H	2.16	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: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:332:MET:HE1	2:M:1:ALA:HB2	1.88	0.52
1:A:227:LEU:HD21	1:A:242:ASP:CG	2.36	0.51
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: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:274:LEU:C	1:B:274:LEU:HD12	2.35	0.50
1:A:173:THR:OG1	1:B:186:ASP:OD1	2.29	0.50
1:A:663:TYR:CD1	1:A:663:TYR:C	2.89	0.50
1:A:824:GLY:O	1:A:825:SER:HB3	2.10	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:B:227:LEU:CD1	1:B:247:MET:C	2.85	0.50
1:B:256:PRO:CD	1:B:316:MET:HE1	2.41	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
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:B:700:VAL:HG12	1:B:738:MET:HE1	1.93	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:B:663:TYR:CD1	1:B:663:TYR:C	2.88	0.49
1:A:707:ILE:HG13	1:A:707:ILE:O	2.12	0.49
1:B:227:LEU:HD13	1:B:246:ASP:C	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:535:ASP:C	1:A:536:THR:CG2	2.75	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:714:ASP:C	1:A:716:VAL:H	2.20	0.48
1:A:736:CYS:HB3	1:A:773:TYR:CD1	2.49	0.48
1:A:707:ILE:C	1:A:709:SER:H	2.22	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: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:256:PRO:CD	1:A:316:MET:HE1	2.45	0.47
1:A:532:ARG:HH21	1:A:598:ILE:HD12	1.79	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: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:A:601:ASN:HB3	1:A:638:GLN:OE1	2.15	0.46
1:A:227:LEU:HD21	1:A:242:ASP:OD1	2.14	0.46
1:A:236:PRO:HG2	1:A:317:PRO:HG2	1.97	0.46
1:A:333:GLU:O	1:A:334:ASN:C	2.58	0.46
1:B:736:CYS:HB3	1:B:773:TYR:CD1	2.50	0.46
1:A:202:SER:HB3	1:A:205:MET:HE3	1.96	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:B:202:SER:HB3	1:B:205:MET:HE3	1.98	0.46
1:A:272:LEU:HD13	1:A:279:ARG:HD3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:VAL:O	1:A:873:LEU:O	2.33	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: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: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:A:332:MET:HE2	2:M:1:ALA:HB2	1.97	0.45
1:A:532:ARG:NE	1:A:534:TYR:CE1	2.85	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:111:ARG:HE	1:B:205:MET:HE2	1.81	0.44
1:A:332:MET:HE2	1:A:332:MET:HA	1.99	0.44
1:B:755:ALA:HB2	1:B:785:TYR:CD2	2.52	0.44
1:A:274:LEU:C	1:A:274:LEU:CD1	2.90	0.44
1:A:534:TYR:O	1:A:537:GLY:N	2.46	0.44
1:A:939:PHE:C	1:A:941:ALA:H	2.26	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:111:ARG:NH1	1:A:205:MET:HE2	2.32	0.44
1:A:755:ALA:HB2	1:A:785:TYR:CD2	2.53	0.43
1:A:175:ASP:HA	1:A:179:TYR:CD1	2.54	0.43
1:B:60:ASP:C	1:B:61:GLU:HG2	2.44	0.43
1:A:408:GLU:HB2	1:A:723:LEU:HD22	2.00	0.43
1:A:256:PRO:HG2	1:A:316:MET:HE3	2.00	0.43
1:A:714:ASP:C	1:A:716:VAL:N	2.72	0.43
1:B:511:THR:HB	1:B:514:GLN:H	1.84	0.43
1:B:333:GLU:O	1:B:334:ASN:C	2.61	0.43
1:B:450:VAL:HA	1:B:454:LYS:HB3	2.00	0.43
1:B:704:ILE:HD11	1:B:738:MET:HE1	2.00	0.43
1:A:60:ASP:C	1:A:61:GLU:HG2	2.42	0.43
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:HE2	1:A:786:LEU:HD11	1.94	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:A:576:ASP:OD1	1:A:576:ASP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:ARG:HA	1:A:693:TYR:CE1	2.54	0.42
1:B:402:MET:HE1	8:B:1161:HOH:O	2.19	0.42
1:A:341:ARG:NH2	2:M:4:LYS:HG3	2.33	0.42
1:A:367:GLU:OE1	2:M:2:ALA:HB2	2.19	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:HD23	1:B:750:LEU:HA	1.90	0.42
1:B:280:VAL:O	1:B:280:VAL:HG23	2.19	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: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: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:B:910:ASN:C	1:B:910:ASN:OD1	2.62	0.41
1:A:305:ASP:OD1	1:A:311:PRO:HA	2.20	0.41
1:B:256:PRO:HD3	1:B:316:MET:HE1	2.01	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: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:B:624:LEU:HD21	1:B:631:ILE:HD12	2.03	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
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:707:ILE:C	1:B:709:SER:N	2.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:707:ILE:C	1:A:709:SER:N	2.80	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	878/957 (92%)	822 (94%)	48 (6%)	8 (1%)	14	24
1	B	885/957 (92%)	833 (94%)	47 (5%)	5 (1%)	21	34
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%)	18	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	GLY
1	A	534	TYR
1	A	536	THR
1	A	715	ALA
1	B	715	ALA
1	A	535	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	718 (96%)	26 (4%)	32	52
1	B	747/802 (93%)	726 (97%)	21 (3%)	38	60
2	M	1/1 (100%)	0	1 (100%)	0	0
3	N	1/1 (100%)	0	1 (100%)	0	0
All	All	1493/1606 (93%)	1444 (97%)	49 (3%)	33	55

All (49) 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	143	THR
1	A	193	LEU
1	A	265	PHE
1	A	302	LYS
1	A	411	GLU
1	A	454	LYS
1	A	458	VAL
1	A	465	VAL
1	A	520	THR
1	A	530	VAL
1	A	532	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	555	THR
1	A	559	MET
1	A	663	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	84	ARG
1	B	143	THR
1	B	193	LEU
1	B	302	LYS
1	B	411	GLU
1	B	454	LYS
1	B	458	VAL
1	B	465	VAL
1	B	520	THR
1	B	530	VAL
1	B	536	THR
1	B	559	MET
1	B	618	GLU
1	B	663	TYR
1	B	710	LEU
1	B	717	SER
1	B	768	SER
1	B	827	THR
1	B	908	ARG
1	B	913	THR
2	M	4	LYS
3	N	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	334	ASN
1	A	529	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	573	ASN
1	A	595	ASN
1	B	96	GLN
1	B	424	GLN
1	B	529	ASN
1	B	912	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	1004	-	5,5,5	0.99	0	5,5,5	1.09	0
5	GOL	B	1002	-	5,5,5	0.54	0	5,5,5	0.28	0
5	GOL	A	1003	-	5,5,5	0.47	0	5,5,5	0.43	0
6	NHE	A	1004	-	13,13,13	2.20	2 (15%)	16,17,17	1.76	2 (12%)
5	GOL	A	1002	-	5,5,5	0.56	0	5,5,5	0.86	0
5	GOL	B	1003	-	5,5,5	0.46	0	5,5,5	0.39	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	B	1004	-	-	0/4/4/4	-
5	GOL	B	1002	-	-	0/4/4/4	-
5	GOL	A	1003	-	-	4/4/4/4	-
6	NHE	A	1004	-	-	4/7/15/15	0/1/1/1
5	GOL	A	1002	-	-	4/4/4/4	-
5	GOL	B	1003	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1004	NHE	C2-S	-6.78	1.68	1.77
6	A	1004	NHE	O3-S	3.61	1.60	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1004	NHE	C1-N-C1'	4.46	122.76	114.18
6	A	1004	NHE	O3-S-C2	4.30	114.42	106.00

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1002	GOL	O1-C1-C2-C3
5	A	1002	GOL	C1-C2-C3-O3
5	A	1003	GOL	C1-C2-C3-O3
6	A	1004	NHE	N-C1-C2-S
5	A	1002	GOL	O2-C2-C3-O3
5	A	1003	GOL	O1-C1-C2-C3
5	A	1002	GOL	O1-C1-C2-O2
6	A	1004	NHE	C2-C1-N-C1'
5	A	1003	GOL	O1-C1-C2-O2
5	A	1003	GOL	O2-C2-C3-O3
6	A	1004	NHE	C6'-C1'-N-C1
6	A	1004	NHE	C2'-C1'-N-C1

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, 95th 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 ²)	Q<0.9
1	A	882/957 (92%)	-0.10	15 (1%) 69 64	31, 54, 96, 133	0
1	B	887/957 (92%)	-0.09	17 (1%) 66 61	32, 56, 91, 134	0
2	M	5/5 (100%)	2.37	3 (60%) 0 0	66, 75, 83, 89	0
3	N	3/3 (100%)	2.15	2 (66%) 0 0	81, 81, 83, 93	0
All	All	1777/1922 (92%)	-0.09	37 (2%) 63 57	31, 55, 94, 134	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	831	ILE	6.7
1	B	715	ALA	4.9
1	B	943	ALA	4.9
2	M	5	ALA	4.1
1	A	715	ALA	4.0
2	M	3	ALA	3.6
1	A	60	ASP	3.6
1	A	508	ASN	3.5
1	A	59	VAL	3.5
1	B	942	GLU	3.2
1	B	127	VAL	3.1
1	B	941	ALA	3.1
1	A	942	GLU	3.0
1	A	591	THR	3.0
1	B	58	ALA	3.0
1	A	786	LEU	3.0
1	B	59	VAL	2.9
1	A	615	HIS	2.7
1	B	714	ASP	2.7
1	B	713	ILE	2.6
3	N	0	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	713	ILE	2.5
3	N	1	ALA	2.5
1	A	941	ALA	2.4
1	B	832	ASN	2.4
1	B	126	GLY	2.4
1	B	130	ALA	2.4
1	A	943	ALA	2.3
1	A	824	GLY	2.3
1	B	538	ASP	2.2
2	M	1	ALA	2.2
1	B	60	ASP	2.1
1	B	825	SER	2.1
1	B	711	LEU	2.1
1	A	893	GLU	2.0
1	A	537	GLY	2.0
1	A	709	SER	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 oligosaccharides 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, 95th 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	B	1003	6/6	0.76	0.13	79,95,99,108	0
5	GOL	B	1002	6/6	0.80	0.21	86,94,98,104	0
5	GOL	A	1002	6/6	0.80	0.18	61,69,72,73	0
5	GOL	B	1004	6/6	0.80	0.19	48,56,65,68	0
7	CU	B	1005	1/1	0.89	0.17	126,126,126,126	0
5	GOL	A	1003	6/6	0.91	0.12	68,72,80,81	0
6	NHE	A	1004	13/13	0.98	0.07	37,44,51,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	A	1001	1/1	0.99	0.03	50,50,50,50	0
4	ZN	B	1001	1/1	1.00	0.02	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.