



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2016 – 05:05 AM EDT

PDB ID : 5HRT
Title : Crystal structure of mouse autotaxin in complex with a DNA aptamer
Authors : Kato, K.; Nishimasu, H.; Morita, J.; Ishitani, R.; Nureki, O.
Deposited on : 2016-01-24
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

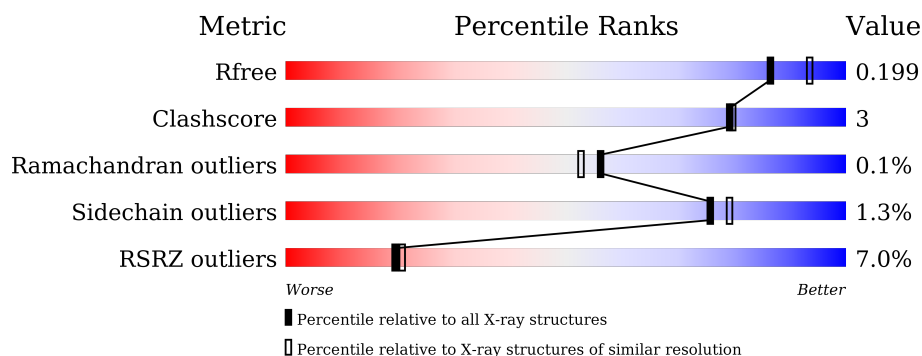
1 Overall quality at a glance

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 ≥ 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	831	<div> <div>6%</div> <div>88%</div> <div>6% • 5%</div> </div>
2	B	34	<div> <div>21%</div> <div>71%</div> <div>29%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	GOL	A	918	-	-	-	X
11	GOL	A	920	-	-	-	X
11	GOL	A	921	-	-	-	X
11	GOL	A	923	-	-	X	X
11	GOL	A	924	-	-	-	X
11	GOL	A	926	-	-	-	X
5	MAN	A	905	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7677 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	786	Total	C	N	O	S	0	5	0
			6306	4005	1090	1163	48			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q9R1E6
A	?	-	VAL	deletion	UNP Q9R1E6
A	?	-	GLU	deletion	UNP Q9R1E6
A	?	-	PRO	deletion	UNP Q9R1E6
A	859	SER	-	expression tag	UNP Q9R1E6
A	860	ARG	-	expression tag	UNP Q9R1E6
A	861	GLU	-	expression tag	UNP Q9R1E6
A	862	ASN	-	expression tag	UNP Q9R1E6
A	863	LEU	-	expression tag	UNP Q9R1E6
A	864	TYR	-	expression tag	UNP Q9R1E6
A	865	PHE	-	expression tag	UNP Q9R1E6
A	866	GLN	-	expression tag	UNP Q9R1E6

- Molecule 2 is a DNA chain called modified DNA (34-MER).

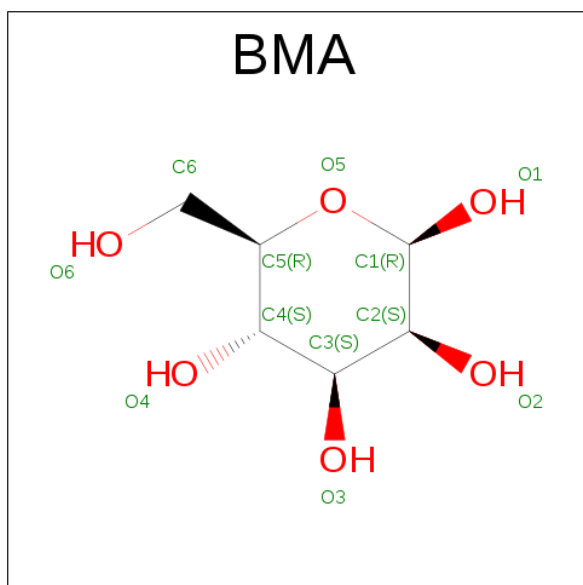
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	34	Total	C	N	O	P	0	0	0
			712	340	128	211	33			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



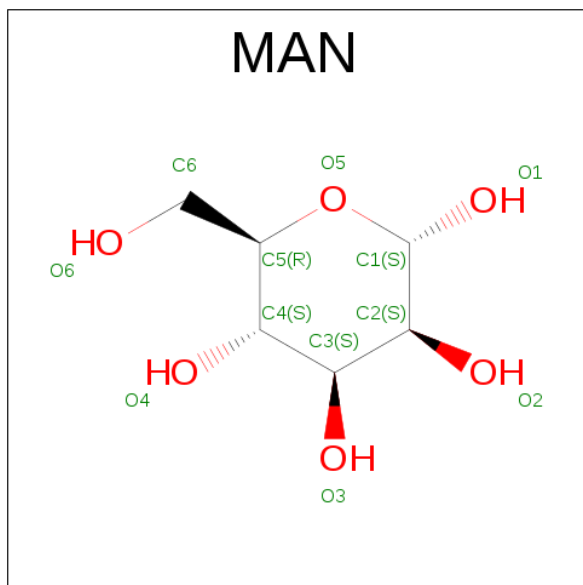
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Zn	0	0
			2	2		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	A	1	Total Ca 1 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0

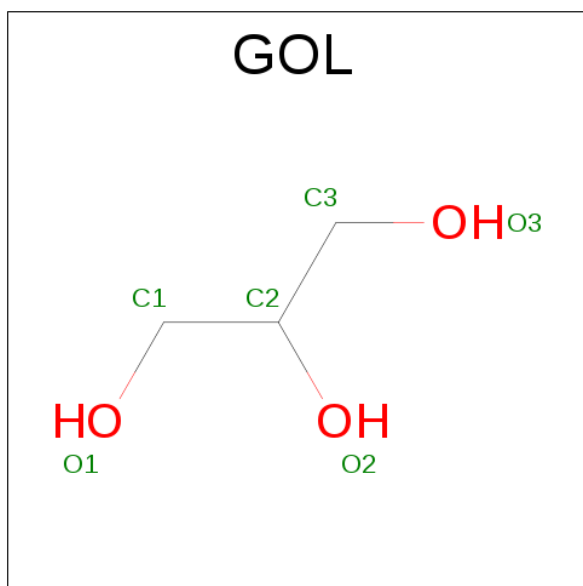
- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total K 1 1	0	0

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

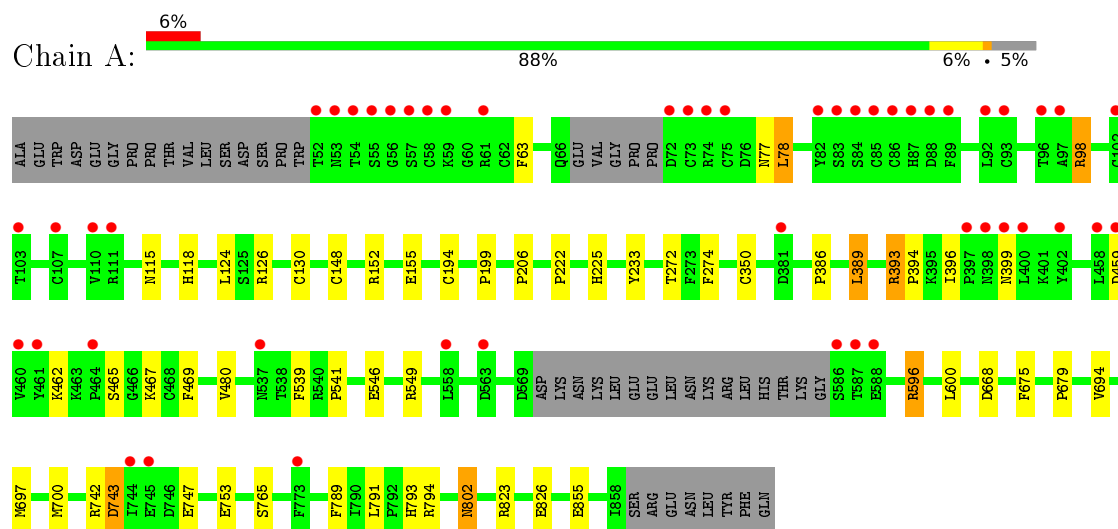
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	441	Total O 441 441	0	0
12	B	18	Total O 18 18	0	0

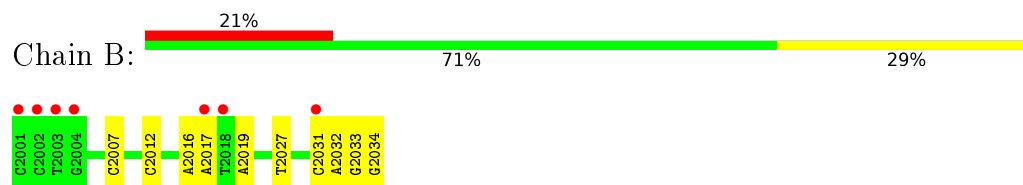
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



- Molecule 2: modified DNA (34-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.06 Å 208.76 Å 90.04 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.15 – 2.00 45.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.15-2.00) 93.3 (45.15-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.00 Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.164 , 0.202 0.159 , 0.199	Depositor DCC
R_{free} test set	1856 reflections (2.59%)	DCC
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.022 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7677	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: OMC, GOL, ZN, BMA, OMG, NAG, CL, NA, K, A2M, CA, MAN

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	0.86	2/6492 (0.0%)	0.82	8/8825 (0.1%)
2	B	1.25	2/564 (0.4%)	1.09	0/868
All	All	0.90	4/7056 (0.1%)	0.85	8/9693 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	480	VAL	CB-CG2	6.96	1.67	1.52
2	B	2012	DC	C3'-O3'	-6.06	1.36	1.44
1	A	130	CYS	CB-SG	5.93	1.92	1.82
2	B	2027	DT	C1'-N1	5.36	1.56	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	743	ASP	CB-CG-OD2	-10.80	108.58	118.30
1	A	194	CYS	CA-CB-SG	-8.89	98.00	114.00
1	A	148	CYS	CA-CB-SG	-7.42	100.64	114.00
1	A	596	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	A	549	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	A	742	ARG	C-N-CA	-6.59	105.22	121.70
1	A	393	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	743	ASP	CB-CA-C	5.03	120.46	110.40

There are no chirality outliers.

There are no planarity outliers.

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	6306	0	5989	38	0
2	B	712	0	402	8	0
3	A	56	0	48	1	0
4	A	22	0	16	1	0
5	A	55	0	48	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	A	1	0	0	0	0
11	A	60	0	79	11	0
12	A	441	0	0	7	0
12	B	18	0	0	0	0
All	All	7677	0	6582	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (48) 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)
2:B:2019:A2M:O4'	2:B:2019:A2M:C1'	1.64	1.22
2:B:2032:A2M:C1'	2:B:2032:A2M:O4'	1.65	1.19
1:A:826:GLU:HB3	11:A:923:GOL:H12	1.50	0.91
1:A:546:GLU:OE2	1:A:596:ARG:NH1	2.05	0.90
2:B:2033:OMG:HM22	2:B:2034:OMG:H5'	1.61	0.81
11:A:920:GOL:H32	12:A:1011:HOH:O	1.93	0.69
1:A:855:GLU:OE2	12:A:1001:HOH:O	2.13	0.67
1:A:823:ARG:HH12	11:A:923:GOL:H32	1.64	0.63
1:A:206:PRO:HB3	1:A:389:LEU:HD23	1.81	0.63
1:A:789[B]:PHE:CD1	1:A:791:LEU:HG	2.34	0.63
1:A:469:PHE:HE2	2:B:2007:OMC:HM22	1.66	0.60
11:A:923:GOL:H11	12:A:1271:HOH:O	2.01	0.60
1:A:794[C]:ARG:NH2	12:A:1002:HOH:O	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2016:DA:H2'	2:B:2017:DA:C8	2.43	0.54
1:A:600:LEU:HD11	11:A:923:GOL:H2	1.90	0.53
1:A:826:GLU:HB3	11:A:923:GOL:C1	2.31	0.53
1:A:600:LEU:CD1	11:A:923:GOL:H2	2.41	0.50
1:A:700:MET:HA	1:A:793:HIS:NE2	2.26	0.50
1:A:668:ASP:HB2	1:A:753:GLU:HB3	1.94	0.50
1:A:823:ARG:NH1	11:A:923:GOL:H32	2.27	0.49
1:A:743:ASP:HB2	1:A:747:GLU:OE2	2.13	0.49
1:A:546:GLU:OE2	12:A:1003:HOH:O	2.20	0.48
1:A:675:PHE:H	11:A:920:GOL:C3	2.27	0.48
2:B:2031:DC:H2'	2:B:2032:A2M:H8	1.96	0.48
1:A:78:LEU:HD21	1:A:274:PHE:CB	2.44	0.48
1:A:98:ARG:HG3	1:A:115:ASN:ND2	2.28	0.47
1:A:77:ASN:ND2	1:A:272:THR:HG21	2.29	0.47
1:A:539:PHE:O	1:A:541:PRO:HD3	2.14	0.47
1:A:679:PRO:HD2	11:A:920:GOL:H11	1.97	0.46
1:A:393:ARG:HB2	1:A:394:PRO:HD2	1.98	0.46
2:B:2032:A2M:H2'	2:B:2033:OMG:O4'	2.15	0.46
2:B:2031:DC:H2'	2:B:2032:A2M:C8	2.45	0.46
1:A:389:LEU:C	1:A:389:LEU:HD12	2.38	0.44
1:A:118:HIS:HD2	12:A:1101:HOH:O	2.00	0.43
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.53	0.43
1:A:233:TYR:HB2	11:A:924:GOL:H2	2.00	0.43
1:A:126:ARG:HB3	1:A:126:ARG:HE	1.60	0.43
3:A:909:NAG:O3	4:A:910:BMA:O2	2.29	0.43
1:A:78:LEU:HD13	1:A:78:LEU:HA	1.85	0.43
1:A:396:ILE:O	1:A:399:ASN:HB2	2.19	0.43
1:A:77:ASN:HD21	1:A:272:THR:CB	2.32	0.42
1:A:459:ASP:OD2	1:A:462:LYS:N	2.53	0.42
1:A:389:LEU:HD12	1:A:389:LEU:O	2.20	0.41
1:A:155:GLU:O	1:A:350:CYS:HB2	2.20	0.41
1:A:802:ASN:ND2	12:A:1023:HOH:O	2.54	0.41
1:A:765:SER:HB2	1:A:789[B]:PHE:CZ	2.56	0.40
1:A:694:VAL:HG23	1:A:697:MET:HE2	2.03	0.40
1:A:63:PHE:CE1	1:A:77:ASN:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	786/831 (95%)	764 (97%)	21 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	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	695/756 (92%)	686 (99%)	9 (1%)	76	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	98	ARG
1	A	124	LEU
1	A	152	ARG
1	A	199	PRO
1	A	389	LEU
1	A	465	SER
1	A	467	LYS
1	A	802	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	115	ASN
1	A	797	ASN
1	A	802	ASN
1	A	852	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	B	2007	2	15,22,23	3.35	6 (40%)	20,31,34	1.50	3 (15%)
2	OMG	B	2009	2,7	18,26,27	3.02	6 (33%)	21,38,41	2.06	6 (28%)
2	A2M	B	2014	2	18,25,26	4.69	9 (50%)	18,36,39	3.76	4 (22%)
2	OMG	B	2015	2	18,26,27	3.36	6 (33%)	21,38,41	1.78	4 (19%)
2	A2M	B	2019	2	18,25,26	4.95	10 (55%)	18,36,39	3.01	2 (11%)
2	OMC	B	2020	2	15,22,23	3.70	6 (40%)	20,31,34	1.30	2 (10%)
2	A2M	B	2032	2	18,25,26	5.09	10 (55%)	18,36,39	3.40	2 (11%)
2	OMG	B	2033	2	18,26,27	3.37	6 (33%)	21,38,41	1.90	4 (19%)
2	OMG	B	2034	2	18,26,27	3.48	6 (33%)	21,38,41	2.05	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	B	2007	2	-	0/5/27/28	0/2/2/2
2	OMG	B	2009	2,7	-	0/5/27/28	0/3/3/3
2	A2M	B	2014	2	-	0/5/27/28	0/3/3/3
2	OMG	B	2015	2	-	0/5/27/28	0/3/3/3
2	A2M	B	2019	2	-	0/5/27/28	0/3/3/3
2	OMC	B	2020	2	-	0/5/27/28	0/2/2/2
2	A2M	B	2032	2	-	0/5/27/28	0/3/3/3
2	OMG	B	2033	2	-	0/5/27/28	0/3/3/3
2	OMG	B	2034	2	-	0/5/27/28	0/3/3/3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2032	A2M	C2'-C1'	-7.06	1.33	1.53
2	B	2032	A2M	O4'-C4'	-6.94	1.29	1.45
2	B	2014	A2M	O4'-C4'	-6.83	1.29	1.45
2	B	2014	A2M	C2'-C1'	-6.62	1.35	1.53
2	B	2019	A2M	O4'-C4'	-6.56	1.30	1.45
2	B	2019	A2M	C2'-C1'	-6.42	1.35	1.53
2	B	2014	A2M	O3'-C3'	-4.71	1.31	1.43
2	B	2032	A2M	O3'-C3'	-4.26	1.32	1.43
2	B	2019	A2M	O3'-C3'	-3.99	1.33	1.43
2	B	2019	A2M	C5-C4	-2.60	1.34	1.40
2	B	2032	A2M	C5-C4	-2.39	1.35	1.40
2	B	2009	OMG	O6-C6	-2.36	1.18	1.24
2	B	2014	A2M	C5-C4	-2.35	1.35	1.40
2	B	2034	OMG	O6-C6	-2.01	1.19	1.24
2	B	2033	OMG	C2-N3	2.02	1.45	1.35
2	B	2014	A2M	C3'-C4'	2.10	1.58	1.53
2	B	2015	OMG	C2-N3	2.12	1.46	1.35
2	B	2020	OMC	C5-C4	2.35	1.46	1.41
2	B	2019	A2M	C5'-C4'	2.47	1.59	1.51
2	B	2032	A2M	C3'-C4'	2.52	1.59	1.53
2	B	2032	A2M	C5'-C4'	2.54	1.59	1.51
2	B	2007	OMC	C4-N4	2.56	1.42	1.35
2	B	2007	OMC	C5-C4	2.57	1.47	1.41
2	B	2019	A2M	C3'-C4'	2.75	1.60	1.53
2	B	2020	OMC	C4-N4	2.83	1.43	1.35
2	B	2014	A2M	O2'-C2'	3.03	1.50	1.42
2	B	2032	A2M	C2-N3	3.14	1.37	1.32
2	B	2019	A2M	C2-N3	3.28	1.38	1.32
2	B	2014	A2M	C2-N3	3.39	1.38	1.32
2	B	2014	A2M	C6-N6	3.55	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2009	OMG	C2-N1	3.79	1.42	1.35
2	B	2019	A2M	O2'-C2'	3.93	1.53	1.42
2	B	2032	A2M	C6-N6	4.08	1.50	1.34
2	B	2032	A2M	O2'-C2'	4.10	1.53	1.42
2	B	2019	A2M	C6-N6	4.17	1.51	1.34
2	B	2007	OMC	C2-N3	4.68	1.47	1.38
2	B	2015	OMG	C2-N1	4.77	1.44	1.35
2	B	2033	OMG	C2-N2	4.91	1.44	1.34
2	B	2009	OMG	C2-N2	4.98	1.44	1.34
2	B	2033	OMG	C2-N1	5.08	1.45	1.35
2	B	2034	OMG	C2-N1	5.28	1.45	1.35
2	B	2007	OMC	C6-C5	5.31	1.49	1.38
2	B	2034	OMG	C2-N2	5.40	1.45	1.34
2	B	2015	OMG	C2-N2	5.40	1.45	1.34
2	B	2007	OMC	C4-N3	5.46	1.45	1.35
2	B	2020	OMC	C6-C5	5.48	1.50	1.38
2	B	2020	OMC	C2-N3	5.55	1.49	1.38
2	B	2015	OMG	C6-N1	5.96	1.43	1.33
2	B	2009	OMG	C6-C5	6.04	1.53	1.41
2	B	2009	OMG	C4-N3	6.07	1.45	1.35
2	B	2033	OMG	C6-N1	6.11	1.44	1.33
2	B	2009	OMG	C6-N1	6.19	1.44	1.33
2	B	2034	OMG	C6-N1	6.21	1.44	1.33
2	B	2034	OMG	C6-C5	6.23	1.54	1.41
2	B	2015	OMG	C6-C5	6.24	1.54	1.41
2	B	2033	OMG	C6-C5	6.44	1.54	1.41
2	B	2020	OMC	C4-N3	6.49	1.47	1.35
2	B	2033	OMG	C4-N3	8.16	1.48	1.35
2	B	2015	OMG	C4-N3	8.20	1.48	1.35
2	B	2034	OMG	C4-N3	8.40	1.49	1.35
2	B	2007	OMC	C6-N1	8.63	1.46	1.35
2	B	2020	OMC	C6-N1	9.28	1.47	1.35
2	B	2014	A2M	O4'-C1'	15.15	1.62	1.41
2	B	2019	A2M	O4'-C1'	16.44	1.64	1.41
2	B	2032	A2M	O4'-C1'	16.81	1.65	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2014	A2M	N3-C2-N1	-12.86	118.77	128.87
2	B	2032	A2M	N3-C2-N1	-12.65	118.93	128.87
2	B	2019	A2M	N3-C2-N1	-10.48	120.64	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2014	A2M	N6-C6-N1	-7.86	105.32	118.52
2	B	2019	A2M	N6-C6-N1	-6.39	107.80	118.52
2	B	2034	OMG	N3-C2-N1	-5.83	119.63	127.56
2	B	2009	OMG	N3-C2-N1	-5.75	119.74	127.56
2	B	2032	A2M	N6-C6-N1	-5.66	109.03	118.52
2	B	2015	OMG	N3-C2-N1	-5.09	120.64	127.56
2	B	2033	OMG	C5-C6-N1	-4.80	117.24	123.52
2	B	2033	OMG	N3-C2-N1	-4.48	121.47	127.56
2	B	2015	OMG	C5-C6-N1	-3.90	118.42	123.52
2	B	2034	OMG	C5-C6-N1	-3.58	118.85	123.52
2	B	2009	OMG	C5-C6-N1	-2.99	119.61	123.52
2	B	2009	OMG	C1'-N9-C4	-2.90	123.57	126.81
2	B	2009	OMG	C6-C5-C4	-2.67	117.81	120.86
2	B	2014	A2M	O4'-C1'-C2'	-2.58	101.95	106.60
2	B	2014	A2M	O3'-C3'-C4'	-2.31	104.10	111.01
2	B	2020	OMC	N4-C4-N3	2.06	120.10	116.50
2	B	2015	OMG	C1'-N9-C4	2.16	129.21	126.81
2	B	2033	OMG	N2-C2-N1	2.31	121.00	117.20
2	B	2009	OMG	N2-C2-N1	2.53	121.38	117.20
2	B	2007	OMC	CM2-O2'-C2'	2.80	122.43	114.58
2	B	2007	OMC	O2'-C2'-C3'	2.83	118.51	111.23
2	B	2034	OMG	N2-C2-N1	3.12	122.34	117.20
2	B	2009	OMG	C6-N1-C2	3.71	120.23	115.88
2	B	2015	OMG	C6-N1-C2	3.80	120.33	115.88
2	B	2020	OMC	C6-C5-C4	4.13	119.05	117.44
2	B	2034	OMG	C6-N1-C2	4.14	120.74	115.88
2	B	2033	OMG	C6-N1-C2	4.38	121.02	115.88
2	B	2007	OMC	C6-C5-C4	4.74	119.29	117.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2007	OMC	1	0
2	B	2019	A2M	1	0
2	B	2032	A2M	4	0
2	B	2033	OMG	2	0
2	B	2034	OMG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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$
3	NAG	A	901	1,3	14,14,15	0.76	1 (7%)	15,19,21	1.02	1 (6%)
3	NAG	A	902	3,4	14,14,15	0.83	1 (7%)	15,19,21	0.73	0
4	BMA	A	903	3,5	11,11,12	1.43	1 (9%)	15,15,17	1.06	1 (6%)
5	MAN	A	904	5,4	11,11,12	0.90	0	15,15,17	1.29	2 (13%)
5	MAN	A	905	5	11,11,12	2.01	2 (18%)	15,15,17	1.08	1 (6%)
5	MAN	A	906	5	11,11,12	1.55	2 (18%)	15,15,17	1.50	3 (20%)
5	MAN	A	907	4	11,11,12	1.50	2 (18%)	15,15,17	1.15	2 (13%)
3	NAG	A	908	1,3	14,14,15	0.57	0	15,19,21	0.75	0
3	NAG	A	909	3,4	14,14,15	0.43	0	15,19,21	1.34	2 (13%)
4	BMA	A	910	3,5	11,11,12	3.72	6 (54%)	15,15,17	3.18	7 (46%)
5	MAN	A	911	4	11,11,12	1.85	4 (36%)	15,15,17	1.41	3 (20%)
11	GOL	A	918	-	5,5,5	0.46	0	5,5,5	0.52	0
11	GOL	A	919	-	5,5,5	0.28	0	5,5,5	0.48	0
11	GOL	A	920	-	5,5,5	0.76	0	5,5,5	1.07	0
11	GOL	A	921	-	5,5,5	0.32	0	5,5,5	0.97	0
11	GOL	A	922	-	5,5,5	0.39	0	5,5,5	0.32	0
11	GOL	A	923	-	5,5,5	0.50	0	5,5,5	1.05	0
11	GOL	A	924	-	5,5,5	0.45	0	5,5,5	0.94	0
11	GOL	A	925	-	5,5,5	0.32	0	5,5,5	0.46	0
11	GOL	A	926	-	5,5,5	0.49	0	5,5,5	0.60	0
11	GOL	A	927	-	5,5,5	0.72	0	5,5,5	0.88	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
3	NAG	A	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	902	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	903	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	904	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	905	5	-	0/2/19/22	0/1/1/1
5	MAN	A	906	5	-	0/2/19/22	0/1/1/1
5	MAN	A	907	4	-	0/2/19/22	0/1/1/1
3	NAG	A	908	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	909	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	910	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	911	4	-	0/2/19/22	1/1/1/1
11	GOL	A	918	-	-	0/4/4/4	0/0/0/0
11	GOL	A	919	-	-	0/4/4/4	0/0/0/0
11	GOL	A	920	-	-	0/4/4/4	0/0/0/0
11	GOL	A	921	-	-	0/4/4/4	0/0/0/0
11	GOL	A	922	-	-	0/4/4/4	0/0/0/0
11	GOL	A	923	-	-	0/4/4/4	0/0/0/0
11	GOL	A	924	-	-	0/4/4/4	0/0/0/0
11	GOL	A	925	-	-	0/4/4/4	0/0/0/0
11	GOL	A	926	-	-	0/4/4/4	0/0/0/0
11	GOL	A	927	-	-	0/4/4/4	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	910	BMA	C2-C3	-5.78	1.44	1.52
4	A	910	BMA	O2-C2	-5.06	1.32	1.43
4	A	903	BMA	O5-C1	-3.29	1.38	1.43
4	A	910	BMA	C4-C5	-2.89	1.46	1.53
3	A	902	NAG	O5-C1	-2.83	1.39	1.43
5	A	907	MAN	O4-C4	-2.42	1.37	1.43
4	A	910	BMA	C4-C3	-2.18	1.46	1.52
5	A	911	MAN	O5-C5	2.08	1.48	1.43
3	A	901	NAG	O5-C1	2.12	1.47	1.43
5	A	911	MAN	C4-C3	2.23	1.58	1.52
5	A	906	MAN	O5-C1	2.39	1.47	1.43
5	A	905	MAN	C1-C2	2.67	1.58	1.52
5	A	911	MAN	O5-C1	2.79	1.48	1.43
5	A	906	MAN	C4-C3	2.84	1.59	1.52
5	A	907	MAN	C1-C2	2.85	1.59	1.52
4	A	910	BMA	O5-C1	3.14	1.48	1.43
5	A	911	MAN	C1-C2	4.10	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	905	MAN	C2-C3	5.07	1.59	1.52
4	A	910	BMA	O5-C5	7.95	1.60	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	910	BMA	O2-C2-C3	-6.35	97.38	110.19
4	A	910	BMA	C3-C4-C5	-3.40	104.16	110.23
3	A	901	NAG	O4-C4-C3	-2.79	104.07	110.36
5	A	911	MAN	O2-C2-C3	-2.49	105.17	110.19
5	A	906	MAN	O2-C2-C3	-2.47	105.21	110.19
5	A	911	MAN	C1-C2-C3	-2.41	106.64	109.55
5	A	906	MAN	C1-C2-C3	-2.29	106.78	109.55
4	A	910	BMA	O4-C4-C3	-2.18	105.43	110.36
5	A	907	MAN	O5-C5-C4	-2.11	106.64	110.13
5	A	904	MAN	O2-C2-C3	-2.08	105.99	110.19
5	A	907	MAN	O2-C2-C1	2.17	113.57	109.23
4	A	903	BMA	C1-O5-C5	2.24	115.44	112.14
4	A	910	BMA	O5-C1-C2	2.28	114.54	110.89
5	A	911	MAN	O2-C2-C1	2.52	114.28	109.23
5	A	905	MAN	O3-C3-C2	2.54	114.67	110.01
5	A	904	MAN	C1-O5-C5	2.79	116.24	112.14
3	A	909	NAG	C1-O5-C5	3.13	116.75	112.14
3	A	909	NAG	O4-C4-C3	3.21	117.59	110.36
5	A	906	MAN	C1-O5-C5	3.44	117.20	112.14
4	A	910	BMA	C1-O5-C5	4.51	118.77	112.14
4	A	910	BMA	O5-C5-C6	5.32	118.74	107.34
4	A	910	BMA	C1-C2-C3	6.02	116.85	109.55

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	911	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	909	NAG	1	0
4	A	910	BMA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	920	GOL	3	0
11	A	923	GOL	7	0
11	A	924	GOL	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	786/831 (94%)	0.41	50 (6%) 23 24	19, 30, 67, 96	0
2	B	25/34 (73%)	1.07	7 (28%) 1 1	33, 60, 105, 108	0
All	All	811/865 (93%)	0.44	57 (7%) 19 21	19, 31, 72, 108	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	TYR	7.2
1	A	52	THR	6.9
1	A	586	SER	6.3
1	A	744	ILE	6.1
1	A	460	VAL	6.0
1	A	587	THR	6.0
1	A	56	GLY	5.8
1	A	110	VAL	5.5
1	A	55	SER	5.2
1	A	73	CYS	5.0
1	A	83	SER	4.6
2	B	2018	DT	4.5
1	A	92	LEU	4.3
1	A	464	PRO	4.2
1	A	57	SER	4.1
2	B	2001	DC	4.1
1	A	400	LEU	4.0
1	A	89	PHE	4.0
1	A	54	THR	4.0
2	B	2004	DG	3.6
1	A	588	GLU	3.4
1	A	53	ASN	3.4
2	B	2002	DC	3.4
1	A	88	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	745	GLU	3.2
1	A	86	CYS	3.2
2	B	2003	DT	3.1
1	A	82	TYR	3.1
1	A	97	ALA	3.1
1	A	399	ASN	3.1
1	A	58	CYS	3.0
1	A	85	CYS	3.0
1	A	72	ASP	2.9
1	A	398	ASN	2.8
1	A	96	THR	2.7
1	A	402	TYR	2.7
1	A	87	HIS	2.7
1	A	381	ASP	2.6
1	A	459	ASP	2.6
1	A	773	PHE	2.6
1	A	75	CYS	2.5
1	A	107	CYS	2.5
1	A	111	ARG	2.5
2	B	2017	DA	2.4
1	A	103	THR	2.4
2	B	2031	DC	2.4
1	A	397	PRO	2.4
1	A	59	LYS	2.3
1	A	563	ASP	2.3
1	A	558	LEU	2.2
1	A	74	ARG	2.2
1	A	458	LEU	2.1
1	A	61	ARG	2.1
1	A	102	CYS	2.1
1	A	93	CYS	2.1
1	A	84	SER	2.0
1	A	537	ASN	2.0

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

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	A2M	B	2019	23/24	0.87	0.30	-	112,124,129,133	0
2	OMG	B	2009	24/25	0.97	0.12	-	39,45,50,54	0
2	OMG	B	2015	24/25	0.94	0.20	-	58,65,75,80	0
2	OMC	B	2020	21/22	0.85	0.28	-	106,124,132,137	0
2	OMG	B	2033	24/25	0.75	0.41	-	77,91,96,98	0
2	OMC	B	2007	21/22	0.94	0.16	-	51,57,70,76	0
2	A2M	B	2014	23/24	0.94	0.18	-	47,59,68,71	0
2	A2M	B	2032	23/24	0.80	0.38	-	73,76,86,92	0
2	OMG	B	2034	24/25	0.54	0.40	-	88,99,102,103	0

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
11	GOL	A	926	6/6	0.66	0.31	14.96	44,56,57,60	0
11	GOL	A	924	6/6	0.79	0.32	13.98	56,64,65,65	0
5	MAN	A	905	11/12	0.85	0.26	13.55	56,63,67,69	0
11	GOL	A	923	6/6	0.82	0.26	9.83	63,66,67,68	0
11	GOL	A	920	6/6	0.84	0.24	6.02	47,59,62,64	0
11	GOL	A	921	6/6	0.77	0.23	5.80	60,62,63,64	0
11	GOL	A	918	6/6	0.77	0.28	4.01	57,62,63,65	0
11	GOL	A	927	6/6	0.82	0.35	1.83	52,58,65,67	0
3	NAG	A	901	14/15	0.97	0.13	0.92	20,23,26,29	0
11	GOL	A	919	6/6	0.86	0.14	0.65	53,57,59,60	0
9	CL	A	916	1/1	0.97	0.12	0.08	42,42,42,42	0
11	GOL	A	925	6/6	0.90	0.12	-0.20	57,61,61,62	0
3	NAG	A	908	14/15	0.94	0.13	-0.23	28,34,40,45	0
10	K	A	917	1/1	0.99	0.11	-0.24	23,23,23,23	0
7	CA	A	914	1/1	0.98	0.10	-0.51	22,22,22,22	0
6	ZN	A	913	1/1	1.00	0.12	-0.60	25,25,25,25	0
6	ZN	A	912	1/1	1.00	0.12	-0.86	27,27,27,27	0
8	NA	A	915	1/1	0.99	0.06	-2.29	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	902	14/15	0.96	0.09	-	32,35,39,46	0
5	MAN	A	911	11/12	0.73	0.25	-	71,73,75,76	0
3	NAG	A	909	14/15	0.94	0.16	-	39,44,51,52	0
5	MAN	A	907	11/12	0.77	0.27	-	78,84,85,87	0
4	BMA	A	903	11/12	0.86	0.13	-	52,59,63,70	0
5	MAN	A	906	11/12	0.91	0.21	-	41,51,54,54	0
4	BMA	A	910	11/12	0.73	0.17	-	45,54,62,68	0
7	CA	B	2101	1/1	0.94	0.06	-	49,49,49,49	0
5	MAN	A	904	11/12	0.89	0.18	-	62,63,67,69	0
11	GOL	A	922	6/6	0.78	0.13	-	68,69,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.