Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:11 PM GMT

PDB ID	:	3T6Q
Title	:	Crystal structure of mouse RP105/MD-1 complex
Authors	:	Ohto, U.; Shimizu, T.
Deposited on	:	2011-07-28
Resolution	:	1.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

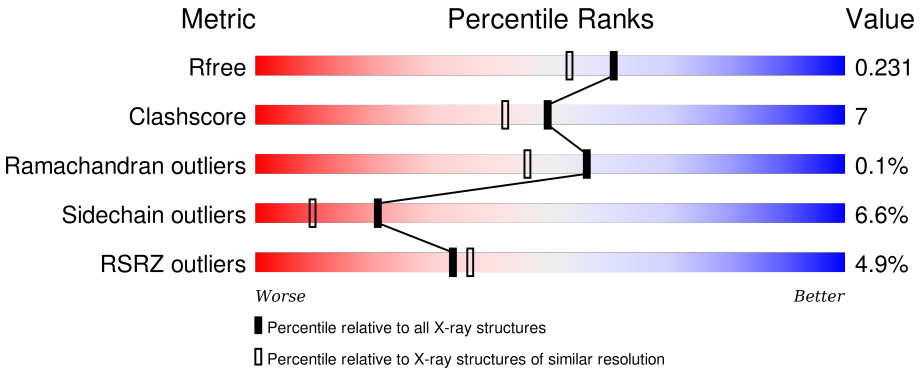
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 <=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	606	% 83% 14%
1	B	606	6% 83% 13%
2	C	145	11% 83% 10%
2	D	145	10% 78% 14%

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
4	GOL	A	10	-	-	-	X
4	GOL	A	6	-	-	-	X
4	GOL	A	9	-	-	-	X
4	GOL	B	11	-	-	-	X
4	GOL	B	5	-	-	-	X
4	GOL	D	14	-	-	-	X
4	GOL	D	7	-	-	-	X
5	NAG	A	701	-	-	-	X
5	NAG	B	701	-	-	-	X
5	NAG	B	703	-	-	-	X
5	NAG	D	202	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13571 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 CD180 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	19	0
			4887	3082	821	957	27			
1	B	601	Total	C	N	O	S	0	7	0
			4789	3030	803	931	25			

- Molecule 2 is a protein called Lymphocyte antigen 86.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	139	Total	C	N	O	S	0	1	0
			1099	692	186	214	7			
2	D	139	Total	C	N	O	S	0	0	0
			1091	688	185	211	7			

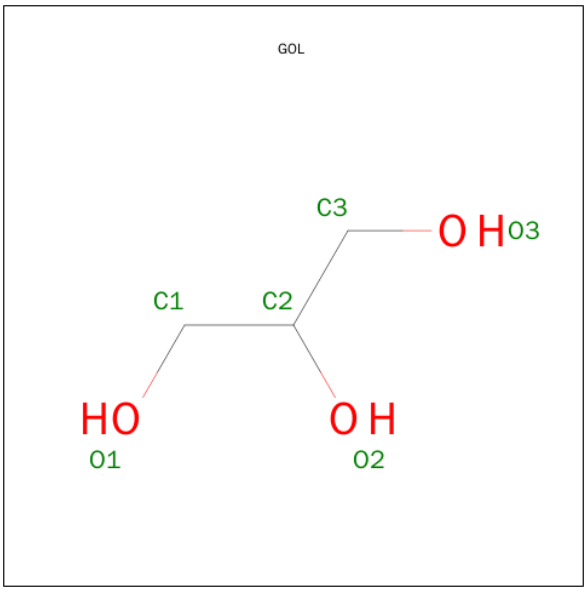
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	163	GLU	-	EXPRESSION TAG	UNP O88188
C	164	PHE	-	EXPRESSION TAG	UNP O88188
D	163	GLU	-	EXPRESSION TAG	UNP O88188
D	164	PHE	-	EXPRESSION TAG	UNP O88188

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cu	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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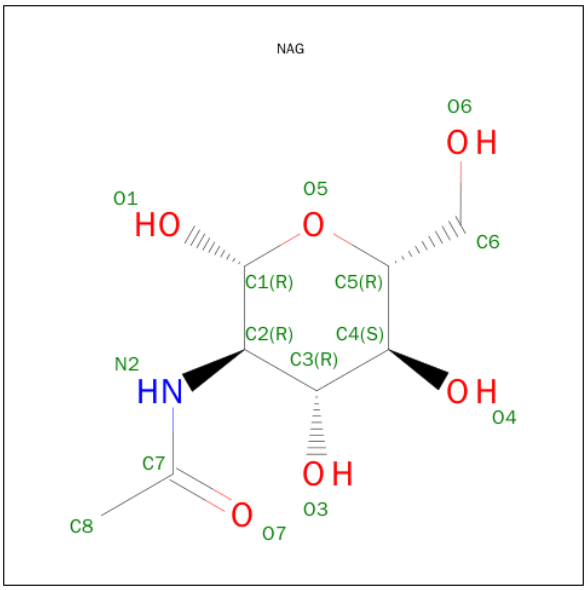
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total C N O 105 58 2 45	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total C N O 28 16 2 10	0	0
7	B	2	Total C N O 28 16 2 10	0	0
7	B	2	Total C N O 28 16 2 10	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	8	Total C N O 94 52 2 40	0	0

- Molecule 9 is water.

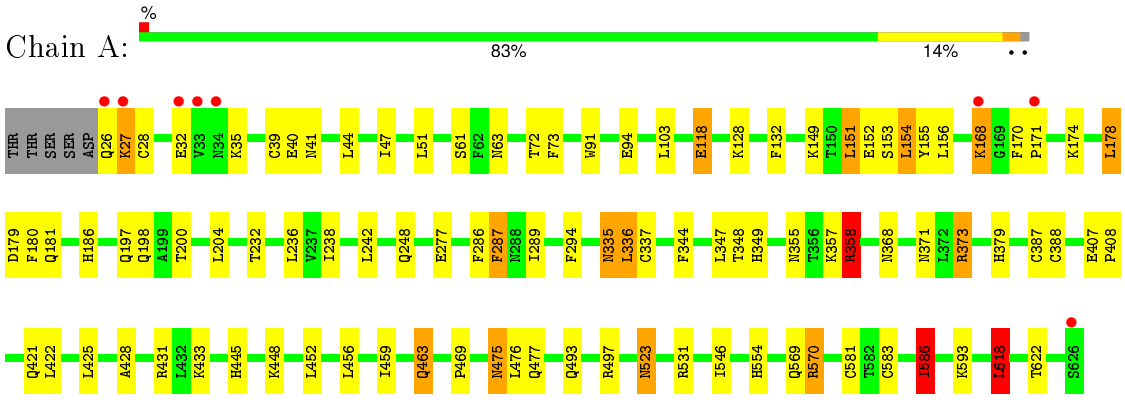
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	556	Total O 556 556	0	0
9	C	97	Total O 97 97	0	0
9	B	419	Total O 419 419	0	0
9	D	77	Total O 77 77	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

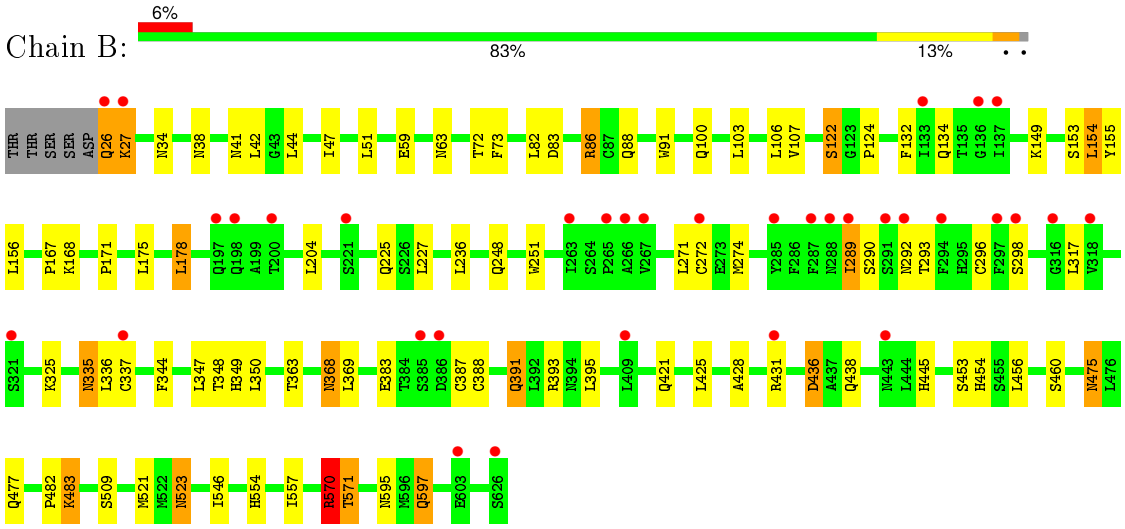
- Molecule 1: CD180 antigen

Chain A:



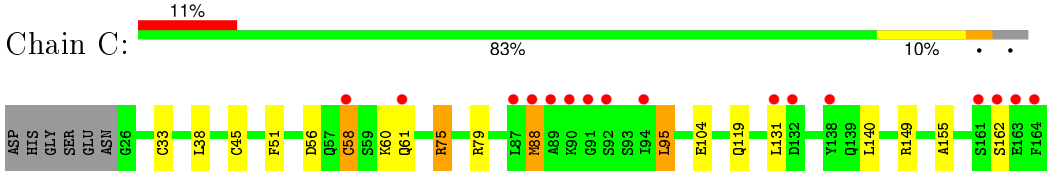
- Molecule 1: CD180 antigen

Chain B:



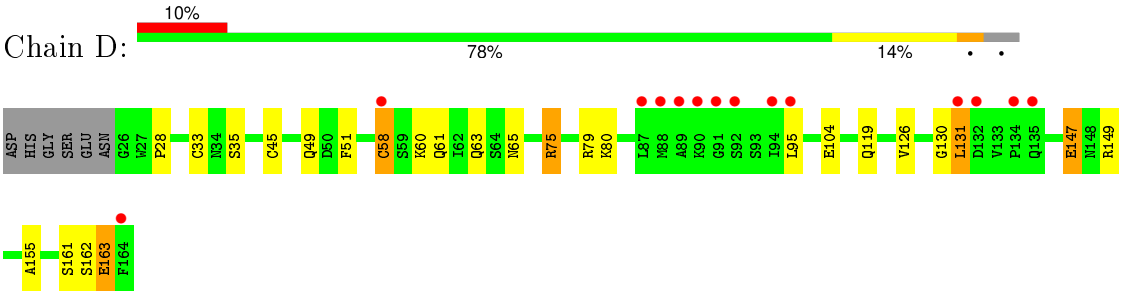
- Molecule 2: Lymphocyte antigen 86

Chain C:



- Molecule 2: Lymphocyte antigen 86

Chain D:


10%
78%
14%
ASP HIS GLY SER GLU ASN G26 V27 P28 C33 M34 S35 C45 Q49 D50 F51 C58 S59 K60 Q61 I62 Q63 S64 N65 R75 R79 K80 L87 M88 A89 K90 G91 S92 S93 I94 L95 E104 Q119 V126 G130 L131 D132 V133 P134 Q135 E147 N148 R149
A155 S161 S162 E163 F164

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	143.75Å 192.79Å 75.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 1.90 49.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.02-1.90) 98.4 (49.02-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.231 0.186 , 0.231	Depositor DCC
R_{free} test set	8204 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 163408 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13571	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, BMA, NAG, CU, 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	0.72	1/4975 (0.0%)	0.79	8/6743 (0.1%)
1	B	0.61	2/4877 (0.0%)	0.73	4/6612 (0.1%)
2	C	0.69	0/1121	0.84	3/1518 (0.2%)
2	D	0.59	0/1113	0.82	2/1507 (0.1%)
All	All	0.66	3/12086 (0.0%)	0.78	17/16380 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	TRP	CD2-CE2	5.72	1.48	1.41
1	B	251	TRP	CD2-CE2	5.41	1.47	1.41
1	B	91	TRP	CD2-CE2	5.03	1.47	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	75	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	570	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	570	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	C	75	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	B	86	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	86	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	531	ARG	NE-CZ-NH1	-6.93	116.84	120.30
1	B	570	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	358	ARG	NE-CZ-NH2	6.63	123.61	120.30
2	C	95	LEU	CA-CB-CG	6.47	130.19	115.30
1	A	358	ARG	NE-CZ-NH1	-6.25	117.17	120.30
2	C	75	ARG	NE-CZ-NH2	-6.19	117.20	120.30
2	D	75	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	570	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	586	ILE	CB-CA-C	-5.43	100.75	111.60
1	A	618	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	531	ARG	NE-CZ-NH2	5.02	122.81	120.30

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	4887	0	4823	81	0
1	B	4789	0	4757	61	0
2	C	1099	0	1058	13	0
2	D	1091	0	1055	20	0
3	A	1	0	0	0	0
4	A	30	0	40	3	0
4	B	24	0	32	4	0
4	C	18	0	24	2	0
4	D	18	0	24	2	0
5	A	70	0	65	0	0
5	B	56	0	52	2	0
5	C	28	0	26	0	0
5	D	28	0	26	0	0
6	A	105	0	88	0	0
7	A	28	0	25	1	0
7	B	56	0	50	1	0
8	B	94	0	79	0	0
9	A	556	0	0	19	0
9	B	419	0	0	10	0
9	C	97	0	0	4	0
9	D	77	0	0	2	0
All	All	13571	0	12224	174	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 7.

All (174) 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:C:79:ARG:NH1	2:C:104:GLU:HG2	1.64	1.11
2:C:79:ARG:HH12	2:C:104:GLU:HG2	1.20	0.99
1:B:391:GLN:HE21	1:B:391:GLN:H	1.15	0.90
1:A:431[B]:ARG:HG3	1:A:431[B]:ARG:HH21	1.37	0.89
1:A:431[B]:ARG:CG	1:A:431[B]:ARG:HH21	1.85	0.89
1:A:168:LYS:HE2	1:A:168:LYS:H	1.37	0.89
1:A:47:ILE:HD11	1:A:73:PHE:HD2	1.40	0.87
1:A:47:ILE:HD11	1:A:73:PHE:CD2	2.10	0.86
1:B:335:ASN:HD22	1:B:337:CYS:H	1.25	0.84
1:A:355:ASN:O	4:A:6:GOL:H32	1.80	0.81
2:D:28:PRO:HB3	4:D:14:GOL:H2	1.64	0.78
2:D:80:LYS:HD2	2:D:147:GLU:HG2	1.66	0.77
1:B:290:SER:O	1:B:293:THR:HG22	1.85	0.76
1:A:335[A]:ASN:HD22	1:A:337:CYS:H	1.31	0.76
1:B:47:ILE:HD11	1:B:73:PHE:CD2	2.24	0.73
1:A:357:LYS:HE3	9:A:751:HOH:O	1.88	0.72
1:A:379:HIS:O	4:A:6:GOL:H31	1.89	0.72
1:B:88:GLN:HG2	9:B:1109:HOH:O	1.89	0.72
1:B:391:GLN:H	1:B:391:GLN:NE2	1.88	0.70
1:B:571:THR:HG23	9:B:848:HOH:O	1.91	0.70
2:D:79:ARG:NH1	2:D:104:GLU:HG2	2.08	0.69
1:A:433:LYS:NZ	9:A:979:HOH:O	2.25	0.69
1:B:570:ARG:HG3	1:B:571:THR:HG22	1.76	0.68
1:B:47:ILE:HG23	1:B:51:LEU:HD12	1.75	0.68
1:B:149:LYS:HB2	9:B:965:HOH:O	1.93	0.68
1:A:181:GLN:NE2	9:A:885:HOH:O	2.27	0.68
1:B:431:ARG:HG2	1:B:456:LEU:HD12	1.76	0.67
1:B:47:ILE:HD12	1:B:72:THR:O	1.95	0.67
1:A:431[A]:ARG:HD2	1:A:433:LYS:HZ3	1.60	0.66
1:A:348:THR:OG1	1:A:349:HIS:HD2	1.78	0.66
1:B:26:GLN:N	1:B:27:LYS:HA	2.09	0.66
1:A:469:PRO:O	1:A:497:ARG:HG3	1.96	0.66
2:D:60:LYS:HD2	2:D:162:SER:O	1.95	0.66
1:B:122:SER:HB3	9:B:983:HOH:O	1.96	0.65
1:B:44:LEU:H	1:B:63:ASN:HD22	1.46	0.64
1:A:431[A]:ARG:NH2	9:A:979:HOH:O	2.30	0.64
1:A:335[A]:ASN:ND2	1:A:337:CYS:H	1.96	0.64
1:B:41:ASN:HD21	2:D:75:ARG:HH21	1.47	0.63
1:B:428:ALA:HB3	7:B:901:NAG:H82	1.80	0.63
2:D:80:LYS:HD2	2:D:147:GLU:CG	2.28	0.62
1:B:47:ILE:HD11	1:B:73:PHE:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431[B]:ARG:CG	1:A:431[B]:ARG:NH2	2.52	0.62
1:A:44:LEU:H	1:A:63:ASN:HD22	1.48	0.62
9:A:1116:HOH:O	4:B:11:GOL:H31	2.00	0.62
1:A:149:LYS:HB2	9:A:1138:HOH:O	2.00	0.61
2:C:58:CYS:HB2	9:C:180:HOH:O	2.00	0.61
1:B:167:PRO:HB3	9:B:1102:HOH:O	2.00	0.61
2:C:79:ARG:HH12	2:C:104:GLU:CG	2.06	0.60
2:D:80:LYS:CD	2:D:147:GLU:HG2	2.31	0.60
1:B:44:LEU:H	1:B:63:ASN:ND2	1.98	0.60
2:D:79:ARG:HH12	2:D:104:GLU:HG2	1.65	0.60
1:A:47:ILE:HG23	1:A:51:LEU:HD12	1.83	0.59
1:B:475:ASN:C	1:B:475:ASN:HD22	2.05	0.59
1:A:371[B]:ASN:CG	9:A:1113:HOH:O	2.39	0.59
1:A:475:ASN:ND2	1:A:477:GLN:H	2.00	0.59
1:B:34:ASN:HD22	5:B:700:NAG:C7	2.15	0.59
2:C:119:GLN:NE2	9:C:370:HOH:O	2.34	0.58
1:B:571:THR:HB	9:B:975:HOH:O	2.04	0.56
1:B:597[A]:GLN:H	1:B:597[A]:GLN:NE2	2.03	0.56
1:A:355:ASN:O	4:A:6:GOL:C3	2.53	0.56
1:A:493[B]:GLN:OE1	9:A:1123:HOH:O	2.18	0.56
2:D:49:GLN:OE1	2:D:75:ARG:HD3	2.07	0.55
1:A:463:GLN:H	1:A:463:GLN:HE21	1.54	0.55
1:A:583:CYS:O	1:A:586:ILE:HG13	2.07	0.55
2:D:119:GLN:NE2	9:D:848:HOH:O	2.40	0.55
1:A:431[A]:ARG:HH21	1:A:433:LYS:HZ3	1.55	0.55
1:A:433:LYS:CE	9:A:979:HOH:O	2.55	0.54
2:C:79:ARG:HH11	2:C:104:GLU:HG2	1.64	0.53
1:A:459:ILE:HG22	1:A:459:ILE:O	2.09	0.53
2:C:56:ASP:HB2	9:C:913:HOH:O	2.10	0.52
1:A:431[B]:ARG:HD2	1:A:456:LEU:HD12	1.90	0.52
1:B:368:ASN:H	1:B:368:ASN:ND2	2.07	0.52
1:A:41:ASN:OD1	2:C:75:ARG:NH2	2.43	0.52
1:A:44:LEU:H	1:A:63:ASN:ND2	2.07	0.52
1:A:118:GLU:HG3	9:A:742:HOH:O	2.08	0.52
1:A:407:GLU:HB3	1:A:408:PRO:CD	2.40	0.52
1:A:128:LYS:HD2	1:A:152:GLU:OE1	2.10	0.52
1:B:523:ASN:C	1:B:523:ASN:HD22	2.13	0.52
5:B:701:NAG:H82	9:B:906:HOH:O	2.10	0.51
1:B:482:PRO:C	1:B:483:LYS:HG2	2.31	0.51
1:A:475:ASN:C	1:A:475:ASN:HD22	2.14	0.51
1:A:151:LEU:HD12	1:A:170:PHE:CZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD12	1:A:72:THR:O	2.11	0.50
1:B:521[B]:MET:HA	1:B:521[B]:MET:CE	2.42	0.50
1:A:431[B]:ARG:NH2	1:A:431[B]:ARG:HG2	2.26	0.50
1:A:178:LEU:HD13	1:A:180:PHE:HE2	1.76	0.50
1:B:348:THR:OG1	1:B:349:HIS:HD2	1.94	0.50
2:D:130:GLY:O	2:D:131:LEU:HB3	2.10	0.50
1:B:26:GLN:CG	1:B:26:GLN:O	2.59	0.49
2:D:80:LYS:HB2	2:D:147:GLU:HG3	1.95	0.49
1:A:546:ILE:H	1:A:569:GLN:HE21	1.61	0.49
1:B:438:GLN:NE2	9:B:934:HOH:O	2.45	0.48
1:B:475:ASN:ND2	1:B:477:GLN:H	2.11	0.48
1:B:154:LEU:HD13	1:B:156:LEU:HD11	1.94	0.48
1:A:431[B]:ARG:HH21	1:A:431[B]:ARG:HG2	1.73	0.48
1:A:186:HIS:HD2	9:A:1105:HOH:O	1.95	0.48
1:A:335[A]:ASN:HD22	1:A:336:LEU:N	2.11	0.48
1:A:428:ALA:HB3	7:A:901:NAG:H82	1.95	0.48
1:B:554:HIS:ND1	4:B:5:GOL:O1	2.45	0.48
1:B:595:ASN:HA	1:B:597[A]:GLN:HE22	1.79	0.48
1:A:28:CYS:HG	1:A:39:CYS:CB	2.27	0.48
2:C:88:MET:HG3	9:C:1137:HOH:O	2.13	0.48
1:A:289:ILE:HD11	1:A:294:PHE:CE2	2.49	0.48
2:D:51:PHE:CZ	2:D:155:ALA:HB2	2.49	0.48
2:C:79:ARG:NH1	2:C:104:GLU:CG	2.57	0.48
1:A:32:GLU:OE2	1:A:35:LYS:HD3	2.14	0.48
1:A:523:ASN:HD22	1:A:523:ASN:C	2.17	0.47
1:A:151:LEU:HD12	1:A:170:PHE:HZ	1.79	0.47
2:D:63:GLN:HG2	9:D:1124:HOH:O	2.14	0.47
1:B:225[A]:GLN:O	1:B:248:GLN:HB3	2.15	0.47
1:A:197:GLN:HG3	1:A:198:GLN:OE1	2.15	0.47
1:A:452:LEU:HB2	1:A:476:LEU:HD23	1.96	0.47
1:A:475:ASN:HD22	1:A:477:GLN:H	1.61	0.47
1:A:448:LYS:HE2	9:A:696:HOH:O	2.16	0.46
1:A:358:ARG:CG	9:A:995:HOH:O	2.62	0.46
1:A:181:GLN:HB3	4:C:12:GOL:H32	1.96	0.46
2:D:35:SER:HB3	2:D:58:CYS:HB3	1.97	0.46
1:B:363:THR:CG2	1:B:393:ARG:HH21	2.29	0.46
1:B:272:CYS:HG	1:B:296:CYS:HG	0.60	0.46
1:B:134:GLN:NE2	4:B:11:GOL:H32	2.31	0.46
1:A:546:ILE:HG12	1:A:569:GLN:NE2	2.31	0.46
2:D:51:PHE:HZ	2:D:155:ALA:HB2	1.81	0.46
1:A:154:LEU:HD13	1:A:156:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:SER:OG	1:B:454:HIS:HD2	1.99	0.45
1:B:100:GLN:HB3	1:B:103:LEU:HB2	1.98	0.45
1:A:200:THR:HG23	9:A:866:HOH:O	2.16	0.45
2:C:60:LYS:HE2	2:C:162:SER:O	2.17	0.45
1:A:358:ARG:HG2	9:A:995:HOH:O	2.16	0.45
1:A:26:GLN:HA	1:A:27:LYS:HA	1.67	0.45
1:A:286:PHE:O	1:A:287:PHE:C	2.55	0.45
1:B:38:ASN:HA	1:B:59:GLU:HB2	1.99	0.45
1:A:593:LYS:HG2	9:A:956:HOH:O	2.18	0.44
2:C:51:PHE:HZ	2:C:155:ALA:HB2	1.82	0.44
1:A:431[A]:ARG:HD2	1:A:433:LYS:NZ	2.31	0.44
1:B:570:ARG:HD2	9:B:1010:HOH:O	2.17	0.44
1:A:463:GLN:H	1:A:463:GLN:NE2	2.14	0.44
1:A:238:ILE:O	1:A:242:LEU:HG	2.17	0.44
1:A:569:GLN:NE2	1:A:569:GLN:HA	2.32	0.44
1:B:103:LEU:HB3	1:B:124:PRO:HB3	2.00	0.44
1:B:175:LEU:HD21	1:B:178:LEU:HG	2.00	0.44
1:A:373:ARG:CZ	9:A:1014:HOH:O	2.66	0.43
1:A:179:ASP:OD2	4:C:12:GOL:H12	2.18	0.43
1:B:335:ASN:ND2	1:B:337:CYS:HB2	2.33	0.43
1:A:149:LYS:HG3	1:A:171:PRO:HG2	2.00	0.43
1:B:570:ARG:HG3	1:B:571:THR:CG2	2.47	0.43
1:B:153:SER:HB3	1:B:155:TYR:CE2	2.54	0.43
1:B:153:SER:HB3	1:B:155:TYR:HE2	1.84	0.43
1:A:40:GLU:HG2	1:A:61[A]:SER:OG	2.19	0.43
2:D:60:LYS:HG2	2:D:161:SER:OG	2.19	0.42
2:C:51:PHE:CZ	2:C:155:ALA:HB2	2.54	0.42
2:D:65:ASN:HA	2:D:126:VAL:O	2.19	0.42
1:A:581:CYS:SG	1:A:618:LEU:HD22	2.60	0.42
1:B:460:SER:HA	9:B:873:HOH:O	2.20	0.42
1:B:554:HIS:CE1	4:B:5:GOL:HO1	2.37	0.42
1:B:149:LYS:HG3	1:B:171:PRO:HG2	2.02	0.42
1:A:569:GLN:HE21	1:A:569:GLN:HA	1.84	0.42
1:A:289:ILE:HG22	9:A:944:HOH:O	2.19	0.42
1:A:344:PHE:HB3	1:A:347:LEU:HG	2.02	0.41
1:B:344:PHE:HB3	1:B:347:LEU:HG	2.01	0.41
1:A:94:GLU:HG2	4:D:14:GOL:H11	2.01	0.41
1:B:42:LEU:H	1:B:63:ASN:HD21	1.67	0.41
1:B:289:ILE:HG23	1:B:289:ILE:O	2.20	0.41
1:A:373:ARG:NH1	9:A:1113:HOH:O	2.46	0.41
2:D:163:GLU:OE2	2:D:163:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:SER:HB3	1:A:155:TYR:CE2	2.55	0.41
1:B:475:ASN:HD22	1:B:477:GLN:H	1.68	0.41
1:B:523:ASN:HA	1:B:546:ILE:HG22	2.02	0.41
1:A:335[A]:ASN:HD22	1:A:337:CYS:N	2.10	0.41
1:B:325:LYS:HE2	1:B:349:HIS:CD2	2.55	0.41
1:B:83:ASP:HA	1:B:107:VAL:HB	2.03	0.41
1:B:41:ASN:HD21	2:D:75:ARG:NH2	2.15	0.40
1:A:546:ILE:H	1:A:569:GLN:NE2	2.19	0.40
1:A:387:CYS:HA	1:A:388:CYS:HA	1.90	0.40
1:B:387:CYS:HA	1:B:388:CYS:HA	1.85	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	618/606 (102%)	592 (96%)	25 (4%)	1 (0%)	52	42
1	B	606/606 (100%)	579 (96%)	26 (4%)	1 (0%)	52	42
2	C	138/145 (95%)	131 (95%)	7 (5%)	0	100	100
2	D	137/145 (94%)	129 (94%)	8 (6%)	0	100	100
All	All	1499/1502 (100%)	1431 (96%)	66 (4%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	PHE
1	B	436	ASP

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	574/560 (102%)	540 (94%)	34 (6%)	24 12
1	B	562/560 (100%)	522 (93%)	40 (7%)	18 8
2	C	122/126 (97%)	112 (92%)	10 (8%)	14 5
2	D	121/126 (96%)	112 (93%)	9 (7%)	17 7
All	All	1379/1372 (100%)	1286 (93%)	93 (7%)	21 9

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	103	LEU
1	A	118	GLU
1	A	132	PHE
1	A	151	LEU
1	A	154	LEU
1	A	168	LYS
1	A	174	LYS
1	A	178	LEU
1	A	204	LEU
1	A	232	THR
1	A	236	LEU
1	A	248	GLN
1	A	277[A]	GLU
1	A	277[B]	GLU
1	A	335[A]	ASN
1	A	335[B]	ASN
1	A	336	LEU
1	A	358	ARG
1	A	368[A]	ASN
1	A	368[B]	ASN
1	A	373	ARG
1	A	421	GLN
1	A	422	LEU

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Mol	Chain	Res	Type
1	A	425	LEU
1	A	445	HIS
1	A	463	GLN
1	A	475	ASN
1	A	523	ASN
1	A	554	HIS
1	A	570	ARG
1	A	586	ILE
1	A	618	LEU
1	A	622	THR
2	C	33	CYS
2	C	38	LEU
2	C	45	CYS
2	C	58	CYS
2	C	61	GLN
2	C	88	MET
2	C	95	LEU
2	C	131	LEU
2	C	140	LEU
2	C	149	ARG
1	B	26	GLN
1	B	27	LYS
1	B	82	LEU
1	B	86	ARG
1	B	106	LEU
1	B	122	SER
1	B	132	PHE
1	B	154	LEU
1	B	168	LYS
1	B	178	LEU
1	B	204	LEU
1	B	227	LEU
1	B	236	LEU
1	B	271	LEU
1	B	274	MET
1	B	289	ILE
1	B	292	ASN
1	B	298	SER
1	B	317	LEU
1	B	335	ASN
1	B	336	LEU
1	B	350	LEU

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Mol	Chain	Res	Type
1	B	368	ASN
1	B	369	LEU
1	B	383	GLU
1	B	391	GLN
1	B	395	LEU
1	B	421	GLN
1	B	425	LEU
1	B	436	ASP
1	B	445	HIS
1	B	475	ASN
1	B	483	LYS
1	B	509	SER
1	B	523	ASN
1	B	557	ILE
1	B	570	ARG
1	B	571	THR
1	B	597[A]	GLN
1	B	597[B]	GLN
2	D	33	CYS
2	D	45	CYS
2	D	58	CYS
2	D	61	GLN
2	D	95	LEU
2	D	131	LEU
2	D	147	GLU
2	D	149	ARG
2	D	163	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	181	GLN
1	A	248	GLN
1	A	288	ASN
1	A	349	HIS
1	A	421	GLN
1	A	445	HIS
1	A	454	HIS
1	A	463	GLN
1	A	475	ASN
1	A	523	ASN

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Mol	Chain	Res	Type
1	A	569	GLN
2	C	43	GLN
2	C	61	GLN
1	B	63	ASN
1	B	88	GLN
1	B	197	GLN
1	B	335	ASN
1	B	349	HIS
1	B	368	ASN
1	B	391	GLN
1	B	421	GLN
1	B	454	HIS
1	B	472	GLN
1	B	475	ASN
1	B	523	ASN
2	D	76	GLN
2	D	119	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

23 carbohydrates 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	$\#\|Z\| > 2$
6	NAG	A	801	1,6	14,14,15	0.94	2 (14%)	15,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	802	6	14,14,15	0.76	0	15,19,21	1.96	4 (26%)
6	BMA	A	803	6	11,11,12	0.64	0	14,15,17	1.23	1 (7%)
6	MAN	A	804	6	11,11,12	1.05	1 (9%)	14,15,17	1.39	2 (14%)
6	MAN	A	805	6	11,11,12	0.59	0	14,15,17	1.38	2 (14%)
6	MAN	A	806	6	11,11,12	1.04	1 (9%)	14,15,17	0.96	1 (7%)
6	MAN	A	807	6	11,11,12	0.59	0	14,15,17	1.47	3 (21%)
6	MAN	A	808	6	11,11,12	0.50	0	14,15,17	1.97	5 (35%)
6	MAN	A	810	6	11,11,12	0.60	0	14,15,17	0.93	0
7	NAG	A	901	1,7	14,14,15	0.76	0	15,19,21	0.90	1 (6%)
7	NAG	A	902	7	14,14,15	0.81	0	15,19,21	1.46	2 (13%)
7	NAG	B	702	1,7	14,14,15	0.66	0	15,19,21	0.85	0
7	NAG	B	705	7	14,14,15	0.62	0	15,19,21	1.24	1 (6%)
8	NAG	B	801	1,8	14,14,15	0.65	0	15,19,21	1.24	1 (6%)
8	NAG	B	802	8	14,14,15	0.58	0	15,19,21	1.19	1 (6%)
8	BMA	B	803	8	11,11,12	0.48	0	14,15,17	1.49	4 (28%)
8	MAN	B	804	8	11,11,12	0.63	0	14,15,17	0.88	0
8	MAN	B	805	8	11,11,12	0.65	0	14,15,17	1.03	1 (7%)
8	MAN	B	806	8	11,11,12	0.71	0	14,15,17	1.60	3 (21%)
8	MAN	B	807	8	11,11,12	0.58	0	14,15,17	1.38	2 (14%)
8	MAN	B	808	8	11,11,12	0.59	0	14,15,17	1.24	3 (21%)
7	NAG	B	901	1,7	14,14,15	0.65	0	15,19,21	1.35	2 (13%)
7	NAG	B	902	7	14,14,15	0.62	0	15,19,21	1.19	2 (13%)

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
6	NAG	A	801	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	802	6	-	0/6/23/26	0/1/1/1
6	BMA	A	803	6	-	0/2/19/22	0/1/1/1
6	MAN	A	804	6	-	0/2/19/22	0/1/1/1
6	MAN	A	805	6	-	0/2/19/22	0/1/1/1
6	MAN	A	806	6	-	0/2/19/22	0/1/1/1
6	MAN	A	807	6	-	0/2/19/22	0/1/1/1
6	MAN	A	808	6	-	0/2/19/22	0/1/1/1
6	MAN	A	810	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	901	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	902	7	-	0/6/23/26	0/1/1/1
7	NAG	B	702	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	705	7	-	0/6/23/26	0/1/1/1
8	NAG	B	801	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	802	8	-	0/6/23/26	0/1/1/1
8	BMA	B	803	8	-	0/2/19/22	0/1/1/1
8	MAN	B	804	8	-	0/2/19/22	0/1/1/1
8	MAN	B	805	8	-	0/2/19/22	0/1/1/1
8	MAN	B	806	8	-	0/2/19/22	0/1/1/1
8	MAN	B	807	8	-	0/2/19/22	0/1/1/1
8	MAN	B	808	8	-	0/2/19/22	0/1/1/1
7	NAG	B	901	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	902	7	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	804	MAN	O5-C1	-2.61	1.39	1.43
6	A	801	NAG	O5-C1	-2.18	1.40	1.43
6	A	801	NAG	C1-C2	2.00	1.55	1.52
6	A	806	MAN	C2-C3	2.22	1.55	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	802	NAG	O6-C6-C5	-3.38	100.16	111.33
6	A	803	BMA	O4-C4-C3	-2.91	103.78	110.34
8	B	806	MAN	O2-C2-C1	-2.90	103.40	109.21
8	B	801	NAG	O4-C4-C5	-2.84	101.70	109.24
6	A	808	MAN	C1-O5-C5	-2.83	108.65	112.25
7	A	902	NAG	O7-C7-C8	-2.73	117.04	122.06
8	B	802	NAG	O6-C6-C5	-2.66	102.53	111.33
6	A	808	MAN	O3-C3-C2	-2.48	105.52	110.00
8	B	807	MAN	C3-C4-C5	-2.16	106.42	110.20
6	A	805	MAN	O2-C2-C3	-2.15	105.79	110.12
8	B	805	MAN	O2-C2-C3	-2.11	105.87	110.12
8	B	803	BMA	O3-C3-C4	-2.06	105.69	110.34
6	A	807	MAN	O6-C6-C5	-2.03	104.62	111.33
6	A	802	NAG	O3-C3-C4	-2.03	105.78	110.34
6	A	806	MAN	O2-C2-C1	-2.02	105.15	109.21
8	B	803	BMA	O6-C6-C5	-2.01	104.68	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	804	MAN	O4-C4-C3	2.01	114.85	110.34
8	B	808	MAN	C2-C3-C4	2.04	114.50	111.04
7	B	902	NAG	C2-N2-C7	2.09	125.73	123.04
6	A	804	MAN	C1-O5-C5	2.20	115.04	112.25
8	B	807	MAN	O2-C2-C3	2.23	114.61	110.12
8	B	808	MAN	O2-C2-C3	2.24	114.62	110.12
7	A	901	NAG	C1-O5-C5	2.29	115.16	112.25
7	B	902	NAG	C1-O5-C5	2.33	115.21	112.25
8	B	808	MAN	O5-C5-C6	2.38	112.50	107.35
8	B	803	BMA	C1-O5-C5	2.55	115.48	112.25
7	B	901	NAG	C2-N2-C7	2.62	126.41	123.04
6	A	807	MAN	O2-C2-C1	2.63	114.47	109.21
8	B	806	MAN	C1-C2-C3	2.72	112.75	109.54
6	A	808	MAN	O2-C2-C1	2.76	114.74	109.21
6	A	808	MAN	C2-C3-C4	2.90	115.97	111.04
6	A	802	NAG	C3-C4-C5	2.91	115.26	110.20
8	B	803	BMA	C1-C2-C3	3.08	113.19	109.54
7	B	901	NAG	C1-O5-C5	3.12	116.21	112.25
7	A	902	NAG	C1-O5-C5	3.30	116.43	112.25
6	A	807	MAN	C1-O5-C5	3.32	116.46	112.25
7	B	705	NAG	C1-O5-C5	3.33	116.47	112.25
6	A	808	MAN	C3-C4-C5	3.37	116.06	110.20
8	B	806	MAN	C1-O5-C5	3.69	116.94	112.25
6	A	805	MAN	C1-O5-C5	4.02	117.36	112.25
6	A	802	NAG	C1-O5-C5	4.47	117.93	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	901	NAG	1	0
7	B	901	NAG	1	0

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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	$\#\|Z\| > 2$
4	GOL	A	10	-	5,5,5	0.35	0	5,5,5	0.34	0
4	GOL	A	15	-	5,5,5	0.28	0	5,5,5	0.54	0
4	GOL	A	3	-	5,5,5	0.35	0	5,5,5	0.75	0
4	GOL	A	6	-	5,5,5	0.53	0	5,5,5	0.48	0
5	NAG	A	700	1	14,14,15	0.52	0	15,19,21	1.22	1 (6%)
5	NAG	A	701	1	14,14,15	0.68	0	15,19,21	0.90	1 (6%)
5	NAG	A	702	1	14,14,15	0.69	0	15,19,21	1.33	1 (6%)
5	NAG	A	703	1	14,14,15	0.52	0	15,19,21	0.97	0
5	NAG	A	704	1	14,14,15	0.47	0	15,19,21	1.22	1 (6%)
4	GOL	A	9	-	5,5,5	0.64	0	5,5,5	0.66	0
4	GOL	B	11	-	5,5,5	0.26	0	5,5,5	0.22	0
4	GOL	B	2	-	5,5,5	0.34	0	5,5,5	0.13	0
4	GOL	B	5	-	5,5,5	0.18	0	5,5,5	1.00	0
5	NAG	B	700	1	14,14,15	0.57	0	15,19,21	1.59	3 (20%)
5	NAG	B	701	1	14,14,15	0.85	0	15,19,21	1.82	4 (26%)
5	NAG	B	703	1	14,14,15	0.54	0	15,19,21	0.94	0
5	NAG	B	704	1	14,14,15	0.51	0	15,19,21	0.83	0
4	GOL	B	8	-	5,5,5	0.21	0	5,5,5	0.34	0
4	GOL	C	12	-	5,5,5	0.32	0	5,5,5	0.36	0
4	GOL	C	13	-	5,5,5	0.25	0	5,5,5	0.51	0
5	NAG	C	201	2	14,14,15	0.49	0	15,19,21	1.33	2 (13%)
5	NAG	C	202	2	14,14,15	0.56	0	15,19,21	2.03	3 (20%)
4	GOL	C	4	-	5,5,5	0.25	0	5,5,5	0.33	0
4	GOL	D	1	-	5,5,5	0.49	0	5,5,5	0.52	0
4	GOL	D	14	-	5,5,5	0.31	0	5,5,5	0.70	0
5	NAG	D	201	2	14,14,15	0.60	0	15,19,21	1.38	2 (13%)
5	NAG	D	202	2	14,14,15	0.72	0	15,19,21	1.63	3 (20%)
4	GOL	D	7	-	5,5,5	0.53	0	5,5,5	0.65	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
4	GOL	A	10	-	-	0/4/4/4	0/0/0/0
4	GOL	A	15	-	-	0/4/4/4	0/0/0/0
4	GOL	A	3	-	-	0/4/4/4	0/0/0/0
4	GOL	A	6	-	-	0/4/4/4	0/0/0/0
5	NAG	A	700	1	-	0/6/23/26	0/1/1/1
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	NAG	A	702	1	-	0/6/23/26	0/1/1/1
5	NAG	A	703	1	-	0/6/23/26	0/1/1/1
5	NAG	A	704	1	-	0/6/23/26	0/1/1/1
4	GOL	A	9	-	-	0/4/4/4	0/0/0/0
4	GOL	B	11	-	-	0/4/4/4	0/0/0/0
4	GOL	B	2	-	-	0/4/4/4	0/0/0/0
4	GOL	B	5	-	-	0/4/4/4	0/0/0/0
5	NAG	B	700	1	-	0/6/23/26	0/1/1/1
5	NAG	B	701	1	-	0/6/23/26	0/1/1/1
5	NAG	B	703	1	-	0/6/23/26	0/1/1/1
5	NAG	B	704	1	-	0/6/23/26	0/1/1/1
4	GOL	B	8	-	-	0/4/4/4	0/0/0/0
4	GOL	C	12	-	-	0/4/4/4	0/0/0/0
4	GOL	C	13	-	-	0/4/4/4	0/0/0/0
5	NAG	C	201	2	-	0/6/23/26	0/1/1/1
5	NAG	C	202	2	-	0/6/23/26	0/1/1/1
4	GOL	C	4	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1	-	-	0/4/4/4	0/0/0/0
4	GOL	D	14	-	-	0/4/4/4	0/0/0/0
5	NAG	D	201	2	-	0/6/23/26	0/1/1/1
5	NAG	D	202	2	-	0/6/23/26	0/1/1/1
4	GOL	D	7	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	701	NAG	O7-C7-C8	-2.96	116.62	122.06
5	A	702	NAG	O7-C7-C8	-2.90	116.75	122.06
5	C	202	NAG	O7-C7-C8	-2.76	117.00	122.06
5	B	700	NAG	O7-C7-C8	-2.31	117.83	122.06
5	C	202	NAG	C6-C5-C4	-2.09	107.87	113.02
5	B	701	NAG	O7-C7-N2	2.08	126.11	121.86
5	C	201	NAG	O5-C5-C6	2.18	112.08	107.35
5	D	202	NAG	C6-C5-C4	2.20	118.44	113.02
5	D	202	NAG	C2-N2-C7	2.30	126.00	123.04
5	D	201	NAG	C2-N2-C7	2.36	126.07	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	701	NAG	C4-C3-C2	2.40	114.96	111.23
5	B	700	NAG	C8-C7-N2	2.64	121.16	116.11
5	D	201	NAG	C4-C3-C2	3.03	115.94	111.23
5	C	201	NAG	C2-N2-C7	3.24	127.21	123.04
5	A	704	NAG	C1-O5-C5	3.28	116.42	112.25
5	B	701	NAG	C4-C3-C2	3.55	116.75	111.23
5	A	700	NAG	C1-O5-C5	3.67	116.91	112.25
5	B	701	NAG	C2-N2-C7	3.74	127.85	123.04
5	B	700	NAG	C3-C4-C5	3.81	116.85	110.20
5	D	202	NAG	C1-O5-C5	4.13	117.49	112.25
5	C	202	NAG	C1-O5-C5	6.39	120.36	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	6	GOL	3	0
4	B	11	GOL	2	0
4	B	5	GOL	2	0
5	B	700	NAG	1	0
5	B	701	NAG	1	0
4	C	12	GOL	2	0
4	D	14	GOL	2	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^{th} 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	601/606 (99%)	-0.05	8 (1%) 79 82	15, 25, 46, 76	0
1	B	601/606 (99%)	0.31	34 (5%) 27 30	19, 35, 61, 88	0
2	C	139/145 (95%)	0.48	16 (11%) 6 7	17, 30, 56, 75	0
2	D	139/145 (95%)	0.58	14 (10%) 9 10	21, 36, 67, 94	0
All	All	1480/1502 (98%)	0.21	72 (4%) 33 36	15, 30, 58, 94	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	PHE	6.5
2	C	92	SER	5.5
1	A	26	GLN	5.2
2	D	94	ILE	5.1
1	B	26	GLN	5.1
1	B	626	SER	5.0
2	D	91	GLY	4.8
2	D	92	SER	4.5
2	C	94	ILE	4.5
2	D	90	LYS	4.4
1	B	263	ILE	4.3
2	C	132[A]	ASP	4.2
2	C	91	GLY	4.2
2	C	89	ALA	4.2
2	C	90	LYS	4.0
1	B	288	ASN	4.0
2	D	95	LEU	3.9
1	A	33	VAL	3.8
1	B	221	SER	3.7
1	B	197	GLN	3.5
1	B	385	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	409	LEU	3.4
2	D	88	MET	3.4
2	C	163	GLU	3.3
1	B	316	GLY	3.3
2	D	131	LEU	3.2
1	B	291	SER	3.2
2	D	132	ASP	3.1
1	B	318	VAL	3.1
2	D	89	ALA	3.1
2	C	162	SER	3.0
1	B	292	ASN	3.0
1	B	289	ILE	2.9
1	B	266	ALA	2.9
1	B	272	CYS	2.8
2	D	58	CYS	2.8
2	C	88	MET	2.8
2	C	87	LEU	2.8
1	B	386	ASP	2.8
1	B	265	PRO	2.8
1	A	32	GLU	2.7
2	C	61	GLN	2.7
1	B	443	ASN	2.6
2	D	164	PHE	2.6
1	B	297	PHE	2.6
1	B	285	TYR	2.6
2	C	164	PHE	2.5
2	D	87	LEU	2.5
1	B	133	ILE	2.5
1	B	137	ILE	2.4
1	B	321	SER	2.4
1	B	198	GLN	2.3
1	B	298	SER	2.3
1	B	200	THR	2.3
1	B	337	CYS	2.3
2	D	135	GLN	2.2
2	C	131	LEU	2.2
1	B	603	GLU	2.2
2	C	161	SER	2.2
2	D	134	PRO	2.2
1	B	267	VAL	2.2
1	A	171	PRO	2.1
1	A	34	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	27	LYS	2.1
2	C	58	CYS	2.1
1	A	168	LYS	2.1
1	A	27	LYS	2.0
1	B	294	PHE	2.0
1	B	431	ARG	2.0
1	A	626	SER	2.0
2	C	138	TYR	2.0
1	B	136	GLY	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)

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^{th} 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^2)	Q<0.9
7	NAG	B	901	14/15	0.97	0.09	0.63	25,27,30,33	0
6	MAN	A	806	11/12	0.98	0.12	0.47	17,18,20,20	0
8	NAG	B	801	14/15	0.97	0.09	0.40	25,27,30,30	0
6	NAG	A	801	14/15	0.98	0.11	0.31	16,19,20,22	0
6	MAN	A	804	11/12	0.98	0.09	-0.06	17,20,22,26	0
6	MAN	A	805	11/12	0.98	0.10	-0.80	17,20,23,24	0
7	NAG	A	901	14/15	0.99	0.09	-0.81	16,19,21,21	0
8	MAN	B	805	11/12	0.97	0.08	-0.81	26,30,36,37	0
8	MAN	B	806	11/12	0.97	0.08	-0.84	26,28,33,34	0
8	MAN	B	804	11/12	0.97	0.07	-4.85	25,29,30,33	0
6	MAN	A	807	11/12	0.97	0.08	-	25,27,37,45	0
8	MAN	B	807	11/12	0.94	0.10	-	27,35,43,49	0
8	NAG	B	802	14/15	0.96	0.09	-	25,29,33,34	0
7	NAG	A	902	14/15	0.95	0.09	-	22,26,31,34	0
7	NAG	B	902	14/15	0.96	0.09	-	28,37,42,42	0
8	BMA	B	803	11/12	0.97	0.07	-	26,31,34,34	0
8	MAN	B	808	11/12	0.90	0.10	-	39,44,57,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	NAG	B	702	14/15	0.91	0.15	-	28,40,53,54	0
6	NAG	A	802	14/15	0.96	0.10	-	17,20,23,36	0
6	BMA	A	803	11/12	0.97	0.09	-	19,23,29,30	0
6	MAN	A	808	11/12	0.84	0.13	-	40,49,66,71	0
7	NAG	B	705	14/15	0.82	0.34	-	51,61,76,81	0
6	MAN	A	810	11/12	0.93	0.13	-	40,56,69,78	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
4	GOL	D	14	6/6	0.82	0.29	6.31	47,54,63,67	0
4	GOL	A	10	6/6	0.84	0.16	6.07	47,51,60,66	0
4	GOL	B	5	6/6	0.89	0.22	5.84	35,41,49,61	0
5	NAG	D	202	14/15	0.58	0.31	5.80	68,81,94,102	0
4	GOL	A	6	6/6	0.79	0.20	4.53	35,45,52,58	0
5	NAG	B	703	14/15	0.88	0.27	4.39	47,60,74,88	0
4	GOL	B	11	6/6	0.91	0.24	3.30	31,44,64,65	0
4	GOL	D	7	6/6	0.84	0.19	3.30	41,51,53,58	0
5	NAG	B	701	14/15	0.84	0.21	3.18	57,69,83,89	0
5	NAG	A	701	14/15	0.81	0.24	2.88	64,74,80,83	0
4	GOL	A	9	6/6	0.82	0.16	2.49	42,50,61,62	0
5	NAG	A	703	14/15	0.94	0.12	1.92	25,32,40,41	0
4	GOL	A	3	6/6	0.88	0.19	1.42	39,48,54,69	0
4	GOL	C	12	6/6	0.89	0.14	0.92	42,52,55,56	0
4	GOL	B	2	6/6	0.90	0.17	0.85	50,53,57,63	0
4	GOL	C	4	6/6	0.98	0.09	-0.53	21,30,32,35	0
5	NAG	A	704	14/15	0.93	0.10	-0.60	28,37,43,50	0
4	GOL	D	1	6/6	0.96	0.10	-0.68	26,33,34,35	0
5	NAG	A	702	14/15	0.86	0.12	-	37,46,57,58	0
5	NAG	D	201	14/15	0.79	0.40	-	88,98,104,120	0
5	NAG	B	700	14/15	0.67	0.37	-	65,85,96,98	0
5	NAG	C	202	14/15	0.75	0.40	-	57,68,86,87	0
5	NAG	B	704	14/15	0.85	0.18	-	58,74,87,88	0
5	NAG	C	201	14/15	0.87	0.24	-	53,67,70,73	0
4	GOL	B	8	6/6	0.95	0.12	-	51,56,60,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	700	14/15	0.79	0.43	-	81,89,96,111	0
3	CU	A	1	1/1	1.00	0.08	-	22,22,22,22	1
4	GOL	A	15	6/6	0.83	0.14	-	51,60,65,67	0
4	GOL	C	13	6/6	0.72	0.21	-	58,63,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.