



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:04 am 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 wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

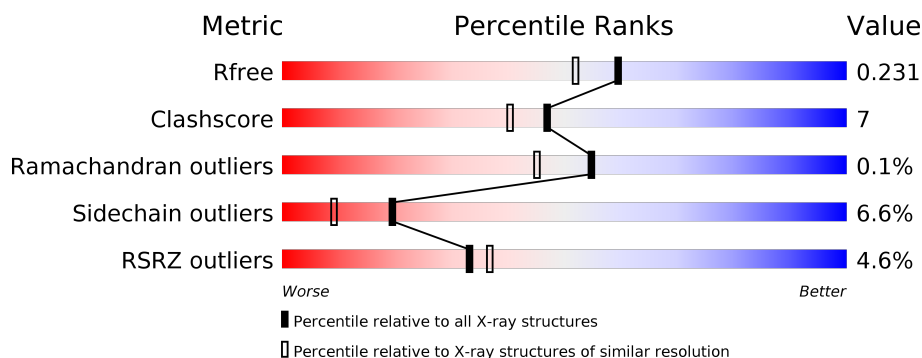
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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 $\leq 5\%$. 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	606	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 83%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
1	B	606	<div> <div style="width: 5%; height: 10px; background-color: red;"></div> <div style="width: 83%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
2	C	145	<div> <div style="width: 10%; height: 10px; background-color: red;"></div> <div style="width: 83%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
2	D	145	<div> <div style="width: 10%; height: 10px; background-color: red;"></div> <div style="width: 78%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 [i](#)

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: C₃H₈O₃).



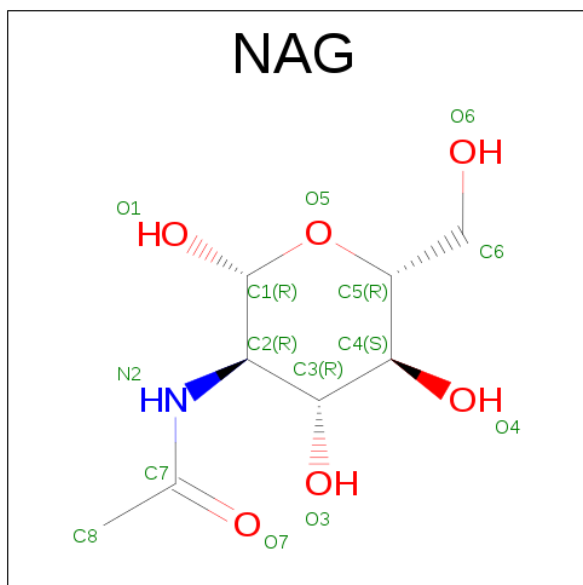
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total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

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

- 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	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- 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	0	0
			105	58	2	45		

- 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	0	0
			28	16	2	10		
7	B	2	Total	C	N	O	0	0
			28	16	2	10		
7	B	2	Total	C	N	O	0	0
			28	16	2	10		

- 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	0	0
			94	52	2	40		

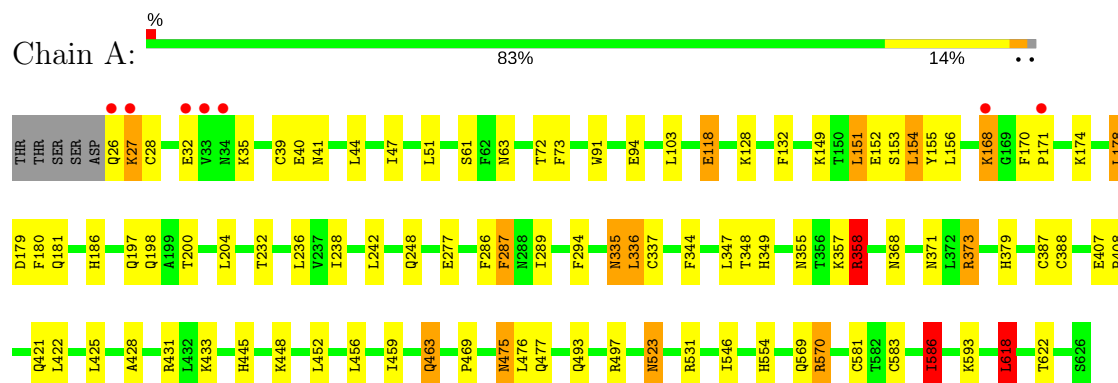
- Molecule 9 is water.

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

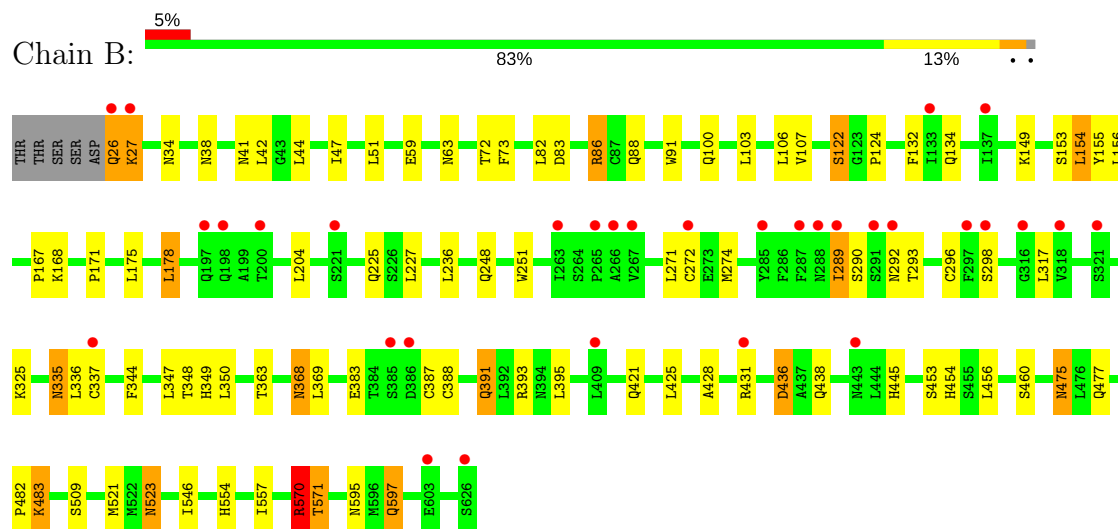
3 Residue-property plots [i](#)

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

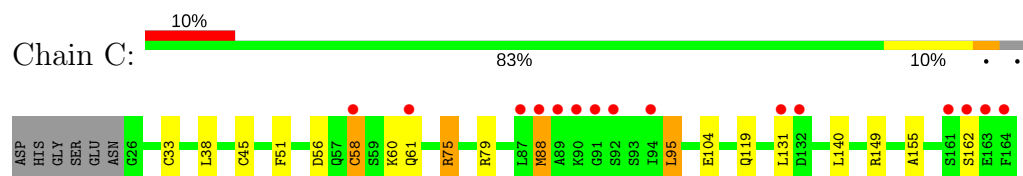
• Molecule 1: CD180 antigen



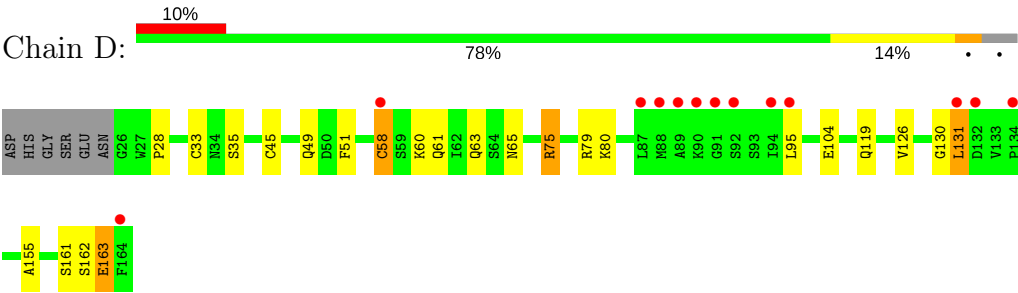
• Molecule 1: CD180 antigen



• Molecule 2: Lymphocyte antigen 86



• Molecule 2: Lymphocyte antigen 86



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	618/606 (102%)	592 (96%)	25 (4%)	1 (0%)	51	41
1	B	606/606 (100%)	579 (96%)	26 (4%)	1 (0%)	51	41
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%)	55	45

All (2) Ramachandran outliers are listed below:

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

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	574/560 (102%)	540 (94%)	34 (6%)	23	12
1	B	562/560 (100%)	522 (93%)	40 (7%)	17	7
2	C	122/126 (97%)	112 (92%)	10 (8%)	13	5
2	D	121/126 (96%)	112 (93%)	9 (7%)	16	7
All	All	1379/1372 (100%)	1286 (93%)	93 (7%)	19	9

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	140	LEU
1	B	168	LYS
2	D	45	CYS
2	C	149	ARG
1	B	86	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	43	GLN
1	B	88	GLN
1	B	523	ASN
2	C	61	GLN
1	B	63	ASN

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	0.95	2 (14%)	15,19,21	0.81	0
6	NAG	A	802	6	14,14,15	0.77	0	15,19,21	2.01	4 (26%)
6	BMA	A	803	6	11,11,12	0.65	0	13,15,17	1.29	1 (7%)
6	MAN	A	804	6	11,11,12	1.07	1 (9%)	13,15,17	1.41	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	805	6	11,11,12	0.61	0	13,15,17	1.35	2 (15%)
6	MAN	A	806	6	11,11,12	1.06	1 (9%)	13,15,17	0.97	0
6	MAN	A	807	6	11,11,12	0.60	0	13,15,17	1.49	2 (15%)
6	MAN	A	808	6	11,11,12	0.52	0	13,15,17	1.99	5 (38%)
6	MAN	A	810	6	11,11,12	0.62	0	13,15,17	0.88	0
7	NAG	A	901	1,7	14,14,15	0.77	0	15,19,21	0.98	1 (6%)
7	NAG	A	902	7	14,14,15	0.82	0	15,19,21	1.43	2 (13%)
7	NAG	B	702	1,7	14,14,15	0.67	0	15,19,21	1.04	0
7	NAG	B	705	7	14,14,15	0.63	0	15,19,21	1.28	1 (6%)
8	NAG	B	801	1,8	14,14,15	0.67	0	15,19,21	1.27	1 (6%)
8	NAG	B	802	8	14,14,15	0.60	0	15,19,21	1.21	1 (6%)
8	BMA	B	803	8	11,11,12	0.49	0	13,15,17	1.49	3 (23%)
8	MAN	B	804	8	11,11,12	0.64	0	13,15,17	0.89	0
8	MAN	B	805	8	11,11,12	0.67	0	13,15,17	1.02	1 (7%)
8	MAN	B	806	8	11,11,12	0.73	0	13,15,17	1.55	3 (23%)
8	MAN	B	807	8	11,11,12	0.59	0	13,15,17	1.34	2 (15%)
8	MAN	B	808	8	11,11,12	0.60	0	13,15,17	1.11	2 (15%)
7	NAG	B	901	1,7	14,14,15	0.67	0	15,19,21	1.34	2 (13%)
7	NAG	B	902	7	14,14,15	0.63	0	15,19,21	1.26	1 (6%)

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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-2.66	1.39	1.43
6	A	801	NAG	O5-C1	-2.23	1.40	1.43
6	A	801	NAG	C1-C2	2.03	1.55	1.52
6	A	806	MAN	C2-C3	2.25	1.55	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	802	NAG	O6-C6-C5	-3.32	100.16	111.34
6	A	803	BMA	O4-C4-C3	-3.02	103.78	110.36
8	B	801	NAG	O4-C4-C5	-3.01	101.70	109.28
8	B	806	MAN	O2-C2-C1	-2.84	103.40	109.18
7	A	902	NAG	O7-C7-C8	-2.75	117.04	122.06

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

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	0.33	0
4	GOL	A	15	-	5,5,5	0.28	0	5,5,5	0.55	0
4	GOL	A	3	-	5,5,5	0.35	0	5,5,5	0.73	0
4	GOL	A	6	-	5,5,5	0.54	0	5,5,5	0.45	0
5	NAG	A	700	1	14,14,15	0.53	0	15,19,21	1.17	1 (6%)
5	NAG	A	701	1	14,14,15	0.69	0	15,19,21	0.99	1 (6%)
5	NAG	A	702	1	14,14,15	0.71	0	15,19,21	1.34	2 (13%)
5	NAG	A	703	1	14,14,15	0.54	0	15,19,21	0.93	0
5	NAG	A	704	1	14,14,15	0.47	0	15,19,21	1.20	1 (6%)
4	GOL	A	9	-	5,5,5	0.66	0	5,5,5	0.63	0
4	GOL	B	11	-	5,5,5	0.27	0	5,5,5	0.24	0
4	GOL	B	2	-	5,5,5	0.35	0	5,5,5	0.11	0
4	GOL	B	5	-	5,5,5	0.18	0	5,5,5	1.02	0
5	NAG	B	700	1	14,14,15	0.58	0	15,19,21	1.90	5 (33%)
5	NAG	B	701	1	14,14,15	0.87	0	15,19,21	2.24	5 (33%)
5	NAG	B	703	1	14,14,15	0.56	0	15,19,21	0.96	0
5	NAG	B	704	1	14,14,15	0.52	0	15,19,21	0.80	0
4	GOL	B	8	-	5,5,5	0.21	0	5,5,5	0.35	0
4	GOL	C	12	-	5,5,5	0.32	0	5,5,5	0.34	0
4	GOL	C	13	-	5,5,5	0.25	0	5,5,5	0.47	0
5	NAG	C	201	2	14,14,15	0.50	0	15,19,21	1.21	1 (6%)
5	NAG	C	202	2	14,14,15	0.57	0	15,19,21	2.20	4 (26%)
4	GOL	C	4	-	5,5,5	0.25	0	5,5,5	0.35	0
4	GOL	D	1	-	5,5,5	0.50	0	5,5,5	0.51	0
4	GOL	D	14	-	5,5,5	0.32	0	5,5,5	0.71	0
5	NAG	D	201	2	14,14,15	0.61	0	15,19,21	1.35	2 (13%)
5	NAG	D	202	2	14,14,15	0.74	0	15,19,21	1.67	4 (26%)
4	GOL	D	7	-	5,5,5	0.54	0	5,5,5	0.64	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.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	700	NAG	O5-C1-C2	-3.76	106.24	111.47
5	B	701	NAG	O7-C7-C8	-2.99	116.62	122.06
5	A	702	NAG	O7-C7-C8	-2.92	116.75	122.06
5	C	202	NAG	O7-C7-C8	-2.78	117.00	122.06
5	B	700	NAG	O7-C7-C8	-2.32	117.83	122.06

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	601/606 (99%)	-0.08	7 (1%) 79 82	15, 25, 46, 76	0
1	B	601/606 (99%)	0.27	32 (5%) 27 31	19, 35, 61, 88	0
2	C	139/145 (95%)	0.44	15 (10%) 6 7	17, 30, 56, 75	0
2	D	139/145 (95%)	0.54	14 (10%) 8 8	21, 36, 67, 94	0
All	All	1480/1502 (98%)	0.17	68 (4%) 33 37	15, 30, 58, 94	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	PHE	6.4
2	C	92	SER	5.4
1	A	26	GLN	5.2
1	B	26	GLN	5.1
2	D	94	ILE	5.0

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, 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
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
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, 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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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.