



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 02:52 PM GMT

PDB ID : 4KR0
Title : Complex structure of MERS-CoV spike RBD bound to CD26
Authors : Lu, G.; Hu, Y.; Wang, Q.; Qi, J.; Gao, F.; Li, Y.; Zhang, Y.; Zhang, W.;
Yuan, Y.; Zhang, B.; Shi, Y.; Yan, J.; Gao, G.F.
Deposited on : 2013-05-15
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

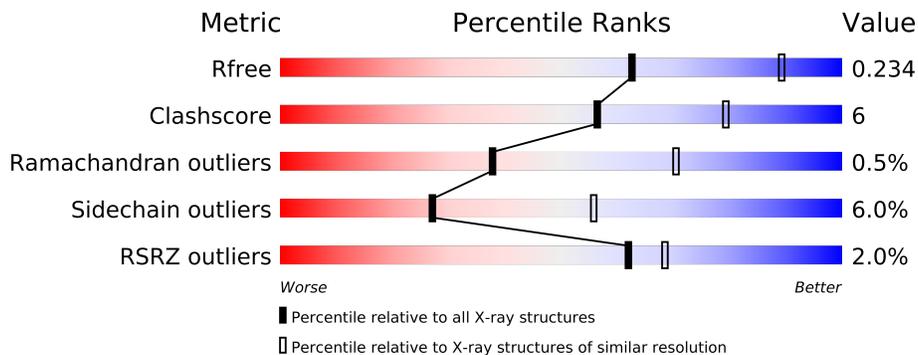
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	739	
2	B	251	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7944 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5963	3827	982	1128	26	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	-	EXPRESSION TAG	UNP P27487
A	35	ASP	-	EXPRESSION TAG	UNP P27487
A	36	GLY	-	EXPRESSION TAG	UNP P27487
A	37	ILE	-	EXPRESSION TAG	UNP P27487
A	38	GLN	-	EXPRESSION TAG	UNP P27487
A	767	HIS	-	EXPRESSION TAG	UNP P27487
A	768	HIS	-	EXPRESSION TAG	UNP P27487
A	769	HIS	-	EXPRESSION TAG	UNP P27487
A	770	HIS	-	EXPRESSION TAG	UNP P27487
A	771	HIS	-	EXPRESSION TAG	UNP P27487
A	772	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is a protein called S protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	208	1608	1026	256	315	11	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	362	ALA	-	EXPRESSION TAG	UNP K0BRG7
B	363	ASP	-	EXPRESSION TAG	UNP K0BRG7
B	364	GLY	-	EXPRESSION TAG	UNP K0BRG7
B	365	ILE	-	EXPRESSION TAG	UNP K0BRG7
B	366	GLN	-	EXPRESSION TAG	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	607	HIS	-	EXPRESSION TAG	UNP K0BRG7
B	608	HIS	-	EXPRESSION TAG	UNP K0BRG7
B	609	HIS	-	EXPRESSION TAG	UNP K0BRG7
B	610	HIS	-	EXPRESSION TAG	UNP K0BRG7
B	611	HIS	-	EXPRESSION TAG	UNP K0BRG7
B	612	HIS	-	EXPRESSION TAG	UNP K0BRG7

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

There are 44 discrepancies between the modelled and reference sequences:

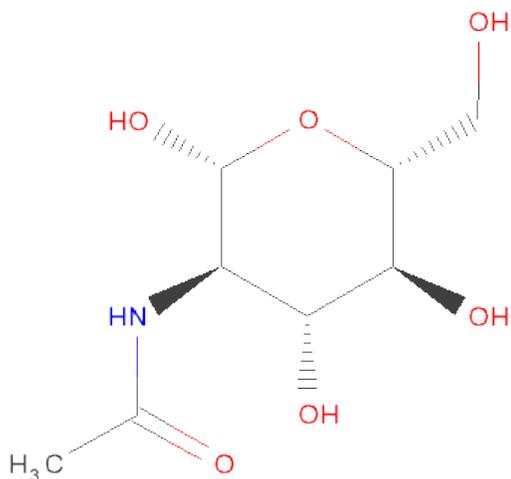
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	-	EXPRESSION TAG	UNP P27487
A	35	ASP	-	EXPRESSION TAG	UNP P27487
A	36	GLY	-	EXPRESSION TAG	UNP P27487
A	37	ILE	-	EXPRESSION TAG	UNP P27487
A	38	GLN	-	EXPRESSION TAG	UNP P27487
A	767	HIS	-	EXPRESSION TAG	UNP P27487
A	768	HIS	-	EXPRESSION TAG	UNP P27487
A	769	HIS	-	EXPRESSION TAG	UNP P27487
A	770	HIS	-	EXPRESSION TAG	UNP P27487
A	771	HIS	-	EXPRESSION TAG	UNP P27487
A	772	HIS	-	EXPRESSION TAG	UNP P27487
A	34	ALA	-	EXPRESSION TAG	UNP P27487
A	35	ASP	-	EXPRESSION TAG	UNP P27487
A	36	GLY	-	EXPRESSION TAG	UNP P27487
A	37	ILE	-	EXPRESSION TAG	UNP P27487
A	38	GLN	-	EXPRESSION TAG	UNP P27487
A	767	HIS	-	EXPRESSION TAG	UNP P27487
A	768	HIS	-	EXPRESSION TAG	UNP P27487
A	769	HIS	-	EXPRESSION TAG	UNP P27487
A	770	HIS	-	EXPRESSION TAG	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
A	771	HIS	-	EXPRESSION TAG	UNP P27487
A	772	HIS	-	EXPRESSION TAG	UNP P27487
A	34	ALA	-	EXPRESSION TAG	UNP P27487
A	35	ASP	-	EXPRESSION TAG	UNP P27487
A	36	GLY	-	EXPRESSION TAG	UNP P27487
A	37	ILE	-	EXPRESSION TAG	UNP P27487
A	38	GLN	-	EXPRESSION TAG	UNP P27487
A	767	HIS	-	EXPRESSION TAG	UNP P27487
A	768	HIS	-	EXPRESSION TAG	UNP P27487
A	769	HIS	-	EXPRESSION TAG	UNP P27487
A	770	HIS	-	EXPRESSION TAG	UNP P27487
A	771	HIS	-	EXPRESSION TAG	UNP P27487
A	772	HIS	-	EXPRESSION TAG	UNP P27487
A	34	ALA	-	EXPRESSION TAG	UNP P27487
A	35	ASP	-	EXPRESSION TAG	UNP P27487
A	36	GLY	-	EXPRESSION TAG	UNP P27487
A	37	ILE	-	EXPRESSION TAG	UNP P27487
A	38	GLN	-	EXPRESSION TAG	UNP P27487
A	767	HIS	-	EXPRESSION TAG	UNP P27487
A	768	HIS	-	EXPRESSION TAG	UNP P27487
A	769	HIS	-	EXPRESSION TAG	UNP P27487
A	770	HIS	-	EXPRESSION TAG	UNP P27487
A	771	HIS	-	EXPRESSION TAG	UNP P27487
A	772	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	-	EXPRESSION TAG	UNP P27487
A	35	ASP	-	EXPRESSION TAG	UNP P27487
A	36	GLY	-	EXPRESSION TAG	UNP P27487
A	37	ILE	-	EXPRESSION TAG	UNP P27487
A	38	GLN	-	EXPRESSION TAG	UNP P27487
A	767	HIS	-	EXPRESSION TAG	UNP P27487
A	768	HIS	-	EXPRESSION TAG	UNP P27487
A	769	HIS	-	EXPRESSION TAG	UNP P27487
A	770	HIS	-	EXPRESSION TAG	UNP P27487
A	771	HIS	-	EXPRESSION TAG	UNP P27487
A	772	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	177	Total	O	0	0
			177	177		
6	B	17	Total	O	0	0
			17	17		

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	110.22Å 110.22Å 527.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.85 – 2.70 48.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.85-2.70) 99.9 (48.85-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, R_{free}	0.198 , 0.232 0.201 , 0.234	Depositor DCC
R_{free} test set	2714 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53442 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7944	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: BMA, NAG

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	0.34	0/6135	0.50	0/8344
2	B	0.33	0/1647	0.50	0/2249
All	All	0.34	0/7782	0.50	0/10593

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5963	0	0	34	0
2	B	1608	0	0	16	0
3	A	112	0	0	0	0
4	A	28	0	0	2	0
5	A	39	0	0	1	0
6	A	177	0	0	15	0
6	B	17	0	0	0	0
All	All	7944	0	0	50	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 6.

All (50) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:TYR:OH	6:A:1016:HOH:O	1.94	0.82
1:A:281:ASN:ND2	6:A:1027:HOH:O	2.22	0.70
1:A:588:ASP:OD2	6:A:1023:HOH:O	2.09	0.69
1:A:400:GLY:O	6:A:923:HOH:O	2.11	0.68
4:A:813:NAG:O6	6:A:953:HOH:O	2.13	0.66
2:B:493:LYS:NZ	2:B:565:GLU:O	2.28	0.66
1:A:457:TYR:OH	6:A:957:HOH:O	2.12	0.65
1:A:435:GLN:NE2	6:A:936:HOH:O	2.29	0.64
2:B:501:ASN:ND2	2:B:559:SER:OG	2.31	0.63
2:B:399:PHE:O	2:B:523:TYR:OH	2.15	0.63
1:A:648:LYS:NZ	1:A:762:CYS:O	2.31	0.63
1:A:242:SER:OG	1:A:243:ASP:N	2.32	0.62
1:A:630:SER:OG	1:A:740:HIS:NE2	2.36	0.58
1:A:329:ASP:OD1	1:A:343:ARG:NH1	2.36	0.58
1:A:381:TYR:OH	6:A:1022:HOH:O	2.17	0.58
1:A:658:ARG:NH1	6:A:1003:HOH:O	2.37	0.57
2:B:384:ASP:OD1	2:B:386:SER:OG	2.23	0.57
2:B:436:ASN:ND2	2:B:577:TYR:OH	2.38	0.57
1:A:299:TYR:OH	6:A:911:HOH:O	2.15	0.56
1:A:336:ARG:NH2	2:B:499:TYR:OH	2.37	0.56
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.37	0.56
1:A:40:ARG:O	1:A:508:GLN:NE2	2.39	0.55
1:A:358:ARG:NH1	6:A:1071:HOH:O	2.40	0.54
1:A:105:TYR:OH	6:A:987:HOH:O	2.18	0.52
1:A:535:ASP:OD1	1:A:537:SER:OG	2.29	0.51
2:B:383:CYS:N	2:B:408:ASN:O	2.44	0.51
1:A:729:ASP:OD2	6:A:941:HOH:O	2.19	0.50
1:A:734:TRP:O	6:A:959:HOH:O	2.20	0.49
1:A:433:LYS:NZ	1:A:488:ASP:OD1	2.46	0.48
2:B:581:THR:O	2:B:583:SER:N	2.47	0.47
2:B:493:LYS:NZ	2:B:564:THR:O	2.48	0.47
1:A:600:THR:OG1	1:A:601:PHE:N	2.48	0.46
1:A:302:ASP:OD1	6:A:926:HOH:O	2.21	0.45
1:A:581:ARG:NH2	1:A:605:ASP:OD1	2.50	0.45
1:A:146:GLU:O	1:A:175:LYS:NZ	2.49	0.45
1:A:201:TRP:NE1	1:A:709:ASP:OD2	2.50	0.45
1:A:74:ASN:ND2	4:A:813:NAG:O7	2.49	0.45
2:B:413:LYS:O	2:B:416:SER:OG	2.35	0.45
1:A:75:ASN:OD1	1:A:92:ASN:N	2.50	0.44
1:A:539:LYS:NZ	1:A:617:GLY:O	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:317:ARG:NH1	2:B:510:ASP:OD2	2.51	0.44
2:B:448:TYR:OH	2:B:452:MET:O	2.36	0.43
1:A:693:GLU:OE2	1:A:696:LYS:NZ	2.52	0.43
1:A:554:LYS:N	1:A:579:ASP:OD1	2.52	0.42
2:B:450:LEU:N	2:B:568:GLN:OE1	2.53	0.41
2:B:426:SER:N	2:B:477:THR:O	2.53	0.41
2:B:395:GLN:O	2:B:398:ASN:N	2.53	0.41
2:B:487:ASN:OD1	2:B:487:ASN:N	2.54	0.41
1:A:331:ASP:OD1	1:A:333:SER:OG	2.39	0.40
5:A:807:NAG:C4	5:A:808:BMA:O2	2.67	0.40

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	726/739 (98%)	690 (95%)	34 (5%)	2 (0%)	50	82
2	B	206/251 (82%)	188 (91%)	15 (7%)	3 (2%)	15	38
All	All	932/990 (94%)	878 (94%)	49 (5%)	5 (0%)	38	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	ASN
2	B	485	PRO
2	B	582	ASN
2	B	382	GLU
1	A	82	GLU

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	653/662 (99%)	620 (95%)	33 (5%)	33	64
2	B	190/224 (85%)	172 (90%)	18 (10%)	12	28
All	All	843/886 (95%)	792 (94%)	51 (6%)	27	56

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	78	VAL
1	A	86	SER
1	A	120	TYR
1	A	142	LEU
1	A	184	ARG
1	A	202	VAL
1	A	265	THR
1	A	277	SER
1	A	313	LEU
1	A	326	ASP
1	A	351	THR
1	A	358	ARG
1	A	385	CYS
1	A	412	SER
1	A	415	LEU
1	A	436	LEU
1	A	442	VAL
1	A	448	GLU
1	A	482	LEU
1	A	489	LYS
1	A	507	VAL
1	A	543	LEU
1	A	546	VAL
1	A	561	LEU
1	A	566	TYR
1	A	630	SER
1	A	660	GLU
1	A	673	LEU
1	A	684	ARG
1	A	685	ASN
1	A	726	VAL
1	A	736	THR

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Mol	Chain	Res	Type
2	B	411	LEU
2	B	423	PHE
2	B	450	LEU
2	B	458	VAL
2	B	465	SER
2	B	473	PHE
2	B	479	LEU
2	B	481	LEU
2	B	484	VAL
2	B	487	ASN
2	B	488	LEU
2	B	490	THR
2	B	510	ASP
2	B	535	TRP
2	B	555	VAL
2	B	565	GLU
2	B	573	ILE
2	B	588	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

11 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
3	NAG	A	801	1,3	12,14,15	0.71	1 (8%)	15,19,21	0.88	1 (6%)
3	NAG	A	802	3	12,14,15	0.68	1 (8%)	15,19,21	1.37	2 (13%)
3	NAG	A	804	1,3	12,14,15	0.72	1 (8%)	15,19,21	1.15	2 (13%)
3	NAG	A	805	3	12,14,15	0.66	1 (8%)	15,19,21	0.77	0
5	NAG	A	806	1,5	12,14,15	0.74	0	15,19,21	1.24	2 (13%)
5	NAG	A	807	5	12,14,15	0.76	1 (8%)	15,19,21	1.38	2 (13%)
5	BMA	A	808	5	10,11,12	0.51	0	11,15,17	0.87	1 (9%)
3	NAG	A	809	1,3	12,14,15	0.69	0	15,19,21	1.22	1 (6%)
3	NAG	A	810	3	12,14,15	0.57	0	15,19,21	1.10	1 (6%)
3	NAG	A	811	1,3	12,14,15	0.59	0	15,19,21	1.11	1 (6%)
3	NAG	A	812	3	12,14,15	0.67	1 (8%)	15,19,21	0.85	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	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	802	3	-	0/6/23/26	0/1/1/1
3	NAG	A	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	805	3	-	0/6/23/26	0/1/1/1
5	NAG	A	806	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	807	5	-	0/6/23/26	0/1/1/1
5	BMA	A	808	5	-	0/2/19/22	0/1/1/1
3	NAG	A	809	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	810	3	-	0/6/23/26	0/1/1/1
3	NAG	A	811	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	812	3	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	NAG	O5-C5	-2.14	1.41	1.45
3	A	804	NAG	O5-C5	-2.13	1.41	1.45
5	A	807	NAG	O5-C5	-2.09	1.41	1.45
3	A	812	NAG	O5-C5	-2.07	1.41	1.45
3	A	802	NAG	O5-C5	-2.05	1.41	1.45
3	A	805	NAG	O5-C5	-2.04	1.41	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	NAG	O5-C5-C6	3.96	111.14	106.98
3	A	809	NAG	O5-C5-C6	3.88	111.05	106.98
5	A	807	NAG	O5-C5-C6	3.78	110.95	106.98
5	A	806	NAG	O5-C5-C6	3.39	110.54	106.98
3	A	811	NAG	O5-C5-C6	3.20	110.34	106.98
3	A	804	NAG	O5-C5-C6	2.73	109.84	106.98
3	A	802	NAG	O5-C5-C4	-2.46	107.54	110.65
5	A	808	BMA	O5-C5-C6	2.37	109.46	106.98
3	A	801	NAG	C3-C4-C5	2.30	114.31	110.20
5	A	807	NAG	O5-C5-C4	-2.20	107.86	110.65
5	A	806	NAG	O4-C4-C3	-2.12	105.59	110.35
3	A	804	NAG	C3-C2-N2	-2.09	108.58	111.76
3	A	810	NAG	C3-C2-N2	2.08	114.93	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry (i)

2 ligands 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$
4	NAG	A	803	1	12,14,15	0.60	0	15,19,21	0.97	1 (6%)
4	NAG	A	813	1	12,14,15	0.61	0	15,19,21	0.86	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
4	NAG	A	803	1	-	0/6/23/26	0/1/1/1
4	NAG	A	813	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	NAG	O5-C5-C6	3.07	110.20	106.98
4	A	813	NAG	O5-C5-C6	2.17	109.25	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	728/739 (98%)	-0.23	12 (1%) 68 74	26, 44, 82, 119	0
2	B	208/251 (82%)	0.08	7 (3%) 43 48	38, 67, 107, 130	0
All	All	936/990 (94%)	-0.16	19 (2%) 62 68	26, 48, 92, 130	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	588	LEU	5.1
1	A	39	SER	4.5
1	A	506	ASN	3.4
2	B	580	ASP	3.1
2	B	587	LYS	3.0
1	A	766	PRO	3.0
1	A	128	TYR	2.9
2	B	486	HIS	2.8
1	A	127	SER	2.6
1	A	95	PHE	2.5
1	A	124	TRP	2.5
2	B	418	PHE	2.5
1	A	96	ASP	2.4
2	B	381	VAL	2.4
1	A	99	GLY	2.3
1	A	123	GLN	2.2
1	A	618	PHE	2.2
1	A	83	TYR	2.0
2	B	391	GLY	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	812	14/15	0.28	6.35	93,106,110,111	0
3	NAG	A	810	14/15	0.23	5.11	40,63,72,82	0
3	NAG	A	811	14/15	0.19	1.33	74,79,90,98	0
3	NAG	A	804	14/15	0.16	0.69	52,65,76,83	0
3	NAG	A	805	14/15	0.17	0.28	70,76,83,88	0
5	NAG	A	807	14/15	0.16	-0.06	47,60,68,69	0
3	NAG	A	801	14/15	0.16	-0.79	89,106,113,117	0
3	NAG	A	809	14/15	0.11	-0.97	42,50,57,62	0
5	NAG	A	806	14/15	0.09	-1.01	30,42,48,50	0
5	BMA	A	808	11/12	0.20	-	85,103,108,113	0
3	NAG	A	802	14/15	0.34	-	108,117,120,122	0

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	A	803	14/15	0.23	1.87	70,85,91,94	0
4	NAG	A	813	14/15	0.27	0.39	89,96,101,102	0

6.5 Other polymers (i)

There are no such residues in this entry.