



Full wwPDB X-ray Structure Validation Report

Oct 22, 2014 – 08:57 AM EDT

PDB ID : 4QZV
Title : Bat-derived coronavirus HKU4 uses MERS-CoV receptor human CD26 for cell entry
Authors : Gao, F.G.; Wang, Q.H.; Qi, J.X.; Lu, G.W.
Deposited on : 2014-07-29
Resolution : 2.59 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>

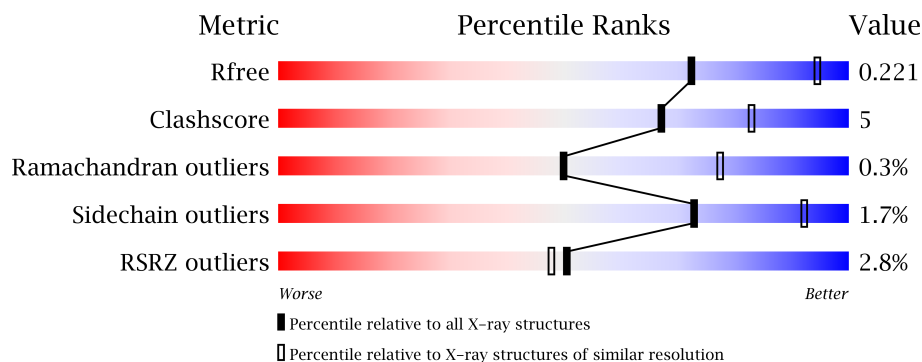
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
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) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.59 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	734	
1	C	734	
2	B	246	
2	D	246	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	C	804	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15900 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
1	A	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	C	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
C	767	HIS	-	EXPRESSION TAG	UNP P27487
C	768	HIS	-	EXPRESSION TAG	UNP P27487
C	769	HIS	-	EXPRESSION TAG	UNP P27487
C	770	HIS	-	EXPRESSION TAG	UNP P27487
C	771	HIS	-	EXPRESSION TAG	UNP P27487
C	772	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1597	1017	260	306	14			
2	D	208	Total	C	N	O	S	0	0	0
			1597	1017	260	306	14			

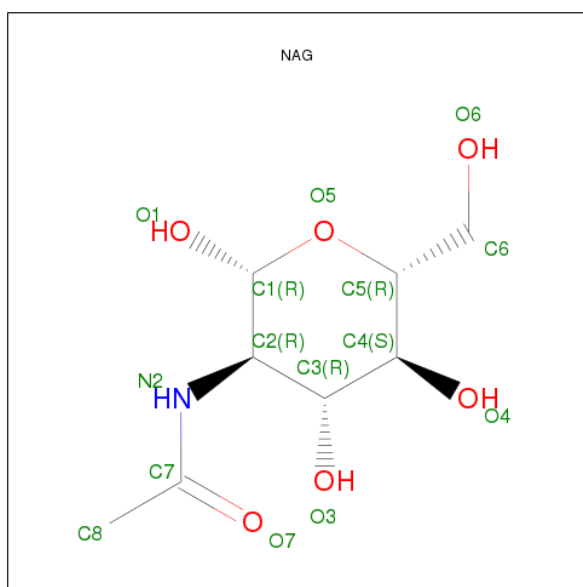
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	241	HIS	-	EXPRESSION TAG	UNP A3EX94
B	242	HIS	-	EXPRESSION TAG	UNP A3EX94
B	243	HIS	-	EXPRESSION TAG	UNP A3EX94
B	244	HIS	-	EXPRESSION TAG	UNP A3EX94
B	245	HIS	-	EXPRESSION TAG	UNP A3EX94
B	246	HIS	-	EXPRESSION TAG	UNP A3EX94
D	241	HIS	-	EXPRESSION TAG	UNP A3EX94
D	242	HIS	-	EXPRESSION TAG	UNP A3EX94
D	243	HIS	-	EXPRESSION TAG	UNP A3EX94
D	244	HIS	-	EXPRESSION TAG	UNP A3EX94
D	245	HIS	-	EXPRESSION TAG	UNP A3EX94
D	246	HIS	-	EXPRESSION TAG	UNP A3EX94

- 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	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

- 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		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	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		
5	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		
6	B	26	Total	O	0	0
			26	26		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	239	Total 239	O 239	0	0
6	D	16	Total 16	O 16	0	0

CYS	VAL	ASP	TYR	HIS	HIS	HIS	HIS	HIS	HIS	GLU	ALA	SER	ALA	THR	GLY	THR	PHE	ILE	GLU	GLN	PRO	ASN	ALA	T15	N22	N44	L49	F52	F57	S58	C59	S63	P64	D65	S66	I67	A68	R69	Y72	S73	Y79	F80	P83	M86	K87	S88	S94	A95	G96	N97	T98	P99	L100	Y101	N102	A116	G117
	V118	L119	L120	N121	V122	T123	T124	T125	K126	R138	L150	Y151	Y157	R161	D162	E170	R177	T180	Q181	F182	E183	T193	D199	S204	Y211	G212	T213	G214	T215	D216	S217	V218	M221	L222	ASP	LEU	GLY	ASP	SER	LEU	THR	ILE	THR	ASN	ARG	LEU	GLY	LYS									

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.80Å 203.17Å 207.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.30 – 2.59 46.30 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.30-2.59) 93.3 (46.30-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.190 , 0.224 0.187 , 0.221	Depositor DCC
R_{free} test set	4863 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.1	EDS
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 102331 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15900	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.29	0/6129	0.46	0/8336
1	C	0.32	0/6129	0.49	1/8336 (0.0%)
2	B	0.39	0/1635	0.49	0/2222
2	D	0.40	0/1635	0.51	0/2222
All	All	0.32	0/15528	0.48	1/21116 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	1
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	ASP	CB-CG-OD2	5.28	123.05	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	121	ASN	Peptide
1	C	96	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	D	121	ASN	Peptide
2	D	215	THR	Peptide

5.2 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 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	5957	0	5673	45	0
1	C	5957	0	5674	54	0
2	B	1597	0	1553	26	0
2	D	1597	0	1553	28	0
3	A	84	0	75	2	0
3	C	84	0	75	0	0
4	A	42	0	39	0	0
4	C	28	0	26	0	0
5	A	39	0	34	0	0
5	C	39	0	34	2	0
6	A	195	0	0	12	0
6	B	26	0	0	1	0
6	C	239	0	0	12	0
6	D	16	0	0	2	0
All	All	15900	0	14736	152	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 5.

All (152) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:658:ARG:NH1	6:A:1029:HOH:O	1.88	1.06
1:A:253:ARG:HH21	1:C:253:ARG:HH21	1.16	0.91
2:D:180:THR:HG22	2:D:183:GLU:HG2	1.59	0.84
2:D:63:SER:OG	2:D:66:SER:OG	1.96	0.84
2:D:138:ARG:NH2	2:D:183:GLU:O	2.11	0.83
2:D:216:ASP:OD1	2:D:217:SER:N	2.11	0.82
2:B:148:THR:OG1	6:B:317:HOH:O	1.98	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:157:TYR:O	6:D:307:HOH:O	2.04	0.76
1:C:40:ARG:NH2	1:C:506:ASN:O	2.19	0.76
1:C:146:GLU:O	1:C:175:LYS:NZ	2.20	0.74
3:A:809:NAG:O4	6:A:935:HOH:O	2.07	0.73
1:A:766:PRO:O	6:A:1040:HOH:O	2.07	0.72
2:D:150:LEU:O	6:D:310:HOH:O	2.07	0.72
1:C:233:VAL:O	6:C:1015:HOH:O	2.08	0.71
1:A:122:LYS:O	6:A:993:HOH:O	2.08	0.71
1:A:597:ARG:NH2	6:A:945:HOH:O	2.23	0.71
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.73	0.69
1:C:302:ASP:OD1	6:C:931:HOH:O	2.10	0.69
1:C:513:LYS:NZ	6:C:930:HOH:O	2.26	0.68
2:B:69:ARG:HH11	2:B:69:ARG:HG2	1.61	0.66
1:A:253:ARG:HH21	1:C:253:ARG:NH2	1.91	0.66
2:D:177:ARG:NH1	2:D:183:GLU:OE2	2.29	0.65
1:A:139:LYS:HG3	1:A:141:GLN:HB2	1.79	0.65
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.78	0.65
1:A:734:TRP:O	6:A:914:HOH:O	2.14	0.65
2:D:126:LYS:NZ	2:D:199:ASP:O	2.30	0.64
1:C:76:ILE:HD12	1:C:90:LEU:HD23	1.80	0.64
2:D:73:SER:HB2	2:D:212:GLY:H	1.63	0.64
2:B:118:VAL:HG12	2:B:122:VAL:HG11	1.80	0.64
1:A:205:GLU:HG2	6:A:1041:HOH:O	1.97	0.64
1:A:329:ASP:OD1	1:A:343:ARG:NH1	2.31	0.63
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.80	0.62
2:D:161:ARG:NH1	2:D:162:ASP:OD1	2.32	0.62
1:A:177:GLU:HB2	1:A:180:LEU:HG	1.82	0.62
1:C:95:PHE:O	1:C:95:PHE:CD2	2.53	0.61
1:C:308:GLN:NE2	6:C:1090:HOH:O	2.30	0.61
1:C:82:GLU:OE1	1:C:467:TYR:OH	2.11	0.61
1:C:135:TYR:CE1	1:C:142:LEU:HB2	2.36	0.60
1:C:95:PHE:HE1	1:C:135:TYR:CZ	2.20	0.60
1:C:555:ALA:O	6:C:983:HOH:O	2.16	0.60
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.85	0.58
1:C:95:PHE:HE1	1:C:135:TYR:HH	1.50	0.58
1:A:146:GLU:O	1:A:175:LYS:NZ	2.35	0.58
2:D:64:PRO:O	2:D:67:ILE:HG22	2.03	0.58
2:D:67:ILE:HG13	2:D:67:ILE:O	2.05	0.57
1:C:658:ARG:NH2	6:C:1091:HOH:O	2.37	0.57
1:A:136:ASP:HB3	1:A:139:LYS:HG2	1.87	0.57
2:B:126:LYS:NZ	2:B:199:ASP:O	2.37	0.57
1:C:729:ASP:OD2	6:C:977:HOH:O	2.16	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:72:TYR:O	2:D:218:VAL:N	2.33	0.56
1:C:67:GLU:OE1	6:C:964:HOH:O	2.18	0.55
1:C:766:PRO:O	6:C:1064:HOH:O	2.18	0.55
1:C:726:VAL:HG12	1:C:728:VAL:HG23	1.89	0.55
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.41	0.54
2:B:118:VAL:CG1	2:B:122:VAL:HG11	2.37	0.54
1:C:95:PHE:HE1	1:C:135:TYR:OH	1.91	0.54
1:A:326:ASP:OD1	1:A:344:GLN:HG2	2.08	0.54
1:C:125:ARG:NE	1:C:205:GLU:OE1	2.32	0.53
1:C:91:GLU:OE1	1:C:91:GLU:N	2.30	0.53
2:B:47:LYS:O	2:B:50:SER:OG	2.22	0.53
1:A:640:LEU:O	6:A:1048:HOH:O	2.19	0.52
2:B:138:ARG:NH2	2:B:183:GLU:O	2.42	0.52
1:C:106:SER:HB3	1:C:115:LEU:HB3	1.90	0.52
1:C:532:PRO:O	6:C:1114:HOH:O	2.19	0.51
1:C:40:ARG:HB3	1:C:508:GLN:NE2	2.26	0.51
1:A:295:ILE:HG22	2:B:189:ILE:HD11	1.92	0.50
1:C:329:ASP:OD1	1:C:343:ARG:NH1	2.44	0.50
1:C:384:ILE:HG13	1:C:404:VAL:HG21	1.93	0.50
2:D:44:ASN:HB2	2:D:221:MET:HE2	1.92	0.50
2:B:90:ILE:HG21	2:B:115:MET:HE1	1.93	0.49
2:D:80:PHE:CE2	2:D:204:SER:HB3	2.48	0.49
1:A:140:ARG:HD3	1:A:140:ARG:N	2.27	0.49
1:A:435:GLN:HE21	1:A:437:SER:HG	1.52	0.48
1:C:75:ASN:HB3	1:C:91:GLU:HA	1.95	0.48
1:A:586:GLN:OE1	6:A:939:HOH:O	2.20	0.48
2:B:22:MET:HA	2:B:79:TYR:CE1	2.48	0.48
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.14	0.48
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.96	0.48
1:A:279:VAL:HG12	1:A:280:THR:HG23	1.95	0.48
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.95	0.48
2:B:181:GLN:OE1	2:B:181:GLN:HA	2.14	0.48
1:A:435:GLN:NE2	1:A:437:SER:OG	2.27	0.47
2:B:92:PRO:HG3	2:B:107:PHE:CZ	2.50	0.47
2:B:215:THR:O	2:B:216:ASP:HB2	2.14	0.47
1:C:277:SER:HG	1:C:280:THR:H	1.63	0.47
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.97	0.47
1:A:82:GLU:HB2	1:A:467:TYR:OH	2.15	0.46
1:C:415:LEU:HB2	1:C:436:LEU:HD21	1.98	0.46
2:B:18:ASP:OD1	2:B:20:SER:OG	2.25	0.46
3:A:802:NAG:O4	6:A:1031:HOH:O	2.20	0.46
2:B:205:PHE:HE1	2:B:207:ILE:HD11	1.79	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:461:PHE:CD2	1:C:468:TYR:HB3	2.51	0.46
1:C:148:ILE:HD11	1:C:164:LEU:HD13	1.97	0.45
1:C:217:SER:HB3	1:C:222:PHE:HB2	1.97	0.45
1:C:280:THR:O	6:C:1050:HOH:O	2.21	0.45
2:D:95:ALA:HA	2:D:96:GLY:HA3	1.63	0.45
2:D:57:PHE:HE2	2:D:59:CYS:SG	2.40	0.45
2:D:98:ILE:HA	2:D:102:ASN:HD22	1.81	0.45
1:C:79:PHE:CE1	1:C:86:SER:HB3	2.51	0.44
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.99	0.44
1:C:51:ASN:OD1	1:C:54:ARG:CZ	2.65	0.44
2:D:22:MET:HA	2:D:79:TYR:CE1	2.51	0.44
1:C:71:LYS:HE3	1:C:105:TYR:CE2	2.52	0.44
1:A:242:SER:OG	1:A:243:ASP:N	2.51	0.44
2:D:49:LEU:HD21	2:D:57:PHE:HE1	1.83	0.44
5:C:806:NAG:H61	2:D:170:GLU:HB2	1.98	0.44
2:D:95:ALA:HB1	2:D:99:PRO:HG2	2.00	0.44
1:A:410:LEU:HD13	1:A:415:LEU:HD23	2.00	0.44
1:C:504:LEU:HA	1:C:507:VAL:HG12	2.00	0.43
5:C:806:NAG:O3	5:C:807:BMA:H2	2.18	0.43
2:B:130:TYR:HB2	2:B:195:VAL:HB	2.00	0.43
2:D:73:SER:HB2	2:D:212:GLY:N	2.30	0.43
2:D:215:THR:O	2:D:216:ASP:HB2	2.18	0.43
1:A:306:ALA:HB3	1:A:310:ARG:HG2	2.00	0.43
1:A:106:SER:HB3	1:A:115:LEU:HB3	2.01	0.42
1:C:377:ASN:ND2	1:C:383:HIS:HD2	2.18	0.42
1:C:630:SER:O	1:C:633:GLY:N	2.52	0.42
2:B:44:ASN:HB2	2:B:221:MET:HE2	2.01	0.42
1:A:105:TYR:HB2	1:A:114:ILE:HD11	2.00	0.42
1:C:95:PHE:CE2	1:C:102:ILE:HD11	2.55	0.42
1:A:429:ARG:HB2	1:A:457:TYR:H	1.84	0.42
1:C:506:ASN:N	1:C:506:ASN:HD22	2.16	0.42
2:B:118:VAL:HG23	2:B:201:LEU:O	2.20	0.42
1:C:72:GLN:HB3	1:C:75:ASN:OD1	2.20	0.42
2:B:23:LEU:HD12	2:B:23:LEU:HA	1.77	0.41
1:C:225:TYR:CZ	1:C:269:PHE:HB2	2.54	0.41
1:C:504:LEU:O	6:C:1005:HOH:O	2.21	0.41
1:A:332:GLU:HG3	1:A:333:SER:N	2.35	0.41
1:A:760:LYS:NZ	6:A:1054:HOH:O	2.45	0.41
2:B:52:PHE:HB3	2:B:116:ALA:HB1	2.03	0.41
1:C:229:ASN:HB3	1:C:265:THR:OG1	2.20	0.41
2:D:52:PHE:HB3	2:D:116:ALA:HB1	2.03	0.41
2:D:83:PRO:HG2	2:D:86:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:49:LEU:HD21	2:B:57:PHE:HE2	1.86	0.41
2:B:56:GLU:HB3	2:B:115:MET:HB2	2.02	0.41
2:B:119:LEU:O	2:B:122:VAL:HG12	2.21	0.41
1:A:501:ASP:O	1:A:505:GLN:HG3	2.21	0.41
1:A:726:VAL:HG13	1:A:728:VAL:HG23	2.02	0.41
1:A:184:ARG:HD3	1:A:187:TRP:CE2	2.56	0.41
1:C:765:LEU:HA	1:C:766:PRO:HD3	1.95	0.41
2:D:100:LEU:HD22	2:D:151:TYR:CD1	2.56	0.41
2:D:161:ARG:O	2:D:161:ARG:HG2	2.19	0.41
1:A:248:TYR:CZ	1:C:234:PRO:HB2	2.56	0.41
1:A:266:VAL:O	6:A:1008:HOH:O	2.22	0.41
1:C:71:LYS:HE3	1:C:105:TYR:CD2	2.56	0.40
1:C:51:ASN:OD1	1:C:54:ARG:NH2	2.54	0.40
2:B:101:TYR:O	2:B:158:SER:HB2	2.21	0.40
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.56	0.40
1:A:95:PHE:CZ	1:A:116:LEU:HD11	2.56	0.40
1:C:640:LEU:HD11	1:C:650:GLY:HA3	2.02	0.40
2:B:163:PHE:CE1	2:B:177:ARG:HB2	2.57	0.40
2:B:215:THR:O	2:B:215:THR:OG1	2.32	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	725/734 (99%)	694 (96%)	31 (4%)	0	100	100
1	C	725/734 (99%)	688 (95%)	34 (5%)	3 (0%)	43	72
2	B	206/246 (84%)	189 (92%)	16 (8%)	1 (0%)	38	67
2	D	206/246 (84%)	195 (95%)	10 (5%)	1 (0%)	38	67
All	All	1862/1960 (95%)	1766 (95%)	91 (5%)	5 (0%)	50	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	216	ASP
1	C	97	GLU
1	C	520	ASN
1	C	73	GLU
2	D	216	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	652/659 (99%)	648 (99%)	4 (1%)	92	98
1	C	652/659 (99%)	644 (99%)	8 (1%)	82	95
2	B	180/212 (85%)	174 (97%)	6 (3%)	50	79
2	D	180/212 (85%)	169 (94%)	11 (6%)	26	50
All	All	1664/1742 (96%)	1635 (98%)	29 (2%)	73	92

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	107	ILE
1	A	279	VAL
1	A	326	ASP
2	B	60	ASN
2	B	111	THR
2	B	118	VAL
2	B	213	THR
2	B	216	ASP
2	B	217	SER
1	C	54	ARG
1	C	74	ASN
1	C	107	ILE
1	C	250	LYS
1	C	277	SER
1	C	506	ASN
1	C	507	VAL
1	C	726	VAL

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Mol	Chain	Res	Type
2	D	49	LEU
2	D	57	PHE
2	D	59	CYS
2	D	66	SER
2	D	67	ILE
2	D	69	ARG
2	D	88	SER
2	D	118	VAL
2	D	161	ARG
2	D	181	GLN
2	D	193	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	731	GLN
2	B	121	ASN
1	C	506	ASN
2	D	153	ASN

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 ⓘ

18 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	0.47	0	15,19,21	0.66	0
3	NAG	A	802	3	12,14,15	0.41	0	15,19,21	0.58	0
5	NAG	A	805	1,5	12,14,15	0.56	0	15,19,21	0.67	0
5	NAG	A	806	5	12,14,15	0.44	0	15,19,21	0.76	1 (6%)
5	BMA	A	807	5	10,11,12	1.57	3 (30%)	11,15,17	2.51	4 (36%)
3	NAG	A	808	1,3	12,14,15	0.44	0	15,19,21	0.54	0
3	NAG	A	809	3	12,14,15	0.28	0	15,19,21	0.39	0
3	NAG	A	810	1,3	12,14,15	0.46	0	15,19,21	0.53	0
3	NAG	A	811	3	12,14,15	0.39	0	15,19,21	0.44	0
3	NAG	C	801	1,3	12,14,15	0.42	0	15,19,21	0.50	0
3	NAG	C	802	3	12,14,15	0.41	0	15,19,21	0.39	0
5	NAG	C	805	1,5	12,14,15	0.78	0	15,19,21	0.61	0
5	NAG	C	806	5	12,14,15	0.41	0	15,19,21	0.47	0
5	BMA	C	807	5	10,11,12	1.59	3 (30%)	11,15,17	2.74	5 (45%)
3	NAG	C	808	1,3	12,14,15	0.40	0	15,19,21	0.49	0
3	NAG	C	809	3	12,14,15	0.31	0	15,19,21	0.39	0
3	NAG	C	810	1,3	12,14,15	0.41	0	15,19,21	0.43	0
3	NAG	C	811	3	12,14,15	0.30	0	15,19,21	0.45	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
5	NAG	A	805	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	806	5	-	0/6/23/26	0/1/1/1
5	BMA	A	807	5	-	0/2/19/22	0/1/1/1
3	NAG	A	808	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	809	3	-	0/6/23/26	0/1/1/1
3	NAG	A	810	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	811	3	-	0/6/23/26	0/1/1/1
3	NAG	C	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	802	3	-	0/6/23/26	0/1/1/1
5	NAG	C	805	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	806	5	-	0/6/23/26	0/1/1/1
5	BMA	C	807	5	-	0/2/19/22	0/1/1/1
3	NAG	C	808	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	809	3	-	0/6/23/26	0/1/1/1
3	NAG	C	810	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	811	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)
5	A	807	BMA	C4-C3	-3.17	1.44	1.52
5	C	807	BMA	C4-C3	-3.07	1.44	1.52
5	C	807	BMA	O5-C5	2.50	1.50	1.45
5	A	807	BMA	C3-C2	-2.37	1.48	1.52
5	C	807	BMA	C3-C2	-2.27	1.48	1.52
5	A	807	BMA	O5-C5	2.14	1.49	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	807	BMA	C4-C3-C2	4.75	115.90	110.61
5	C	807	BMA	C3-C4-C5	4.69	118.59	110.17
5	A	807	BMA	C3-C4-C5	4.39	118.05	110.17
5	A	807	BMA	C4-C3-C2	4.32	115.43	110.61
5	A	807	BMA	O5-C5-C4	4.22	116.01	110.65
5	C	807	BMA	O5-C5-C4	4.13	115.89	110.65
5	C	807	BMA	O5-C5-C6	3.34	110.49	106.98
5	A	807	BMA	O5-C5-C6	2.32	109.42	106.98
5	C	807	BMA	O6-C6-C5	2.21	119.05	111.37
5	A	806	NAG	O5-C5-C4	-2.07	108.03	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

5 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	0.42	0	15,19,21	0.39	0
4	NAG	A	804	1	12,14,15	0.39	0	15,19,21	0.39	0
4	NAG	A	812	1	12,14,15	0.35	0	15,19,21	0.35	0
4	NAG	C	803	1	12,14,15	0.36	0	15,19,21	0.36	0
4	NAG	C	804	1	12,14,15	0.39	0	15,19,21	0.34	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	NAG	A	803	1	-	0/6/23/26	0/1/1/1
4	NAG	A	804	1	-	0/6/23/26	0/1/1/1
4	NAG	A	812	1	-	0/6/23/26	0/1/1/1
4	NAG	C	803	1	-	0/6/23/26	0/1/1/1
4	NAG	C	804	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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	727/734 (99%)	-0.01	11 (1%)	70 71	22, 41, 69, 142	0
1	C	727/734 (99%)	-0.00	18 (2%)	54 52	21, 39, 68, 199	0
2	B	208/246 (84%)	0.30	10 (4%)	29 26	34, 55, 96, 119	0
2	D	208/246 (84%)	0.49	14 (6%)	17 15	33, 58, 124, 171	0
All	All	1870/1960 (95%)	0.08	53 (2%)	50 48	21, 43, 84, 199	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	213	THR	8.4
1	C	95	PHE	8.1
2	D	214	GLY	6.8
1	C	135	TYR	6.4
1	C	94	THR	5.8
2	B	123	THR	5.5
2	D	222	LEU	5.4
2	D	215	THR	5.3
2	D	121	ASN	5.1
2	D	120	ALA	5.1
1	C	96	ASP	4.9
1	A	95	PHE	4.6
2	D	124	ILE	4.4
2	B	119	LEU	3.9
1	C	98	PHE	3.9
1	C	142	LEU	3.9
2	B	124	ILE	3.9
2	D	212	GLY	3.7
1	A	142	LEU	3.6
1	C	99	GLY	3.5
1	C	143	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	94	SER	3.4
2	B	205	PHE	3.4
2	B	222	LEU	3.3
2	D	182	PHE	3.2
1	C	139	LYS	3.2
1	C	97	GLU	3.1
1	C	141	GLN	3.0
1	A	135	TYR	2.9
1	A	506	ASN	2.9
1	C	73	GLU	2.9
1	A	96	ASP	2.8
1	C	100	HIS	2.7
1	A	72	GLN	2.7
1	C	93	SER	2.6
2	B	125	THR	2.6
1	C	72	GLN	2.6
1	A	134	ILE	2.5
2	D	211	TYR	2.4
2	B	120	ALA	2.4
2	D	180	THR	2.4
2	D	123	THR	2.4
1	C	137	LEU	2.4
2	B	215	THR	2.3
1	C	101	SER	2.3
1	A	94	THR	2.2
2	B	69	ARG	2.2
1	A	90	LEU	2.2
2	B	121	ASN	2.2
1	A	173	TYR	2.2
1	C	140	ARG	2.1
2	D	181	GLN	2.1
1	A	395	THR	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 ⓘ

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	C	811	14/15	0.25	28.28	76,91,94,95	0
3	NAG	C	809	14/15	0.20	9.63	51,70,77,92	0
3	NAG	A	809	14/15	0.25	9.27	62,73,79,85	0
5	BMA	A	807	11/12	0.28	7.51	110,122,127,129	0
5	BMA	C	807	11/12	0.23	7.43	98,109,123,126	0
5	NAG	C	806	14/15	0.21	6.44	60,71,79,80	0
3	NAG	A	810	14/15	0.23	4.13	57,67,76,82	0
3	NAG	C	810	14/15	0.24	2.65	49,58,66,78	0
3	NAG	A	811	14/15	0.27	1.98	80,86,91,94	0
5	NAG	A	806	14/15	0.16	1.73	51,65,79,84	0
3	NAG	A	801	14/15	0.16	0.68	60,63,69,73	0
5	NAG	A	805	14/15	0.14	0.43	33,39,54,59	0
3	NAG	A	802	14/15	0.18	0.05	50,60,68,70	0
3	NAG	C	808	14/15	0.15	0.00	51,59,62,62	0
3	NAG	A	808	14/15	0.15	-0.15	46,51,59,61	0
3	NAG	C	801	14/15	0.14	-0.22	65,81,92,102	0
5	NAG	C	805	14/15	0.11	-0.71	23,40,52,59	0
3	NAG	C	802	14/15	0.23	-	105,114,123,127	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	C	804	14/15	0.20	3.68	71,81,90,92	0
4	NAG	A	804	14/15	0.16	0.96	61,70,78,80	0
4	NAG	C	803	14/15	0.23	0.96	61,80,84,86	0
4	NAG	A	812	14/15	0.29	0.52	98,105,114,114	0
4	NAG	A	803	14/15	0.20	-0.43	59,82,88,89	0

6.5 Other polymers ⓘ

There are no such residues in this entry.