



Full wwPDB X-ray Structure Validation Report

Sep 16, 2014 – 03:50 PM EDT

PDB ID : 4MWF
Title : Structure of Hepatitis C Virus Envelope Glycoprotein E2 core bound to broadly neutralizing antibody AR3C
Authors : Kong, L.; Wilson, I.A.; Law, M.
Deposited on : 2013-09-24
Resolution : 2.65 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>

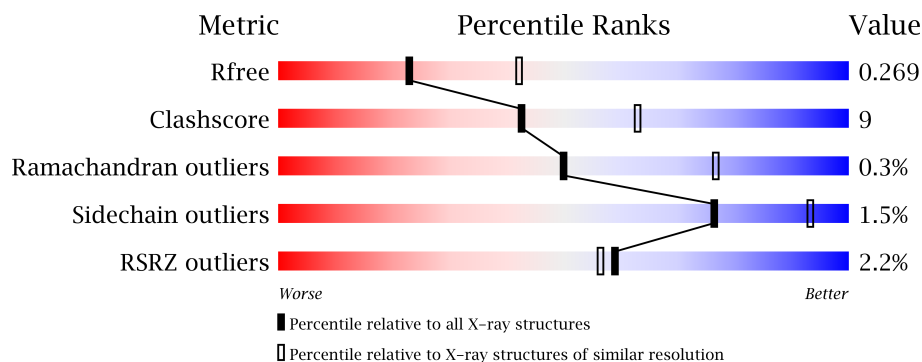
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
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) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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	2393 (2.68-2.60)
Clashscore	79885	2915 (2.68-2.60)
Ramachandran outliers	78287	2865 (2.68-2.60)
Sidechain outliers	78261	2865 (2.68-2.60)
RSRZ outliers	66119	2393 (2.68-2.60)

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	233	
1	H	233	
2	B	214	
2	L	214	
3	C	212	
3	D	212	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9433 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 Fab AR3C heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1663	1047	282	327	7			
1	H	228	Total	C	N	O	S	0	0	0
			1697	1065	288	337	7			

- Molecule 2 is a protein called Fab AR3C light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1612	1005	277	326	4			
2	L	212	Total	C	N	O	S	0	0	0
			1620	1011	278	327	4			

- Molecule 3 is a protein called Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	169	Total	C	N	O	S	0	0	0
			1288	818	218	235	17			
3	D	171	Total	C	N	O	S	0	0	0
			1305	831	222	235	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	448	ASP	ASN	ENGINEERED MUTATION	UNP P27958
C	482	GLY	-	LINKER	UNP P27958
C	483	SER	-	LINKER	UNP P27958
C	484	SER	-	LINKER	UNP P27958
C	485	GLY	-	LINKER	UNP P27958
C	576	ASP	ASN	ENGINEERED MUTATION	UNP P27958
C	589	HIS	TYR	VARIANT	UNP P27958
C	602	TRP	ARG	VARIANT	UNP P27958

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Chain	Residue	Modelled	Actual	Comment	Reference
D	448	ASP	ASN	ENGINEERED MUTATION	UNP P27958
D	482	GLY	-	LINKER	UNP P27958
D	483	SER	-	LINKER	UNP P27958
D	484	SER	-	LINKER	UNP P27958
D	485	GLY	-	LINKER	UNP P27958
D	576	ASP	ASN	ENGINEERED MUTATION	UNP P27958
D	589	HIS	TYR	VARIANT	UNP P27958
D	602	TRP	ARG	VARIANT	UNP P27958

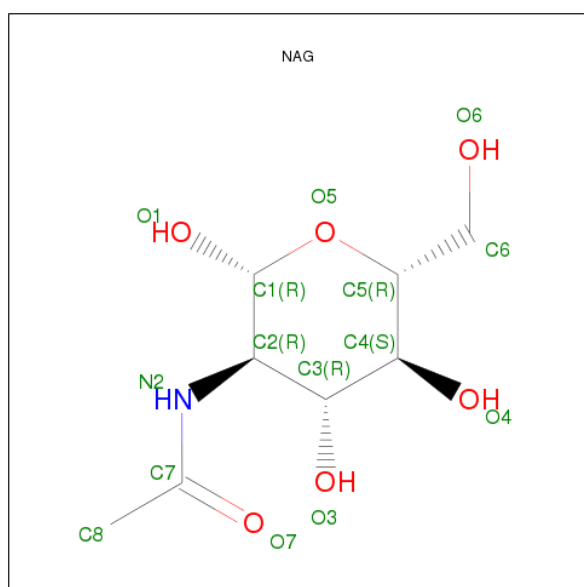
- Molecule 4 is a polymer of unknown type called SUGAR (8-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



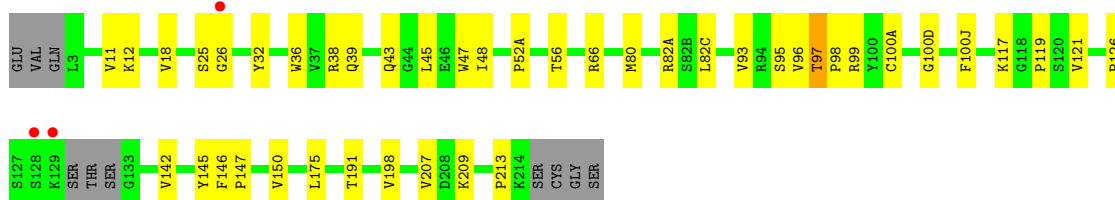
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

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.

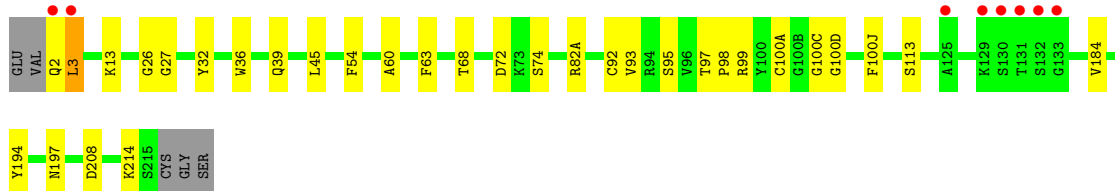
- Molecule 1: Fab AR3C heavy chain

Chain A: 



- Molecule 1: Fab AR3C heavy chain

Chain H: 



- Molecule 2: Fab AR3C light chain

Chain B: 



- Molecule 2: Fab AR3C light chain

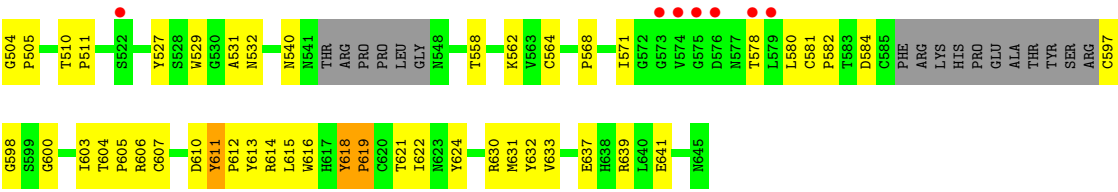
Chain L: 



- Molecule 3: Envelope glycoprotein E2

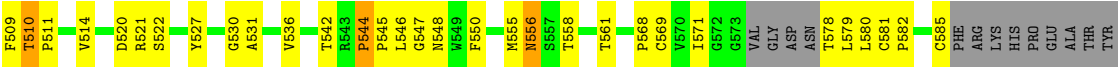
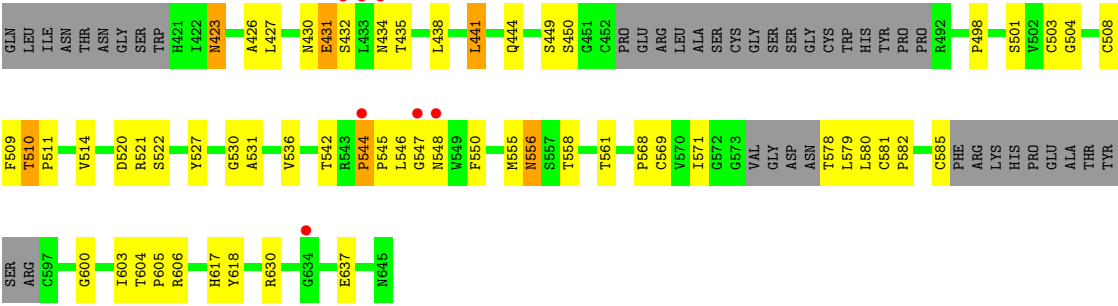
Chain C: 





• Molecule 3: Envelope glycoprotein E2

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.13Å 166.55Å 209.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 2.65 49.08 – 2.64	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.08-2.65) 92.8 (49.08-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.231 , 0.270 0.231 , 0.269	Depositor DCC
R_{free} test set	2309 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 45972 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9433	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.00% 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, 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	0.34	0/1702	0.51	0/2314
1	H	0.38	0/1737	0.56	0/2363
2	B	0.31	0/1646	0.49	0/2235
2	L	0.36	0/1654	0.55	0/2246
3	C	0.45	2/1328 (0.2%)	0.67	2/1816 (0.1%)
3	D	0.37	0/1347	0.69	0/1843
All	All	0.37	2/9414 (0.0%)	0.58	2/12817 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	619	PRO	N-CD	5.18	1.55	1.47
3	C	612	PRO	N-CD	5.14	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	611	TYR	C-N-CD	5.68	140.33	128.40
3	C	618	TYR	C-N-CD	5.64	140.24	128.40

There are no chirality outliers.

There are no planarity outliers.

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	1663	0	1626	32	0
1	H	1697	0	1653	24	0
2	B	1612	0	1570	11	0
2	L	1620	0	1581	10	0
3	C	1288	0	1193	53	0
3	D	1305	0	1219	44	0
4	C	94	0	79	1	0
5	C	28	0	25	0	0
5	D	28	0	25	5	0
6	C	42	0	39	1	0
6	D	56	0	52	0	0
All	All	9433	0	9062	165	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 9.

All (165) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:433:LEU:HD12	1:H:99:ARG:HD2	1.43	1.01
1:H:97:THR:HG22	1:H:99:ARG:HH12	1.35	0.90
3:C:433:LEU:CD1	1:H:99:ARG:HD2	2.02	0.90
3:C:610:ASP:HB3	3:C:641:GLU:HB3	1.65	0.78
1:A:66:ARG:HE	1:A:82(A):ARG:HB2	1.52	0.74
1:H:68:THR:OG1	1:H:82(A):ARG:NH2	2.20	0.73
1:A:99:ARG:HA	3:D:432:SER:HB2	1.71	0.73
3:C:578:THR:OG1	3:C:581:CYS:O	2.07	0.73
1:H:97:THR:HG22	1:H:99:ARG:NH1	2.03	0.73
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.74	0.70
3:D:578:THR:HG23	3:D:579:LEU:HG	1.75	0.68
5:D:704:NAG:H62	5:D:705:NAG:H82	1.76	0.68
3:C:597:CYS:SG	3:C:598:GLY:N	2.67	0.67
3:D:530:GLY:N	3:D:531:ALA:HB3	2.10	0.67
3:C:430:ASN:OD1	3:C:431:GLU:N	2.29	0.66
1:A:191:THR:HG21	3:C:630:ARG:HG3	1.77	0.66
1:A:99:ARG:NH1	3:D:432:SER:O	2.28	0.66
3:C:495:GLY:N	3:C:540:ASN:OD1	2.29	0.65
3:C:429:CYS:HB2	1:H:100(A):CYS:HB2	1.77	0.65
3:D:604:THR:HG22	3:D:606:ARG:H	1.61	0.65
1:H:99:ARG:HG3	2:L:91:TYR:CE2	2.31	0.65
3:C:604:THR:HB	3:C:607:CYS:HB2	1.78	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:503:CYS:O	3:D:555:MET:HB3	1.97	0.64
3:D:509:PHE:C	3:D:511:PRO:HA	2.19	0.63
1:H:2:GLN:N	1:H:3:LEU:HA	2.14	0.63
3:C:630:ARG:HH12	3:C:639:ARG:HH21	1.48	0.61
3:D:520:ASP:O	3:D:522:SER:HA	2.00	0.61
3:D:510:THR:N	3:D:511:PRO:HA	2.16	0.60
3:D:430:ASN:OD1	3:D:431:GLU:HB3	2.02	0.59
3:C:426:ALA:O	3:C:504:GLY:HA2	2.02	0.59
1:H:32:TYR:CD1	1:H:98:PRO:HG3	2.37	0.59
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.85	0.58
1:A:11:VAL:HB	1:A:147:PRO:HG3	1.85	0.58
1:A:56:THR:HG21	1:A:100(D):GLY:HA3	1.86	0.58
1:A:38:ARG:HB3	1:A:48:ILE:HD11	1.85	0.58
3:D:498:PRO:HA	3:D:536:VAL:HG12	1.85	0.58
3:D:521:ARG:HB3	3:D:536:VAL:HG21	1.86	0.57
3:D:578:THR:OG1	3:D:579:LEU:N	2.33	0.57
3:D:444:GLN:N	3:D:444:GLN:OE1	2.29	0.57
1:H:197:ASN:ND2	1:H:208:ASP:OD1	2.38	0.57
3:C:496:ILE:HD11	6:C:712:NAG:H82	1.86	0.57
2:B:14:SER:OG	2:B:107:LYS:NZ	2.38	0.57
3:C:611:TYR:CE1	3:C:614:ARG:HB2	2.40	0.57
3:C:429:CYS:SG	3:C:438:LEU:HD11	2.45	0.57
3:D:544:PRO:O	3:D:546:LEU:HA	2.05	0.56
1:H:26:GLY:N	1:H:27:GLY:HA2	2.20	0.56
1:A:142:VAL:HG11	1:A:150:VAL:HG21	1.87	0.56
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.87	0.56
3:C:511:PRO:HB3	3:C:568:PRO:HB3	1.89	0.55
1:A:66:ARG:NE	1:A:82(A):ARG:HB2	2.21	0.55
3:D:511:PRO:HB3	3:D:568:PRO:HB3	1.89	0.55
1:H:97:THR:CG2	1:H:99:ARG:HH12	2.15	0.54
3:C:440:GLY:HA3	3:C:616:TRP:CD1	2.42	0.54
3:C:615:LEU:CD2	3:C:622:ILE:HA	2.37	0.54
1:A:198:VAL:HB	1:A:207:VAL:HG13	1.90	0.54
1:A:93:VAL:HG21	1:A:100(J):PHE:HB3	1.89	0.54
1:A:121:VAL:O	1:A:209:LYS:NZ	2.41	0.54
3:C:432:SER:HB2	3:C:438:LEU:HB2	1.90	0.53
3:D:510:THR:N	3:D:511:PRO:CA	2.71	0.53
3:D:582:PRO:HA	3:D:605:PRO:HA	1.90	0.53
3:D:509:PHE:HB3	3:D:511:PRO:O	2.09	0.52
2:B:21:LEU:HD22	2:B:102:THR:HG21	1.91	0.52
3:C:441:LEU:HD21	1:H:54:PHE:HZ	1.75	0.52
3:D:568:PRO:HB2	3:D:603:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.45	0.51
3:C:611:TYR:CD1	3:C:614:ARG:HB2	2.45	0.51
1:A:191:THR:CG2	3:C:630:ARG:HG3	2.40	0.50
3:C:568:PRO:HB2	3:C:603:ILE:HG22	1.94	0.50
3:D:544:PRO:HG2	3:D:550:PHE:CE1	2.47	0.50
3:D:434:ASN:OD1	3:D:435:THR:N	2.45	0.50
3:C:578:THR:HG23	3:C:578:THR:O	2.11	0.50
3:C:571:ILE:HB	3:C:580:LEU:HD12	1.93	0.49
1:A:66:ARG:HH21	1:A:82(A):ARG:HH11	1.61	0.49
3:D:544:PRO:HA	3:D:547:GLY:H	1.77	0.49
3:C:447:PHE:CZ	3:C:619:PRO:HB2	2.48	0.49
3:C:423:ASN:OD1	3:C:527:TYR:HD1	1.95	0.49
3:C:434:ASN:OD1	3:C:435:THR:N	2.46	0.49
2:B:123:GLU:O	2:B:126:LYS:HG2	2.12	0.49
2:L:18:ARG:HH11	2:L:74:THR:HG21	1.77	0.49
3:D:558:THR:HG23	5:D:704:NAG:HN2	1.76	0.49
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.94	0.49
3:C:434:ASN:OD1	3:C:435:THR:HG22	2.14	0.48
3:D:423:ASN:HB3	3:D:527:TYR:O	2.13	0.48
3:C:448:ASP:OD1	3:C:449:SER:N	2.41	0.48
3:D:441:LEU:HD12	3:D:441:LEU:O	2.13	0.48
3:C:630:ARG:HD3	3:C:637:GLU:OE2	2.13	0.48
3:C:632:TYR:CE2	3:C:637:GLU:HB2	2.48	0.48
1:A:25:SER:HA	1:A:26:GLY:HA2	1.61	0.47
5:D:704:NAG:H61	5:D:705:NAG:N2	2.30	0.47
1:A:126:PRO:HG2	1:A:213:PRO:HB3	1.96	0.47
3:D:569:CYS:O	3:D:571:ILE:N	2.47	0.47
5:D:704:NAG:H61	5:D:705:NAG:HN2	1.80	0.47
1:A:98:PRO:HB2	3:D:438:LEU:HG	1.97	0.47
3:D:544:PRO:HA	3:D:547:GLY:O	2.15	0.46
2:L:33:LEU:HD22	2:L:71:PHE:CG	2.50	0.46
3:D:510:THR:HG22	3:D:548:ASN:O	2.15	0.46
1:H:32:TYR:CG	1:H:98:PRO:HG3	2.50	0.46
1:H:13:LYS:HD3	1:H:113:SER:HA	1.98	0.46
3:C:447:PHE:CE1	3:C:619:PRO:HB2	2.51	0.46
3:C:494:CYS:HA	3:C:495:GLY:HA3	1.65	0.46
3:C:615:LEU:HD21	3:C:622:ILE:HA	1.97	0.46
3:D:600:GLY:HA2	3:D:618:TYR:CZ	2.51	0.46
3:C:438:LEU:HD12	3:C:438:LEU:HA	1.70	0.46
3:D:449:SER:HA	3:D:450:SER:HA	1.49	0.45
3:C:529:TRP:HB3	1:H:100(C):GLY:HA3	1.98	0.45
1:H:36:TRP:CH2	1:H:92:CYS:HB2	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:18:VAL:HG13	1:A:82(C):LEU:HD11	1.99	0.45
3:C:494:CYS:O	3:C:540:ASN:HA	2.17	0.45
3:C:500:LYS:HE2	3:C:531:ALA:O	2.17	0.45
3:D:501:SER:O	3:D:556:ASN:HA	2.16	0.45
3:C:600:GLY:HA2	3:C:618:TYR:CZ	2.51	0.45
3:D:503:CYS:HA	3:D:504:GLY:HA2	1.66	0.45
1:A:96:VAL:O	1:A:97:THR:HB	2.16	0.44
3:D:582:PRO:HG2	3:D:585:CYS:SG	2.57	0.44
1:H:93:VAL:HG21	1:H:100(J):PHE:HB3	2.00	0.44
1:A:12:LYS:HG3	1:A:18:VAL:CG1	2.47	0.44
1:H:100(C):GLY:HA2	1:H:100(D):GLY:HA2	1.62	0.44
3:C:584:ASP:OD1	3:C:584:ASP:N	2.45	0.44
3:D:426:ALA:O	3:D:504:GLY:HA2	2.17	0.44
5:D:704:NAG:C6	5:D:705:NAG:N2	2.81	0.44
1:A:47:TRP:CD1	2:B:96:LEU:HD12	2.53	0.44
2:L:83:SER:HB2	2:L:106:ILE:HD13	2.00	0.44
1:A:66:ARG:HG2	1:A:82(A):ARG:HB2	2.00	0.44
4:C:707:MAN:C1	4:C:708:MAN:H5	2.48	0.44
3:C:582:PRO:HA	3:C:605:PRO:HA	1.98	0.43
3:C:432:SER:O	3:C:432:SER:OG	2.36	0.43
3:D:630:ARG:NH2	3:D:637:GLU:OE2	2.51	0.43
1:A:146:PHE:HA	1:A:147:PRO:HA	1.85	0.43
3:C:432:SER:CB	3:C:438:LEU:HB2	2.47	0.43
1:A:66:ARG:HE	1:A:82(A):ARG:CB	2.26	0.43
3:C:614:ARG:NH1	3:C:621:THR:OG1	2.52	0.43
1:H:72:ASP:OD1	1:H:74:SER:OG	2.28	0.43
3:C:621:THR:O	3:C:624:TYR:HB2	2.20	0.42
1:H:99:ARG:HA	1:H:99:ARG:HD3	1.71	0.42
3:C:604:THR:HG22	3:C:606:ARG:H	1.85	0.42
3:D:542:THR:O	3:D:547:GLY:HA3	2.20	0.42
2:B:201:LEU:HD13	2:B:205:VAL:HG23	1.99	0.42
1:A:32:TYR:O	1:A:52(A):PRO:HD2	2.19	0.42
2:B:19:ALA:HB2	2:B:78:LEU:HD11	2.01	0.42
3:D:580:LEU:O	3:D:605:PRO:HD3	2.20	0.42
1:A:117:LYS:HD3	1:A:175:LEU:HD21	2.02	0.42
1:A:47:TRP:CG	2:B:96:LEU:HB2	2.55	0.42
3:D:430:ASN:HA	3:D:431:GLU:HA	1.82	0.42
3:D:544:PRO:C	3:D:546:LEU:HA	2.40	0.42
1:H:184:VAL:HG11	1:H:194:TYR:CE1	2.55	0.42
3:C:571:ILE:HD11	3:C:633:VAL:HG22	2.01	0.42
3:C:503:CYS:HA	3:C:504:GLY:HA2	1.69	0.41
1:A:36:TRP:CE2	1:A:80:MET:HB2	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.01	0.41
3:D:508:CYS:O	3:D:514:VAL:HG12	2.20	0.41
2:B:94:SER:HB2	2:B:95:PRO:HD3	2.02	0.41
3:C:558:THR:O	3:C:558:THR:HG22	2.21	0.41
2:L:112:ALA:HA	2:L:113:PRO:HD3	1.94	0.41
1:A:100(A):CYS:HB3	3:D:427:LEU:HG	2.03	0.41
2:B:89:GLN:HB2	2:B:98:PHE:CD2	2.55	0.41
2:L:96:LEU:HD12	2:L:96:LEU:H	1.86	0.40
3:D:561:THR:HG21	3:D:617:HIS:O	2.20	0.40
1:A:66:ARG:HH21	1:A:82(A):ARG:HG3	1.85	0.40
3:C:562:LYS:HA	3:C:562:LYS:HD2	1.85	0.40
1:H:60:ALA:HB3	1:H:63:PHE:HD2	1.86	0.40
2:L:140:TYR:CG	2:L:141:PRO:HA	2.57	0.40
2:L:155:GLN:OE1	2:L:158:ASN:ND2	2.47	0.40
1:A:39:GLN:HB2	1:A:45:LEU:HD23	2.04	0.40
3:C:505:PRO:HG2	3:C:613:TYR:CE2	2.57	0.40
3:C:604:THR:HG23	3:C:605:PRO:HD2	2.03	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	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	38	66
1	H	226/233 (97%)	221 (98%)	5 (2%)	0	100	100
2	B	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
2	L	210/214 (98%)	206 (98%)	4 (2%)	0	100	100
3	C	161/212 (76%)	152 (94%)	8 (5%)	1 (1%)	33	61
3	D	163/212 (77%)	150 (92%)	11 (7%)	2 (1%)	19	37
All	All	1188/1318 (90%)	1146 (96%)	38 (3%)	4 (0%)	50	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	THR
3	D	510	THR
3	C	510	THR
3	D	545	PRO

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	186/195 (95%)	184 (99%)	2 (1%)	84	96
1	H	191/195 (98%)	188 (98%)	3 (2%)	75	93
2	B	181/184 (98%)	181 (100%)	0	100	100
2	L	182/184 (99%)	182 (100%)	0	100	100
3	C	143/180 (79%)	139 (97%)	4 (3%)	56	83
3	D	145/180 (81%)	139 (96%)	6 (4%)	41	71
All	All	1028/1118 (92%)	1013 (98%)	15 (2%)	76	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	95	SER
3	C	429	CYS
3	C	532	ASN
3	C	564	CYS
3	C	631	MET
3	D	423	ASN
3	D	431	GLU
3	D	441	LEU
3	D	544	PRO
3	D	556	ASN
3	D	581	CYS
1	H	3	LEU
1	H	95	SER
1	H	214	LYS

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 ⓘ

12 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	$\# Z > 2$
4	NAG	C	701	3,4	12,14,15	0.78	0	15,19,21	1.27	2 (13%)
4	NAG	C	702	4	12,14,15	0.86	0	15,19,21	1.69	3 (20%)
4	BMA	C	703	4	10,11,12	0.97	1 (10%)	11,15,17	0.93	0
4	MAN	C	704	4	10,11,12	0.63	0	11,15,17	1.35	2 (18%)
4	MAN	C	705	4	10,11,12	0.52	0	11,15,17	0.98	1 (9%)
4	MAN	C	706	4	10,11,12	0.75	0	11,15,17	1.27	1 (9%)
4	MAN	C	707	4	10,11,12	0.68	0	11,15,17	1.24	2 (18%)
4	MAN	C	708	4	10,11,12	0.57	0	11,15,17	0.93	1 (9%)
5	NAG	C	709	3,5	12,14,15	0.77	1 (8%)	15,19,21	1.10	0
5	NAG	C	710	5	12,14,15	0.82	1 (8%)	15,19,21	1.08	2 (13%)
5	NAG	D	704	3,5	12,14,15	0.58	0	15,19,21	0.89	1 (6%)
5	NAG	D	705	5	12,14,15	0.56	0	15,19,21	0.88	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	C	701	3,4	-	0/6/23/26	0/1/1/1
4	NAG	C	702	4	-	0/6/23/26	0/1/1/1
4	BMA	C	703	4	-	0/2/19/22	0/1/1/1
4	MAN	C	704	4	-	0/2/19/22	0/1/1/1
4	MAN	C	705	4	-	0/2/19/22	0/1/1/1
4	MAN	C	706	4	-	0/2/19/22	0/1/1/1
4	MAN	C	707	4	-	0/2/19/22	0/1/1/1
4	MAN	C	708	4	-	0/2/19/22	0/1/1/1
5	NAG	C	709	3,5	-	0/6/23/26	0/1/1/1
5	NAG	C	710	5	-	0/6/23/26	0/1/1/1
5	NAG	D	704	3,5	-	0/6/23/26	0/1/1/1
5	NAG	D	705	5	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	710	NAG	O5-C5	-2.45	1.41	1.45
5	C	709	NAG	O5-C5	-2.09	1.42	1.45
4	C	703	BMA	C4-C5	2.07	1.57	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	NAG	C2-N2-C7	-3.57	119.07	123.39
4	C	702	NAG	C2-N2-C7	-3.56	119.09	123.39
4	C	702	NAG	O5-C5-C6	3.35	110.50	106.98
4	C	706	MAN	C4-C3-C2	-2.93	107.34	110.61
5	C	710	NAG	C2-N2-C7	-2.90	119.88	123.39
4	C	705	MAN	C4-C3-C2	-2.71	107.58	110.61
4	C	704	MAN	O5-C5-C6	2.65	109.76	106.98
4	C	702	NAG	O5-C5-C4	-2.62	107.33	110.65
4	C	704	MAN	O6-C6-C5	2.43	119.82	111.37
5	D	704	NAG	O5-C5-C6	2.40	109.50	106.98
5	D	705	NAG	O5-C5-C6	2.35	109.45	106.98
4	C	708	MAN	O5-C5-C6	2.34	109.44	106.98
4	C	707	MAN	O5-C5-C6	2.26	109.36	106.98
5	C	710	NAG	O5-C5-C6	2.24	109.33	106.98
4	C	707	MAN	O5-C5-C4	-2.17	107.90	110.65
4	C	701	NAG	O5-C5-C6	2.01	109.09	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

7 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
6	NAG	C	711	3	12,14,15	0.76	1 (8%)	15,19,21	1.44	2 (13%)
6	NAG	C	712	3	12,14,15	0.55	0	15,19,21	0.83	1 (6%)
6	NAG	C	713	3	12,14,15	0.75	1 (8%)	15,19,21	0.91	1 (6%)
6	NAG	D	701	3	12,14,15	0.80	1 (8%)	15,19,21	0.74	0
6	NAG	D	702	3	12,14,15	0.85	1 (8%)	15,19,21	1.32	3 (20%)
6	NAG	D	703	3	12,14,15	0.58	0	15,19,21	0.87	1 (6%)
6	NAG	D	706	3	12,14,15	0.82	1 (8%)	15,19,21	1.03	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	C	711	3	-	0/6/23/26	0/1/1/1
6	NAG	C	712	3	-	0/6/23/26	0/1/1/1
6	NAG	C	713	3	-	0/6/23/26	0/1/1/1
6	NAG	D	701	3	-	0/6/23/26	0/1/1/1
6	NAG	D	702	3	-	0/6/23/26	0/1/1/1
6	NAG	D	703	3	-	0/6/23/26	0/1/1/1
6	NAG	D	706	3	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	702	NAG	O5-C5	-2.68	1.41	1.45
6	D	706	NAG	O5-C5	-2.57	1.41	1.45
6	C	711	NAG	O5-C5	-2.33	1.41	1.45
6	C	713	NAG	O5-C5	-2.23	1.42	1.45
6	D	701	NAG	O5-C5	-2.20	1.42	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	711	NAG	O5-C5-C6	4.80	112.02	106.98
6	D	702	NAG	O5-C5-C6	2.72	109.83	106.98
6	C	713	NAG	C2-N2-C7	-2.45	120.43	123.39
6	D	706	NAG	O5-C5-C6	2.34	109.43	106.98
6	D	703	NAG	O5-C5-C6	2.33	109.42	106.98
6	D	702	NAG	C2-N2-C7	-2.26	120.67	123.39
6	C	712	NAG	O5-C5-C6	2.23	109.32	106.98
6	D	702	NAG	O5-C5-C4	-2.22	107.83	110.65
6	D	706	NAG	O5-C5-C4	-2.16	107.91	110.65
6	C	711	NAG	O5-C5-C4	-2.08	108.01	110.65

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	223/233 (95%)	0.09	3 (1%) 74 75	46, 77, 109, 123	0
1	H	228/233 (97%)	0.15	8 (3%) 42 39	39, 55, 96, 134	0
2	B	211/214 (98%)	-0.20	0 100 100	48, 72, 95, 114	0
2	L	212/214 (99%)	-0.08	0 100 100	39, 57, 76, 101	1 (0%)
3	C	169/212 (79%)	0.18	9 (5%) 25 22	45, 69, 123, 165	0
3	D	171/212 (80%)	0.28	7 (4%) 35 32	50, 81, 120, 141	0
All	All	1214/1318 (92%)	0.06	27 (2%) 59 56	39, 67, 109, 165	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	131	THR	6.0
3	C	575	GLY	5.6
3	C	574	VAL	5.5
3	D	433	LEU	4.9
3	C	578	THR	4.6
3	C	522	SER	4.6
1	A	129	LYS	4.5
3	C	576	ASP	4.0
1	H	132	SER	3.6
3	D	432	SER	3.3
3	D	548	ASN	3.3
3	D	544	PRO	3.0
3	C	573	GLY	2.9
1	H	133	GLY	2.8
3	C	579	LEU	2.8
3	C	434	ASN	2.7
1	H	129	LYS	2.7
3	D	547	GLY	2.6
1	H	2	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	26	GLY	2.4
1	H	125	ALA	2.4
1	H	130	SER	2.3
3	C	446	LYS	2.3
1	H	3	LEU	2.3
3	D	634	GLY	2.2
1	A	128	SER	2.1
3	D	434	ASN	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
4	NAG	C	701	14/15	0.11	-	60,71,86,92	0
4	MAN	C	705	11/12	0.19	-	131,135,140,148	0
5	NAG	C	709	14/15	0.14	-	63,88,114,115	0
4	MAN	C	708	11/12	0.14	-	81,98,105,108	0
4	MAN	C	704	11/12	0.15	-	96,111,124,130	0
5	NAG	C	710	14/15	0.17	-	102,121,136,144	0
4	MAN	C	707	11/12	0.15	-	64,78,85,91	0
4	NAG	C	702	14/15	0.16	-	78,86,102,108	0
5	NAG	D	704	14/15	0.15	-	63,93,112,114	0
4	MAN	C	706	11/12	0.15	-	55,69,80,90	0
4	BMA	C	703	11/12	0.15	-	78,86,99,107	0
5	NAG	D	705	14/15	0.26	-	113,137,153,153	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
6	NAG	C	712	14/15	0.40	-	115,135,162,176	0
6	NAG	D	702	14/15	0.30	-	132,144,155,158	0
6	NAG	D	706	14/15	0.26	-	101,122,127,130	0
6	NAG	D	701	14/15	0.26	-	95,105,126,128	0
6	NAG	C	713	14/15	0.15	-	93,102,114,116	0
6	NAG	D	703	14/15	0.20	-	83,109,115,120	0
6	NAG	C	711	14/15	0.31	-	104,126,132,133	0

6.5 Other polymers ⓘ

There are no such residues in this entry.