



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2017 – 02:00 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 : unknown  
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : rb-20029824  
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) : rb-20029824

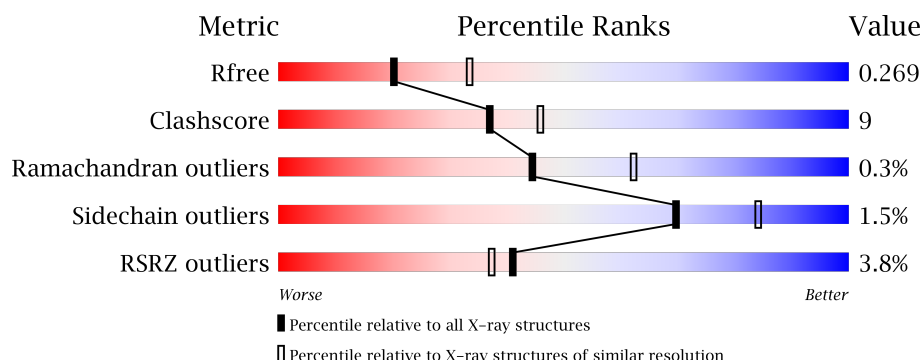
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1044 (2.66-2.62)
Clashscore	112137	1092 (2.66-2.62)
Ramachandran outliers	110173	1077 (2.66-2.62)
Sidechain outliers	110143	1077 (2.66-2.62)
RSRZ outliers	101464	1047 (2.66-2.62)

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  $\geq 3$ , 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	233	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>.</div> </div> </div>
1	H	233	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>.</div> </div> </div>
2	B	214	<div> <div></div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
2	L	214	<div> <div></div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
3	C	212	<div> <div>6%</div> <div> <div></div> <div>49%</div> <div>29%</div> <div>.</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	212	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	D	701	-	-	-	X
4	NAG	D	706	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9433 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 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:

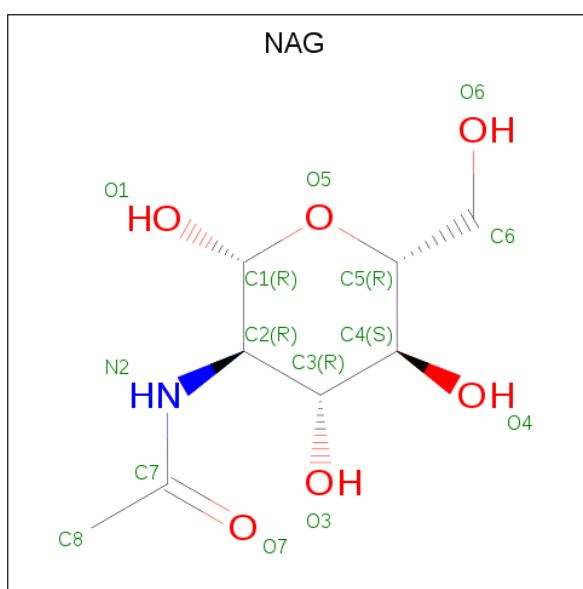
Chain	Residue	Modelled	Actual	Comment	Reference
C	448	ASP	ASN	ENGINEERED MUTATION	UNP P27958
C	482	GLY	-	LINKER	UNP P27958
C	483	SER	-	LINKER	UNP P27958
C	484	SER	-	LINKER	UNP P27958
C	485	GLY	-	LINKER	UNP P27958
C	576	ASP	ASN	ENGINEERED MUTATION	UNP P27958
C	589	HIS	TYR	VARIANT	UNP P27958
C	602	TRP	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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



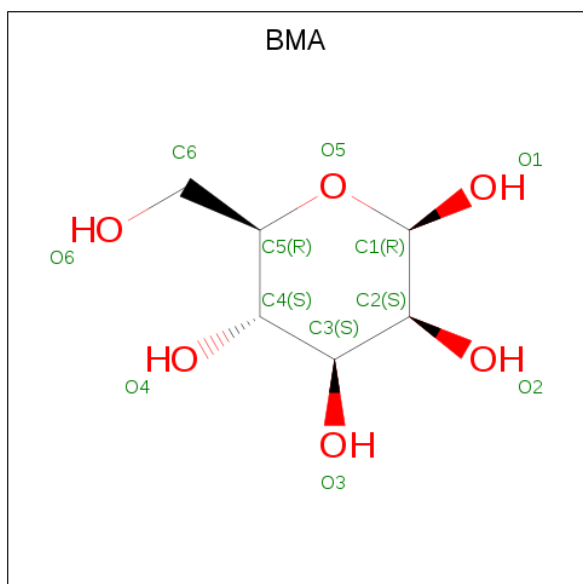
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			11	6	5		

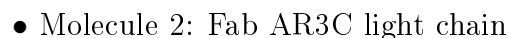
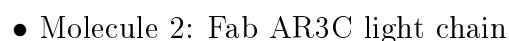
- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		



- Molecule 1: Fab AR3C heavy chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	55.5	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9433	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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 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	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	98	0	88	1	0
4	D	84	0	77	5	0
5	C	11	0	8	0	0
6	C	55	0	47	1	0
All	All	9433	0	9062	165	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 9.

All (165) 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)
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
4:D:704:NAG:H62	4: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	4: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
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	4: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
4:D:704:NAG:H61	4: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
4:D:704:NAG:H61	4: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	Interatomic distance (Å)	Clash overlap (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
4:D:704:NAG:C6	4: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
6:C:707:MAN:C1	6: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TRP:CE2	1:A:80:MET:HB2	2.55	0.41
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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	32	48
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%)	28	43
3	D	163/212 (77%)	150 (92%)	11 (7%)	2 (1%)	15	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1188/1318 (90%)	1146 (96%)	38 (3%)	4 (0%)	44 62

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%)	78 89
1	H	191/195 (98%)	188 (98%)	3 (2%)	68 83
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%)	49 69
3	D	145/180 (81%)	139 (96%)	6 (4%)	35 55
All	All	1028/1118 (92%)	1013 (98%)	15 (2%)	70 84

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

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Mol	Chain	Res	Type
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 [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

19 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	C	701	3,4	14,14,15	0.42	0	15,19,21	1.01	1 (6%)
4	NAG	C	702	5,4	14,14,15	0.50	0	15,19,21	1.13	1 (6%)
5	BMA	C	703	4,6	11,11,12	0.84	1 (9%)	13,15,17	1.72	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	C	704	5,6	11,11,12	0.86	0	13,15,17	2.39	2 (15%)
6	MAN	C	705	6	11,11,12	0.29	0	13,15,17	0.98	1 (7%)
6	MAN	C	706	5,6	11,11,12	0.41	0	13,15,17	1.23	2 (15%)
6	MAN	C	707	6	11,11,12	0.35	0	13,15,17	0.96	1 (7%)
6	MAN	C	708	6	11,11,12	0.22	0	13,15,17	0.81	0
4	NAG	C	709	3,4	14,14,15	0.51	0	15,19,21	1.22	1 (6%)
4	NAG	C	710	4	14,14,15	0.58	0	15,19,21	0.84	2 (13%)
4	NAG	C	711	3	14,14,15	0.49	0	15,19,21	0.67	0
4	NAG	C	712	3	14,14,15	0.28	0	15,19,21	0.52	0
4	NAG	C	713	3	14,14,15	0.45	0	15,19,21	1.04	1 (6%)
4	NAG	D	701	3	14,14,15	0.48	0	15,19,21	0.94	1 (6%)
4	NAG	D	702	3	14,14,15	0.70	0	15,19,21	0.85	0
4	NAG	D	703	3	14,14,15	0.29	0	15,19,21	0.57	0
4	NAG	D	704	3,4	14,14,15	0.27	0	15,19,21	0.58	0
4	NAG	D	705	4	14,14,15	0.29	0	15,19,21	0.55	0
4	NAG	D	706	3	14,14,15	0.54	0	15,19,21	0.71	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	C	701	3,4	-	0/6/23/26	0/1/1/1
4	NAG	C	702	5,4	-	0/6/23/26	0/1/1/1
5	BMA	C	703	4,6	-	0/2/19/22	0/1/1/1
6	MAN	C	704	5,6	-	0/2/19/22	0/1/1/1
6	MAN	C	705	6	-	0/2/19/22	0/1/1/1
6	MAN	C	706	5,6	-	0/2/19/22	0/1/1/1
6	MAN	C	707	6	-	0/2/19/22	0/1/1/1
6	MAN	C	708	6	-	0/2/19/22	0/1/1/1
4	NAG	C	709	3,4	-	0/6/23/26	0/1/1/1
4	NAG	C	710	4	-	0/6/23/26	0/1/1/1
4	NAG	C	711	3	-	0/6/23/26	0/1/1/1
4	NAG	C	712	3	-	0/6/23/26	0/1/1/1
4	NAG	C	713	3	-	0/6/23/26	0/1/1/1
4	NAG	D	701	3	-	0/6/23/26	0/1/1/1
4	NAG	D	702	3	-	0/6/23/26	0/1/1/1
4	NAG	D	703	3	-	0/6/23/26	0/1/1/1
4	NAG	D	704	3,4	-	0/6/23/26	0/1/1/1
4	NAG	D	705	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	706	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	703	BMA	C4-C5	2.12	1.57	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	709	NAG	O5-C1-C2	-3.40	106.74	111.47
4	C	701	NAG	C2-N2-C7	-2.65	119.07	122.94
4	C	702	NAG	C2-N2-C7	-2.64	119.09	122.94
6	C	707	MAN	O2-C2-C3	-2.17	105.91	110.17
4	C	710	NAG	C2-N2-C7	-2.10	119.88	122.94
4	C	710	NAG	O5-C1-C2	-2.07	108.60	111.47
6	C	706	MAN	C2-C3-C4	-2.03	107.34	110.88
6	C	705	MAN	C1-O5-C5	2.24	115.25	112.17
4	D	701	NAG	C1-O5-C5	2.39	115.46	112.17
6	C	706	MAN	C1-O5-C5	2.45	115.55	112.17
6	C	704	MAN	O6-C6-C5	2.52	119.82	111.34
4	C	713	NAG	C1-O5-C5	3.12	116.46	112.17
5	C	703	BMA	C1-O5-C5	3.72	117.30	112.17
5	C	703	BMA	C1-C2-C3	3.99	114.71	109.65
6	C	704	MAN	C1-O5-C5	7.63	122.68	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	707	MAN	1	0
6	C	708	MAN	1	0
4	C	712	NAG	1	0
4	D	704	NAG	5	0
4	D	705	NAG	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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(Å²)	Q<0.9
1	A	223/233 (95%)	0.19	9 (4%)	39	35	46, 77, 109, 123	0
1	H	228/233 (97%)	0.25	8 (3%)	44	40	39, 55, 96, 134	0
2	B	211/214 (98%)	-0.13	1 (0%)	90	90	48, 72, 95, 114	0
2	L	212/214 (99%)	0.00	0	100	100	39, 57, 76, 101	1 (0%)
3	C	169/212 (79%)	0.34	12 (7%)	17	13	45, 69, 123, 165	0
3	D	171/212 (80%)	0.46	16 (9%)	9	7	50, 81, 120, 141	0
All	All	1214/1318 (92%)	0.17	46 (3%)	41	37	39, 67, 109, 165	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	575	GLY	6.4
3	C	578	THR	6.2
3	C	574	VAL	6.0
1	H	131	THR	6.0
3	C	576	ASP	5.6
1	A	129	LYS	5.0
3	D	544	PRO	4.5
3	C	522	SER	4.3
3	D	433	LEU	4.2
3	D	432	SER	4.0
1	H	132	SER	3.8
1	A	50	GLY	3.6
3	D	547	GLY	3.3
3	D	446	LYS	3.3
3	C	573	GLY	3.3
1	A	75	THR	3.3
3	D	445	HIS	3.2
1	H	133	GLY	3.2
3	D	579	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	578	THR	3.0
3	C	577	ASN	3.0
3	C	579	LEU	3.0
3	D	421	HIS	3.0
1	A	67	VAL	3.0
1	H	2	GLN	2.9
1	H	129	LYS	2.7
3	C	434	ASN	2.7
3	D	548	ASN	2.7
3	C	446	LYS	2.6
3	D	542	THR	2.6
1	H	27	GLY	2.6
3	D	449	SER	2.5
3	D	540	ASN	2.4
1	A	26	GLY	2.4
3	C	541	ASN	2.3
2	B	127	SER	2.3
3	C	433	LEU	2.2
3	D	522	SER	2.2
1	A	78	GLY	2.1
1	H	130	SER	2.1
3	D	434	ASN	2.1
1	A	28	THR	2.1
1	H	3	LEU	2.0
1	A	24	THR	2.0
1	A	70	SER	2.0
3	D	634	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	D	706	14/15	0.80	0.42	2.41	101,122,127,130	0
4	NAG	D	701	14/15	0.82	0.24	2.22	95,105,126,128	0
4	NAG	C	713	14/15	0.90	0.20	0.41	93,102,114,116	0
4	NAG	D	704	14/15	0.89	0.17	-0.01	63,93,112,114	0
4	NAG	C	709	14/15	0.90	0.14	-0.09	63,88,114,115	0
4	NAG	C	701	14/15	0.94	0.11	-1.39	60,71,86,92	0
6	MAN	C	708	11/12	0.83	0.15	-	81,98,105,108	0
4	NAG	C	702	14/15	0.94	0.17	-	78,86,102,108	0
4	NAG	C	712	14/15	0.71	0.44	-	115,135,162,176	0
6	MAN	C	707	11/12	0.91	0.17	-	64,78,85,91	0
4	NAG	D	703	14/15	0.88	0.27	-	83,109,115,120	0
4	NAG	C	710	14/15	0.83	0.18	-	102,121,136,144	0
6	MAN	C	706	11/12	0.91	0.15	-	55,69,80,90	0
4	NAG	C	711	14/15	0.78	0.31	-	104,126,132,133	0
6	MAN	C	704	11/12	0.83	0.16	-	96,111,124,130	0
4	NAG	D	702	14/15	0.65	0.29	-	132,144,155,158	0
6	MAN	C	705	11/12	0.75	0.21	-	131,135,140,148	0
5	BMA	C	703	11/12	0.85	0.18	-	78,86,99,107	0
4	NAG	D	705	14/15	0.78	0.27	-	113,137,153,153	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.