



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:25 AM UTC

PDB ID : 4HC1 / pdb_00004hc1
Title : Crystal structure of a loop deleted mutant of human MAdCAM-1 D1D2 complexed with Fab 10G3
Authors : Springer, T.; Yu, Y.; Zhu, J.
Deposited on : 2012-09-28
Resolution : 2.87 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

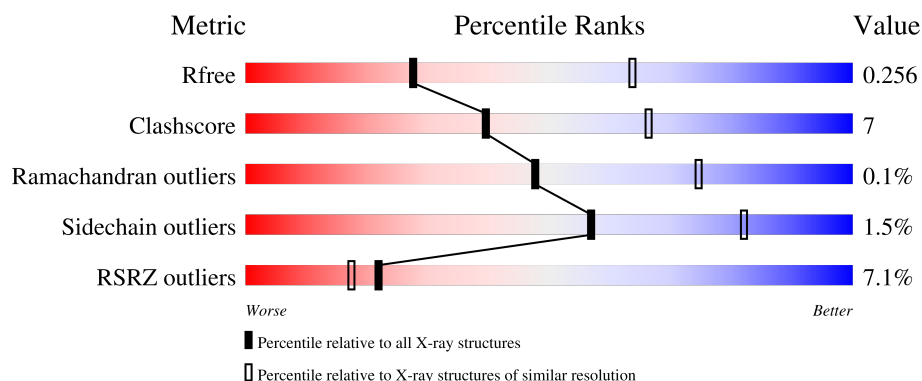
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	206	8% 79% 17% .
1	B	206	8% 79% 17% ..
2	H	220	4% 86% 13% .
2	M	220	9% 87% 13%
3	L	214	3% 82% 17%

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Mol	Chain	Length	Quality of chain
3	N	214	 A horizontal bar chart showing the quality of chain N. The bar is divided into three segments: a red segment on the left labeled '9%', a green segment in the middle labeled '86%', and a yellow segment on the right labeled '13%'.

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18948 atoms, of which 9300 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 Mucosal addressin cell adhesion molecule 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	H	N	O	S	0	1	0
			2939	922	1468	265	277	7			
1	B	198	Total	C	H	N	O	S	0	1	0
			2918	922	1448	264	277	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ASN	ASP	engineered mutation	UNP Q13477
A	148	GLN	GLU	engineered mutation	UNP Q13477
A	?	-	GLU	deletion	UNP Q13477
A	?	-	GLU	deletion	UNP Q13477
A	?	-	GLU	deletion	UNP Q13477
A	?	-	PRO	deletion	UNP Q13477
A	?	-	GLN	deletion	UNP Q13477
A	?	-	GLY	deletion	UNP Q13477
A	?	-	GLN	deletion	UNP Q13477
A	?	-	GLY	deletion	UNP Q13477
A	150	PRO	-	insertion	UNP Q13477
A	151	ILE	-	insertion	UNP Q13477
A	152	GLY	-	insertion	UNP Q13477
A	153	GLY	-	insertion	UNP Q13477
A	203	GLY	-	expression tag	UNP Q13477
A	204	GLY	-	expression tag	UNP Q13477
A	205	GLU	-	expression tag	UNP Q13477
A	206	ASN	-	expression tag	UNP Q13477
A	207	LEU	-	expression tag	UNP Q13477
A	208	TYR	-	expression tag	UNP Q13477
A	209	PHE	-	expression tag	UNP Q13477
A	210	GLN	-	expression tag	UNP Q13477
B	94	ASN	ASP	engineered mutation	UNP Q13477
B	148	GLN	GLU	engineered mutation	UNP Q13477
B	?	-	GLU	deletion	UNP Q13477

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP Q13477
B	?	-	GLU	deletion	UNP Q13477
B	?	-	PRO	deletion	UNP Q13477
B	?	-	GLN	deletion	UNP Q13477
B	?	-	GLY	deletion	UNP Q13477
B	?	-	GLN	deletion	UNP Q13477
B	?	-	GLY	deletion	UNP Q13477
B	150	PRO	-	insertion	UNP Q13477
B	151	ILE	-	insertion	UNP Q13477
B	152	GLY	-	insertion	UNP Q13477
B	153	GLY	-	insertion	UNP Q13477
B	203	GLY	-	expression tag	UNP Q13477
B	204	GLY	-	expression tag	UNP Q13477
B	205	GLU	-	expression tag	UNP Q13477
B	206	ASN	-	expression tag	UNP Q13477
B	207	LEU	-	expression tag	UNP Q13477
B	208	TYR	-	expression tag	UNP Q13477
B	209	PHE	-	expression tag	UNP Q13477
B	210	GLN	-	expression tag	UNP Q13477

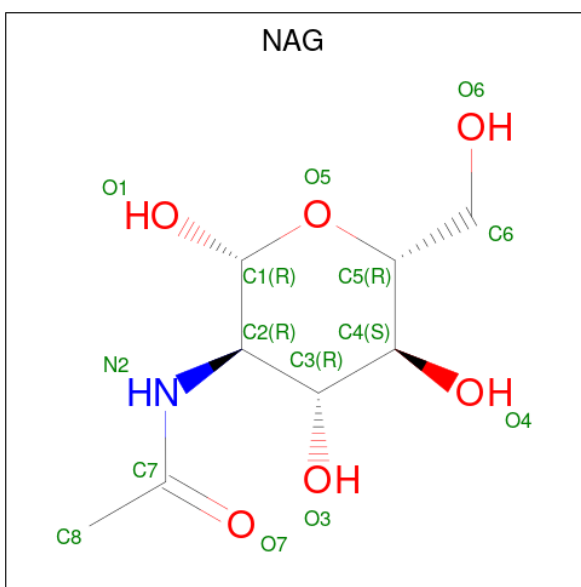
- Molecule 2 is a protein called 10G3 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	220	Total	C	H	N	O	S	0	1	0
			3288	1061	1612	276	333	6			
2	M	220	Total	C	H	N	O	S	0	1	0
			3295	1061	1621	275	332	6			

- Molecule 3 is a protein called 10G3 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	213	Total	C	H	N	O	S	0	0	0
			3218	1030	1569	277	335	7			
3	N	213	Total	C	H	N	O	S	0	0	0
			3218	1030	1569	277	335	7			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	N	O		0	0
			14	8	1	5			

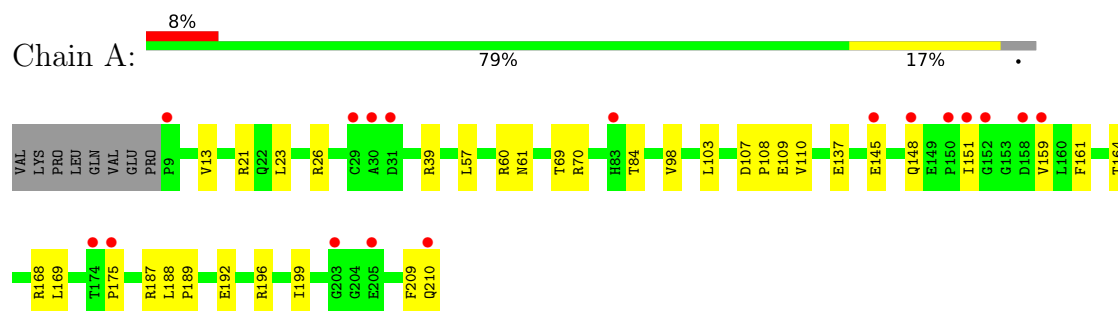
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	H	1	Total	O	0	0
			1	1		
5	L	7	Total	O	0	0
			7	7		
5	B	5	Total	O	0	0
			5	5		
5	M	6	Total	O	0	0
			6	6		
5	N	7	Total	O	0	0
			7	7		

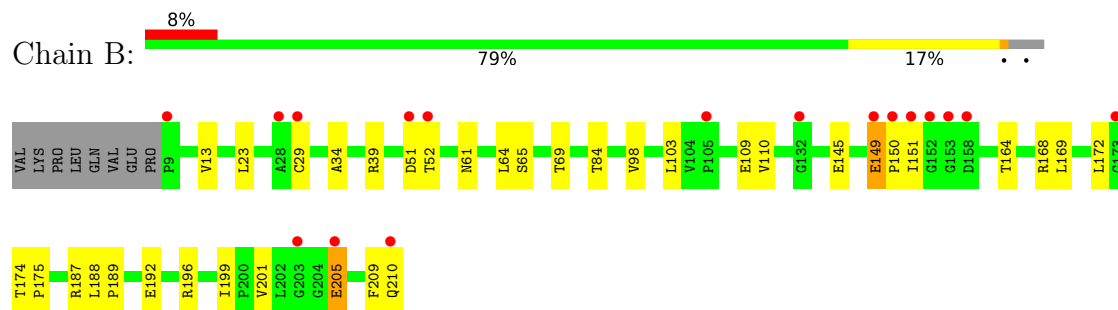
3 Residue-property plots [i](#)

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

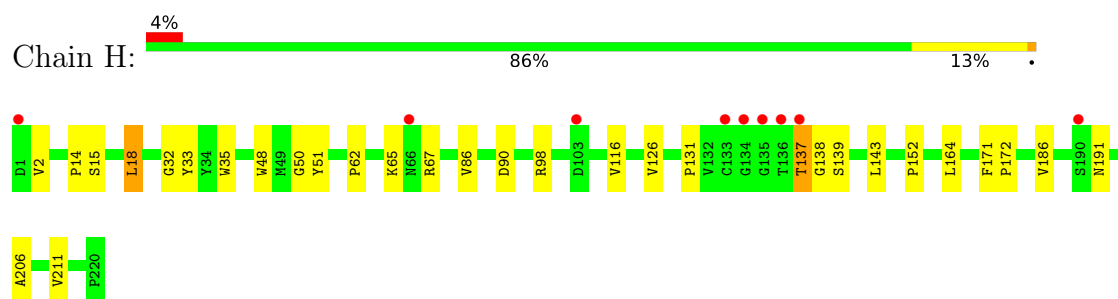
- Molecule 1: Mucosal addressin cell adhesion molecule 1



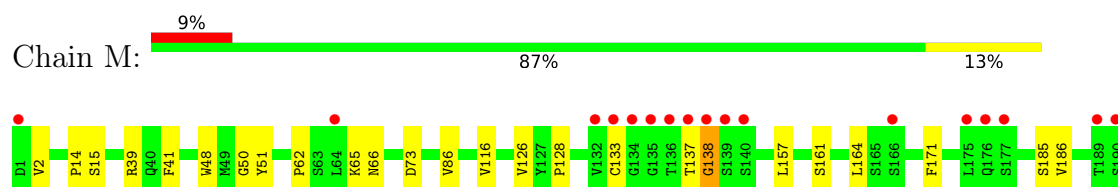
- Molecule 1: Mucosal addressin cell adhesion molecule 1



- Molecule 2: 10G3 heavy chain

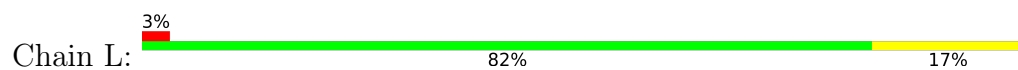


- Molecule 2: 10G3 heavy chain

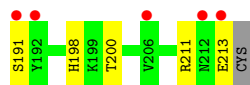
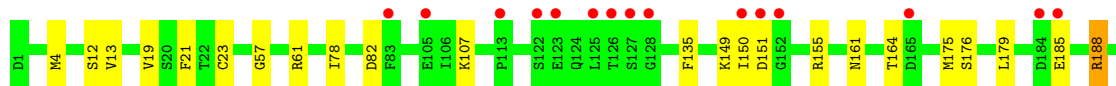
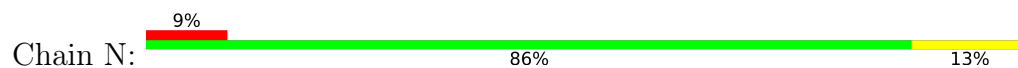




• Molecule 3: 10G3 light chain



• Molecule 3: 10G3 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	317.85Å 71.73Å 70.56Å 90.00° 93.29° 90.00°	Depositor
Resolution (Å)	49.33 – 2.87 49.33 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.33-2.87) 98.0 (49.33-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.200 , 0.253 0.210 , 0.256	Depositor DCC
R_{free} test set	1791 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtrriage
Anisotropy	0.565	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18948	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.33	0/1501	0.77	0/2049
1	B	0.32	0/1501	0.78	2/2052 (0.1%)
2	H	0.28	0/1722	0.73	3/2359 (0.1%)
2	M	0.29	0/1723	0.80	3/2360 (0.1%)
3	L	0.29	0/1687	0.67	0/2284
3	N	0.30	0/1687	0.69	0/2284
All	All	0.30	0/9821	0.74	8/13388 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	138	GLY	CA-C-N	12.82	142.50	120.58
2	M	138	GLY	C-N-CA	12.82	142.50	120.58
2	M	2	VAL	N-CA-C	6.72	119.08	108.87
1	B	149	GLU	CA-C-N	6.13	127.51	119.84
1	B	149	GLU	C-N-CA	6.13	127.51	119.84
2	H	139	SER	N-CA-C	-5.79	105.10	111.82
2	H	137	THR	CA-C-N	5.02	128.39	121.26
2	H	137	THR	C-N-CA	5.02	128.39	121.26

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1471	1468	1471	25	1
1	B	1470	1448	1468	30	0
2	H	1676	1612	1624	23	1
2	M	1674	1621	1627	19	0
3	L	1649	1569	1573	23	1
3	N	1649	1569	1573	16	0
4	A	14	13	12	0	0
4	B	14	0	13	2	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
5	H	1	0	0	0	0
5	L	7	0	0	0	0
5	M	6	0	0	0	0
5	N	7	0	0	0	0
All	All	9648	9300	9361	128	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HG21	2:H:98:ARG:HH12	1.38	0.89
3:L:151:ASP:HA	3:L:191:SER:OG	1.75	0.87
1:A:187:ARG:NH1	5:A:405:HOH:O	2.15	0.78
2:H:2:VAL:HG21	2:H:98:ARG:NH1	2.00	0.77
3:L:151:ASP:OD1	3:L:191:SER:OG	2.04	0.75
1:A:98:VAL:HG11	1:A:199:ILE:HG12	1.71	0.72
2:M:164:LEU:HD23	2:M:186:VAL:HG21	1.73	0.70
3:L:110:ASP:HB3	3:L:200:THR:HG22	1.75	0.69
1:A:210[A]:GLN:HG3	1:A:210[A]:GLN:OXT	1.93	0.68
3:N:151:ASP:HA	3:N:191:SER:OG	1.98	0.63
2:H:131:PRO:HD3	2:H:143:LEU:CD2	2.28	0.62
3:L:15:LEU:HG	3:L:106:ILE:HD11	1.81	0.62
1:B:69:THR:HG23	1:B:84:THR:HG23	1.82	0.62
3:L:151:ASP:CA	3:L:191:SER:OG	2.46	0.62
1:B:205[A]:GLU:CA	1:B:205[A]:GLU:OE1	2.48	0.60
2:M:62:PRO:HA	2:M:65:LYS:HB2	1.85	0.58
2:H:18:LEU:C	2:H:18:LEU:HD23	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:164:LEU:CD2	2:M:186:VAL:HG21	2.33	0.57
1:B:51:ASP:OD1	1:B:52:THR:N	2.38	0.57
1:A:137:GLU:OE1	1:B:69:THR:OG1	2.23	0.56
1:B:172:LEU:HD13	1:B:201:VAL:HG11	1.88	0.56
3:N:150:ILE:HD12	3:N:155:ARG:HD2	1.88	0.56
3:L:83:PHE:CE1	3:L:106:ILE:HB	2.40	0.55
1:A:151:ILE:HG13	1:A:151:ILE:O	2.06	0.55
2:H:164:LEU:HD23	2:H:186:VAL:HG21	1.88	0.55
2:M:48:TRP:CZ2	2:M:50:GLY:HA2	2.42	0.54
2:M:51:TYR:C	2:M:51:TYR:CD1	2.85	0.54
2:M:86:VAL:CG1	2:M:116:VAL:HG21	2.37	0.54
1:B:205[A]:GLU:OE1	1:B:205[A]:GLU:N	2.40	0.54
3:L:13:VAL:HG21	3:L:19:VAL:HG13	1.88	0.54
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.41	0.54
2:H:51:TYR:C	2:H:51:TYR:CD1	2.86	0.53
1:A:192:GLU:O	3:N:57:GLY:N	2.42	0.53
2:H:86:VAL:CG1	2:H:116:VAL:HG21	2.39	0.53
3:N:151:ASP:OD1	3:N:191:SER:OG	2.26	0.53
1:B:209:PHE:O	1:B:210:GLN:C	2.52	0.52
3:L:111:ALA:O	3:L:200:THR:HG21	2.09	0.52
3:L:140:TYR:CG	3:L:141:PRO:HA	2.44	0.52
1:B:13:VAL:HG11	1:B:23:LEU:HD21	1.92	0.52
2:H:86:VAL:HG12	2:H:116:VAL:HG11	1.91	0.52
1:B:98:VAL:HG11	1:B:199:ILE:HG12	1.92	0.51
1:A:175:PRO:HG2	1:B:64:LEU:O	2.11	0.51
1:B:149:GLU:HB2	1:B:150:PRO:HD2	1.92	0.51
2:M:126:VAL:HB	2:M:211:VAL:HG11	1.93	0.50
2:M:137:THR:HG22	2:M:138:GLY:N	2.27	0.50
3:L:113:PRO:HD2	3:L:205:ILE:HD12	1.94	0.50
2:H:191[A]:ASN:OD1	2:H:191[A]:ASN:C	2.55	0.49
2:H:48:TRP:CZ2	2:H:50:GLY:HA2	2.47	0.49
3:N:198:HIS:CD2	3:N:200:THR:HG23	2.48	0.49
1:B:149:GLU:HB2	1:B:150:PRO:CD	2.42	0.49
3:L:161:ASN:HB3	3:L:175:MET:HE3	1.95	0.49
1:B:110:VAL:CG2	1:B:169:LEU:HD11	2.43	0.49
1:A:13:VAL:HG13	1:A:21:ARG:NH1	2.28	0.48
3:L:198:HIS:CD2	3:L:200:THR:HG23	2.49	0.48
3:N:61:ARG:NH1	3:N:82:ASP:OD2	2.46	0.48
1:B:205[A]:GLU:OE1	1:B:205[A]:GLU:HA	2.13	0.47
1:A:103:LEU:HD21	1:A:110:VAL:HG22	1.96	0.47
1:B:109:GLU:OE2	1:B:168:ARG:NH1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:19:VAL:HG22	3:N:78:ILE:HD11	1.96	0.47
3:L:190:ASN:O	3:L:210:ASN:HA	2.14	0.47
3:N:161:ASN:HB3	3:N:175:MET:HE3	1.97	0.47
3:N:175:MET:HG2	3:N:176:SER:N	2.29	0.47
1:A:110:VAL:CG2	1:A:169:LEU:HD11	2.45	0.47
1:A:103:LEU:HD11	1:A:110:VAL:HG21	1.96	0.46
3:L:106:ILE:HG22	3:L:166:GLN:CD	2.40	0.46
1:B:188:LEU:HB3	1:B:189:PRO:HD2	1.97	0.46
3:L:13:VAL:HG21	3:L:19:VAL:CG1	2.45	0.46
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.50	0.45
1:A:109:GLU:OE2	1:A:168:ARG:NH1	2.50	0.45
2:M:161:SER:N	2:M:201:ASN:OD1	2.46	0.45
1:A:148:GLN:HG2	1:A:161:PHE:CE2	2.52	0.45
3:N:12:SER:HB3	3:N:107:LYS:HG3	1.99	0.45
1:A:69:THR:HG23	1:A:84:THR:HG23	1.99	0.45
2:M:86:VAL:HG12	2:M:116:VAL:HG11	1.98	0.45
3:N:185:GLU:HB3	3:N:188:ARG:NH2	2.32	0.45
3:L:188:ARG:HG2	3:L:188:ARG:O	2.17	0.44
1:B:110:VAL:HG11	1:B:199:ILE:HD13	1.98	0.44
2:M:128:PRO:HD3	2:M:213:LYS:HD3	2.00	0.44
2:H:14:PRO:O	2:H:15:SER:HB2	2.17	0.44
3:L:6:GLN:NE2	3:L:88:CYS:SG	2.88	0.44
1:B:29:CYS:SG	1:B:34:ALA:HB2	2.58	0.44
3:N:4:MET:HE3	3:N:23:CYS:SG	2.58	0.44
2:H:126:VAL:HB	2:H:211:VAL:HG11	2.00	0.44
2:H:62:PRO:HA	2:H:65:LYS:HB2	2.00	0.43
1:A:145:GLU:HG3	1:A:164:THR:HB	2.00	0.43
3:L:13:VAL:HG11	3:L:78:ILE:CD1	2.48	0.43
1:B:61:ASN:ND2	4:B:2061:NAG:C7	2.81	0.43
1:A:110:VAL:HG23	1:A:169:LEU:HG	1.99	0.43
2:M:185:SER:HB3	3:N:135:PHE:CE2	2.54	0.43
3:N:13:VAL:HG11	3:N:78:ILE:HD12	1.99	0.43
1:B:145:GLU:HG3	1:B:164:THR:HB	2.00	0.43
1:A:175:PRO:HG2	1:B:65:SER:HA	1.99	0.43
2:M:14:PRO:O	2:M:15:SER:HB2	2.19	0.43
1:A:188:LEU:HB3	1:A:189:PRO:HD2	1.99	0.43
2:H:32:GLY:O	2:H:33:TYR:HB2	2.18	0.43
3:L:4:MET:HE3	3:L:23:CYS:SG	2.59	0.42
3:L:142:LYS:HB2	3:L:173:TYR:CE2	2.53	0.42
1:B:61:ASN:ND2	4:B:2061:NAG:O7	2.52	0.42
1:B:110:VAL:HG23	1:B:169:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:149:LYS:HB2	3:L:193:THR:HB	2.01	0.42
1:B:103:LEU:HD21	1:B:110:VAL:HG22	2.00	0.42
2:M:191:ASN:OD1	2:M:191:ASN:C	2.62	0.42
2:H:152:PRO:HD2	2:H:206:ALA:CB	2.50	0.42
2:H:171:PHE:HA	2:H:172:PRO:HD3	1.95	0.42
1:B:187:ARG:HG2	1:B:192:GLU:HG3	2.02	0.42
2:M:157:LEU:C	2:M:157:LEU:HD23	2.45	0.42
2:H:35:TRP:CZ3	2:H:98:ARG:HB2	2.54	0.42
1:B:210:GLN:OXT	1:B:210:GLN:HG3	2.20	0.42
1:B:151:ILE:O	1:B:151:ILE:HG13	2.20	0.42
1:B:174:THR:HG23	1:B:175:PRO:HA	2.02	0.42
1:A:13:VAL:HG21	1:A:23:LEU:HD21	2.02	0.41
2:H:131:PRO:HD3	2:H:143:LEU:HD22	2.03	0.41
1:A:107:ASP:HA	1:A:108:PRO:HD3	1.92	0.41
2:H:33:TYR:HB3	2:H:98:ARG:HG3	2.02	0.41
2:M:66:ASN:OD1	2:M:66:ASN:N	2.50	0.41
3:N:150:ILE:HD11	3:N:179:LEU:HD21	2.03	0.41
1:A:175:PRO:CG	1:B:64:LEU:O	2.69	0.41
2:H:18:LEU:C	2:H:18:LEU:CD2	2.93	0.41
2:H:131:PRO:HD3	2:H:143:LEU:HD23	2.02	0.41
1:A:209:PHE:O	1:A:210[A]:GLN:C	2.64	0.41
1:A:57:LEU:HD21	1:A:70:ARG:NH1	2.35	0.41
2:M:171:PHE:CD2	3:N:164:THR:HG23	2.56	0.41
1:A:60:ARG:O	1:A:61:ASN:C	2.63	0.41
2:H:137:THR:HG22	2:H:138:GLY:N	2.36	0.41
2:M:73:ASP:OD1	2:M:73:ASP:C	2.64	0.41
3:L:175:MET:HG2	3:L:176:SER:N	2.35	0.40
2:M:39:ARG:HD3	2:M:41:PHE:CZ	2.56	0.40
1:A:137:GLU:CD	1:B:69:THR:HG1	2.26	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:191[A]:ASN:OD1	3:L:24:HIS:NE2[4_555]	2.14	0.06
1:A:26:ARG:HH12	1:A:210[A]:GLN:O[1_554]	1.59	0.01

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	196/206 (95%)	183 (93%)	12 (6%)	1 (0%)	24	51
1	B	197/206 (96%)	185 (94%)	12 (6%)	0	100	100
2	H	219/220 (100%)	212 (97%)	7 (3%)	0	100	100
2	M	219/220 (100%)	209 (95%)	10 (5%)	0	100	100
3	L	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
3	N	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
All	All	1253/1280 (98%)	1194 (95%)	58 (5%)	1 (0%)	48	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	VAL

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	158/165 (96%)	156 (99%)	2 (1%)	61	84
1	B	158/165 (96%)	154 (98%)	4 (2%)	42	72
2	H	192/191 (100%)	191 (100%)	1 (0%)	81	93
2	M	192/191 (100%)	191 (100%)	1 (0%)	81	93
3	L	187/188 (100%)	183 (98%)	4 (2%)	47	75
3	N	187/188 (100%)	182 (97%)	5 (3%)	39	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1074/1088 (99%)	1057 (98%)	17 (2%)	57 81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	196	ARG
2	H	18	LEU
3	L	21	PHE
3	L	149	LYS
3	L	199	LYS
3	L	211	ARG
1	B	39	ARG
1	B	196	ARG
1	B	205[A]	GLU
1	B	205[B]	GLU
2	M	133	CYS
3	N	21	PHE
3	N	149	LYS
3	N	188	ARG
3	N	211	ARG
3	N	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	58	ASN
2	H	169	HIS
2	H	176	GLN
3	L	190	ASN
2	M	40	GLN
2	M	58	ASN
2	M	59	ASN
2	M	169	HIS
3	N	38	GLN
3	N	50	HIS
3	N	53	ASN
3	N	93	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	2061	1	14,14,15	0.88	1 (7%)	17,19,21	0.74	0
4	NAG	B	2061	1	14,14,15	0.48	0	17,19,21	1.07	1 (5%)

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	2061	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2061	1	-	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)
4	A	2061	NAG	O3-C3	-2.83	1.35	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2061	NAG	C1-O5-C5	3.53	116.91	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2061	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2061	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	198/206 (96%)	0.27	17 (8%)	16 13	24, 50, 121, 193	1 (0%)
1	B	198/206 (96%)	0.35	17 (8%)	16 13	27, 58, 118, 192	1 (0%)
2	H	220/220 (100%)	0.01	9 (4%)	41 33	24, 45, 86, 148	1 (0%)
2	M	220/220 (100%)	0.42	19 (8%)	16 13	20, 52, 140, 191	1 (0%)
3	L	213/214 (99%)	0.11	7 (3%)	49 40	19, 49, 102, 164	0
3	N	213/214 (99%)	0.60	20 (9%)	14 12	21, 65, 120, 159	0
All	All	1262/1280 (98%)	0.29	89 (7%)	22 17	19, 54, 118, 193	4 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	139	SER	5.2
3	L	83	PHE	5.2
2	M	136	THR	5.1
1	A	9	PRO	4.8
2	M	175	LEU	4.6
2	M	134	GLY	4.5
3	N	83	PHE	4.4
1	B	151	ILE	4.3
2	H	137	THR	4.3
1	B	150	PRO	4.1
1	A	151	ILE	4.0
3	N	122	SER	3.7
1	B	132	GLY	3.7
2	H	135	GLY	3.7
3	N	128	GLY	3.6
1	A	31	ASP	3.6
2	H	1	ASP	3.6
1	A	150	PRO	3.4
1	A	83	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
3	L	201	SER	3.4
1	B	105	PRO	3.4
1	A	205	GLU	3.4
1	A	210[A]	GLN	3.4
1	A	158	ASP	3.3
2	M	135	GLY	3.3
3	N	184	ASP	3.3
1	A	175	PRO	3.2
1	A	159	VAL	3.2
2	H	103	ASP	3.2
1	B	205[A]	GLU	3.2
2	M	64	LEU	3.1
2	M	140	SER	3.0
2	M	177	SER	3.0
2	H	136	THR	3.0
2	M	137	THR	2.9
3	L	199	LYS	2.9
1	B	153	GLY	2.9
1	B	9	PRO	2.9
3	N	191	SER	2.9
2	M	176	GLN	2.8
3	N	127	SER	2.8
3	N	212	ASN	2.8
3	L	200	THR	2.8
1	A	152	GLY	2.8
1	B	203	GLY	2.8
1	B	51	ASP	2.7
1	A	29	CYS	2.7
2	H	133	CYS	2.6
3	N	165	ASP	2.6
2	M	191	ASN	2.6
3	N	213	GLU	2.6
1	A	30	ALA	2.6
3	N	125	LEU	2.6
1	B	52	THR	2.6
1	A	174	THR	2.5
2	M	189	THR	2.5
2	M	133	CYS	2.5
1	B	152	GLY	2.4
2	M	190	SER	2.4
3	N	185	GLU	2.4
2	H	134	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	N	152	GLY	2.4
3	N	123	GLU	2.4
2	M	192	THR	2.3
3	L	15	LEU	2.3
1	B	149	GLU	2.3
3	N	150	ILE	2.3
3	N	113	PRO	2.3
2	M	132	VAL	2.3
1	A	148	GLN	2.2
3	N	126	THR	2.2
3	L	42	LYS	2.2
2	H	190	SER	2.2
2	M	166	SER	2.2
3	L	191	SER	2.2
2	H	66	ASN	2.1
3	N	151	ASP	2.1
1	B	29	CYS	2.1
1	A	203	GLY	2.1
1	B	173	GLY	2.1
2	M	138	GLY	2.1
3	N	192	TYR	2.1
1	B	210	GLN	2.1
1	B	158	ASP	2.1
1	B	28	ALA	2.1
2	M	1	ASP	2.0
3	N	105	GLU	2.0
1	A	145	GLU	2.0
3	N	206	VAL	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 oligosaccharides 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. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	2061	14/15	0.46	0.18	37,44,48,49	0
4	NAG	A	2061	14/15	0.70	0.13	77,97,121,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.