



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:51 AM GMT

PDB ID : 1L6Z  
Title : CRYSTAL STRUCTURE OF MURINE CEACAM1A[1,4]: A CORON-  
AVIRUS RECEPTOR AND CELL ADHESION MOLECULE IN THE CEA  
FAMILY  
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Deposited on : 2002-03-14  
Resolution : 3.32 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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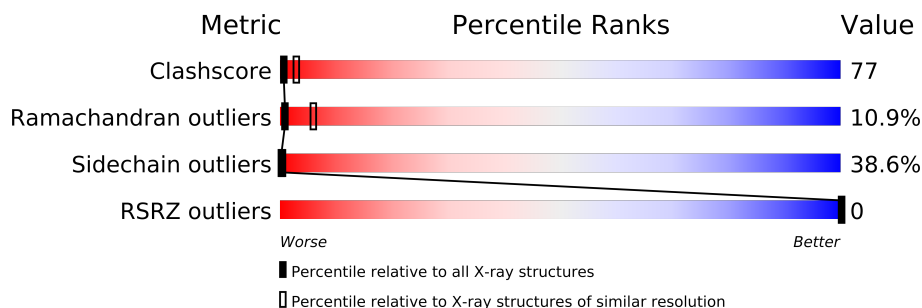
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.32 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))
Clashscore	79885	1016 (3.42-3.22)
Ramachandran outliers	78287	1699 (3.44-3.20)
Sidechain outliers	78261	1697 (3.44-3.20)
RSRZ outliers	66119	1373 (3.44-3.20)

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. 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	216	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1716 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.

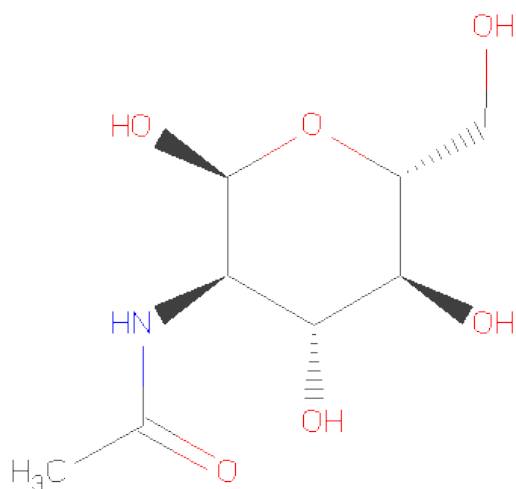
- Molecule 1 is a protein called biliary glycoprotein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1609	1011	276	314	8			

There are 14 discrepancies between the modelled and reference sequences:

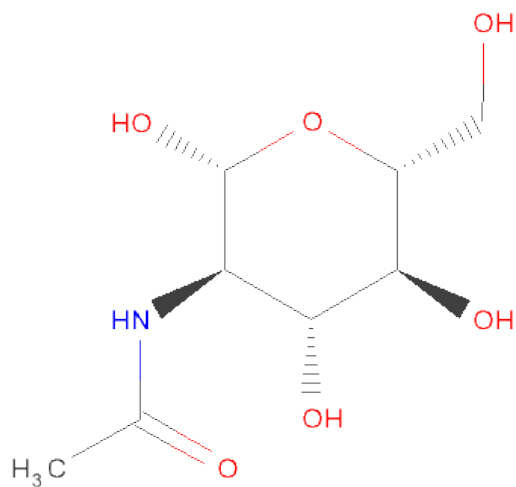
Chain	Residue	Modelled	Actual	Comment	Reference
A	203	SER	-	CLONING ARTIFACT	PIR JC1507
A	204	ARG	-	CLONING ARTIFACT	PIR JC1507
A	205	LEU	-	CLONING ARTIFACT	PIR JC1507
A	206	VAL	-	CLONING ARTIFACT	PIR JC1507
A	207	PRO	-	CLONING ARTIFACT	PIR JC1507
A	208	ARG	-	CLONING ARTIFACT	PIR JC1507
A	209	GLY	-	CLONING ARTIFACT	PIR JC1507
A	210	SER	-	CLONING ARTIFACT	PIR JC1507
A	211	HIS	-	CLONING ARTIFACT	PIR JC1507
A	212	HIS	-	CLONING ARTIFACT	PIR JC1507
A	213	HIS	-	CLONING ARTIFACT	PIR JC1507
A	214	HIS	-	CLONING ARTIFACT	PIR JC1507
A	215	HIS	-	CLONING ARTIFACT	PIR JC1507
A	216	HIS	-	CLONING ARTIFACT	PIR JC1507

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is a polymer of unknown type called SUGAR (NAG-NAG-MAN).

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

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	SER	-	CLONING ARTIFACT	PIR JC1507
A	204	ARG	-	CLONING ARTIFACT	PIR JC1507
A	205	LEU	-	CLONING ARTIFACT	PIR JC1507
A	206	VAL	-	CLONING ARTIFACT	PIR JC1507
A	207	PRO	-	CLONING ARTIFACT	PIR JC1507
A	208	ARG	-	CLONING ARTIFACT	PIR JC1507
A	209	GLY	-	CLONING ARTIFACT	PIR JC1507
A	210	SER	-	CLONING ARTIFACT	PIR JC1507
A	211	HIS	-	CLONING ARTIFACT	PIR JC1507
A	212	HIS	-	CLONING ARTIFACT	PIR JC1507
A	213	HIS	-	CLONING ARTIFACT	PIR JC1507
A	214	HIS	-	CLONING ARTIFACT	PIR JC1507
A	215	HIS	-	CLONING ARTIFACT	PIR JC1507
A	216	HIS	-	CLONING ARTIFACT	PIR JC1507

- Molecule 5 is water.

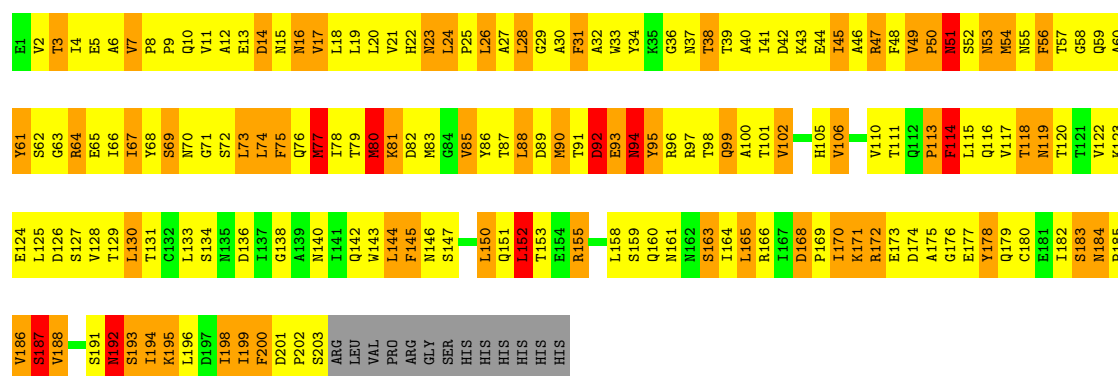
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		

### 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: biliary glycoprotein C

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.26Å 111.26Å 65.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.32 28.85 – 3.32	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.32) 97.4 (28.85-3.32)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 3.31Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.295 , 0.329 0.306 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	95.6	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 50.4	EDS
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 6979 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	1716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, NDG

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	0.50	1/1638 (0.1%)	0.98	8/2229 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	ILE	N-CA	-5.72	1.34	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ASN	C-N-CD	8.87	147.02	128.40
1	A	138	GLY	N-CA-C	-8.21	92.58	113.10
1	A	184	ASN	N-CA-C	-7.92	89.61	111.00
1	A	185	PRO	N-CA-C	-6.65	94.81	112.10
1	A	94	ASN	N-CA-C	-6.17	94.33	111.00
1	A	198	ILE	N-CA-C	5.51	125.87	111.00
1	A	187	SER	N-CA-C	-5.37	96.52	111.00
1	A	92	ASP	N-CA-C	-5.07	97.31	111.00

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	1609	0	1586	254	0
2	A	14	0	13	2	0
3	A	28	0	26	1	0
4	A	39	0	34	6	0
5	A	26	0	0	0	0
All	All	1716	0	1659	258	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 77.

All (258) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:371:NAG:O6	4:A:372:BMA:H2	1.46	1.16
1:A:45:ILE:HA	1:A:60:ALA:HB3	1.25	1.09
1:A:4:ILE:HG12	1:A:102:VAL:HG21	1.34	1.06
1:A:192:ASN:H	1:A:192:ASN:HD22	1.03	0.99
1:A:192:ASN:H	1:A:192:ASN:ND2	1.56	0.98
1:A:88:LEU:H	1:A:100:ALA:CB	1.77	0.97
1:A:192:ASN:N	1:A:192:ASN:HD22	1.59	0.97
1:A:11:VAL:HG11	1:A:17:VAL:HG22	1.48	0.96
1:A:45:ILE:HG21	1:A:65:GLU:OE1	1.66	0.95
1:A:3:THR:HB	1:A:22:HIS:CD2	2.03	0.92
1:A:28:LEU:O	1:A:50:PRO:HG2	1.73	0.89
1:A:21:VAL:HG21	1:A:71:GLY:O	1.75	0.87
1:A:29:GLY:O	1:A:50:PRO:HD2	1.76	0.86
1:A:45:ILE:HA	1:A:60:ALA:CB	2.06	0.85
1:A:88:LEU:H	1:A:100:ALA:HB3	1.39	0.85
1:A:123:LYS:HA	1:A:199:ILE:O	1.77	0.84
1:A:3:THR:HB	1:A:22:HIS:HD2	1.42	0.84
1:A:165:LEU:HD12	1:A:166:ARG:N	1.94	0.82
1:A:31:PHE:CE2	1:A:48:PHE:HB3	2.13	0.82
1:A:64:ARG:HH12	1:A:75:PHE:HE2	1.25	0.81
1:A:4:ILE:CG1	1:A:102:VAL:HG21	2.11	0.80
1:A:66:ILE:HA	3:A:355:NAG:O7	1.82	0.80
1:A:30:ALA:HB2	1:A:49:VAL:HG13	1.66	0.78
1:A:16:ASN:ND2	1:A:76:GLN:HA	1.98	0.78
1:A:114:PHE:HA	1:A:192:ASN:HD21	1.49	0.78
1:A:179:GLN:HG3	1:A:192:ASN:O	1.83	0.78
1:A:182:ILE:O	1:A:188:VAL:HG12	1.84	0.77
1:A:130:LEU:HD23	1:A:130:LEU:N	2.00	0.77
1:A:4:ILE:HD11	1:A:33:TRP:HH2	1.49	0.77
1:A:66:ILE:O	1:A:73:LEU:HA	1.86	0.76
1:A:74:LEU:HG	1:A:75:PHE:N	2.00	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:183:SER:HA	1:A:188:VAL:HG12	1.68	0.75
1:A:4:ILE:HG23	1:A:102:VAL:HG23	1.69	0.75
1:A:91:THR:HG23	1:A:96:ARG:HB2	1.68	0.74
1:A:64:ARG:NH1	1:A:75:PHE:HE2	1.83	0.74
1:A:117:VAL:HG21	1:A:194:ILE:HG21	1.69	0.74
1:A:9:PRO:O	1:A:10:GLN:HB2	1.86	0.73
1:A:4:ILE:CD1	1:A:33:TRP:HH2	2.01	0.73
4:A:371:NAG:O6	4:A:372:BMA:C2	2.34	0.73
1:A:123:LYS:HD3	1:A:201:ASP:HB2	1.70	0.73
1:A:34:TYR:HD2	1:A:43:LYS:O	1.72	0.72
1:A:160:GLN:O	1:A:163:SER:HB2	1.88	0.72
1:A:78:ILE:HG23	1:A:82:ASP:HB3	1.72	0.71
1:A:110:VAL:HG12	1:A:111:THR:N	2.07	0.70
1:A:67:ILE:HG13	1:A:68:TYR:N	2.04	0.70
1:A:28:LEU:HA	1:A:92:ASP:HB3	1.71	0.70
1:A:51:ASN:HD22	1:A:51:ASN:H	1.40	0.69
1:A:152:LEU:HD21	1:A:158:LEU:HD21	1.74	0.69
1:A:110:VAL:HG11	1:A:182:ILE:CG2	2.24	0.68
1:A:75:PHE:O	1:A:78:ILE:HD11	1.93	0.68
1:A:155:ARG:HB2	1:A:169:PRO:HD2	1.75	0.68
1:A:50:PRO:O	1:A:52:SER:N	2.26	0.68
1:A:79:THR:H	1:A:82:ASP:HB2	1.58	0.67
1:A:110:VAL:HG11	1:A:182:ILE:HG21	1.76	0.67
1:A:80:MET:HG3	1:A:81:LYS:N	2.09	0.67
1:A:36:GLY:O	1:A:37:ASN:HB3	1.94	0.67
1:A:110:VAL:HG12	1:A:111:THR:H	1.60	0.66
1:A:91:THR:CG2	1:A:96:ARG:HB2	2.25	0.66
1:A:45:ILE:CA	1:A:60:ALA:HB3	2.15	0.66
1:A:123:LYS:HB2	1:A:126:ASP:OD2	1.97	0.64
1:A:17:VAL:HG23	1:A:78:ILE:CD1	2.27	0.64
1:A:4:ILE:HD11	1:A:33:TRP:CH2	2.32	0.63
1:A:79:THR:O	1:A:82:ASP:N	2.24	0.63
1:A:179:GLN:NE2	1:A:193:SER:OG	2.32	0.63
1:A:115:LEU:HD11	1:A:180:CYS:H	1.63	0.63
1:A:64:ARG:NH1	1:A:75:PHE:CE2	2.65	0.62
1:A:64:ARG:NH1	1:A:82:ASP:OD2	2.31	0.62
2:A:337:NDG:O7	2:A:337:NDG:C3	2.46	0.62
1:A:11:VAL:CG1	1:A:17:VAL:HG22	2.28	0.62
1:A:87:THR:HG23	1:A:100:ALA:HB3	1.81	0.62
1:A:102:VAL:HG12	1:A:102:VAL:O	2.00	0.62
1:A:31:PHE:HE2	1:A:48:PHE:HB3	1.64	0.62
1:A:30:ALA:HB1	1:A:48:PHE:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:110:VAL:CG2	1:A:184:ASN:HB2	2.30	0.61
1:A:200:PHE:N	1:A:200:PHE:CD2	2.68	0.61
1:A:49:VAL:HG21	1:A:56:PHE:CZ	2.36	0.61
1:A:128:VAL:HG23	1:A:170:ILE:HD13	1.81	0.60
1:A:145:PHE:HD1	1:A:146:ASN:N	1.98	0.60
1:A:78:ILE:HD12	1:A:78:ILE:N	2.16	0.60
1:A:31:PHE:O	1:A:47:ARG:HA	2.01	0.60
1:A:131:THR:HG23	1:A:164:ILE:HG12	1.82	0.60
1:A:122:VAL:HG21	1:A:128:VAL:HG22	1.82	0.60
1:A:78:ILE:HG23	1:A:82:ASP:CB	2.32	0.59
1:A:183:SER:HA	1:A:188:VAL:CG1	2.32	0.59
1:A:145:PHE:HE1	1:A:176:GLY:HA3	1.67	0.59
1:A:88:LEU:H	1:A:100:ALA:HB1	1.66	0.58
1:A:113:PRO:HG2	1:A:191:SER:HB3	1.85	0.58
1:A:178:TYR:N	1:A:178:TYR:HD2	2.01	0.58
1:A:34:TYR:CD2	1:A:44:GLU:HA	2.38	0.58
1:A:125:LEU:HD23	1:A:169:PRO:HB2	1.85	0.58
1:A:117:VAL:HG22	1:A:130:LEU:HD22	1.86	0.57
1:A:4:ILE:CD1	1:A:33:TRP:CH2	2.86	0.57
1:A:122:VAL:HG12	1:A:123:LYS:N	2.19	0.57
1:A:60:ALA:O	1:A:62:SER:N	2.38	0.57
1:A:122:VAL:HG11	1:A:170:ILE:CD1	2.35	0.57
1:A:4:ILE:HA	1:A:20:LEU:O	2.05	0.56
1:A:76:GLN:O	1:A:78:ILE:HD12	2.05	0.56
1:A:11:VAL:HG21	1:A:17:VAL:HG21	1.87	0.56
1:A:34:TYR:HE2	1:A:44:GLU:HB2	1.71	0.56
1:A:115:LEU:HB2	1:A:194:ILE:HD13	1.88	0.56
1:A:178:TYR:N	1:A:178:TYR:CD2	2.71	0.56
1:A:63:GLY:C	1:A:64:ARG:HG3	2.25	0.55
1:A:29:GLY:O	1:A:30:ALA:HB2	2.07	0.55
1:A:31:PHE:CD2	1:A:67:ILE:HD11	2.42	0.55
1:A:165:LEU:C	1:A:165:LEU:HD12	2.28	0.55
1:A:19:LEU:HD12	1:A:102:VAL:HG11	1.89	0.54
1:A:54:MET:HG2	1:A:56:PHE:CE2	2.43	0.54
1:A:17:VAL:O	1:A:75:PHE:N	2.37	0.54
1:A:11:VAL:HG11	1:A:17:VAL:CG2	2.31	0.54
2:A:337:NDG:O7	2:A:337:NDG:H3	2.07	0.54
1:A:12:ALA:O	1:A:15:ASN:HB2	2.08	0.54
1:A:117:VAL:CG2	1:A:130:LEU:HD22	2.37	0.53
1:A:145:PHE:HB2	1:A:150:LEU:HD22	1.89	0.53
1:A:28:LEU:HD23	1:A:92:ASP:OD1	2.09	0.53
1:A:16:ASN:CG	1:A:76:GLN:HA	2.29	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:LYS:HE3	1:A:173:GLU:HB2	1.90	0.53
1:A:4:ILE:HG23	1:A:102:VAL:CG2	2.37	0.53
1:A:115:LEU:CB	1:A:194:ILE:HD13	2.38	0.52
1:A:32:ALA:O	1:A:88:LEU:HA	2.09	0.52
1:A:51:ASN:N	1:A:51:ASN:HD22	2.00	0.52
1:A:6:ALA:O	1:A:9:PRO:N	2.43	0.52
1:A:92:ASP:OD1	1:A:92:ASP:N	2.41	0.52
1:A:65:GLU:O	1:A:66:ILE:HG13	2.09	0.52
1:A:88:LEU:N	1:A:100:ALA:HB3	2.16	0.52
1:A:140:ASN:HB3	1:A:183:SER:HB2	1.91	0.52
1:A:32:ALA:HA	1:A:46:ALA:O	2.10	0.52
1:A:124:GLU:O	1:A:125:LEU:HB2	2.10	0.52
1:A:75:PHE:HB3	1:A:78:ILE:HD11	1.92	0.51
1:A:152:LEU:CD2	1:A:158:LEU:HD21	2.40	0.51
1:A:140:ASN:HD22	1:A:183:SER:HB2	1.75	0.51
1:A:168:ASP:C	1:A:168:ASP:OD1	2.49	0.51
1:A:110:VAL:CG1	1:A:182:ILE:HG21	2.40	0.51
1:A:14:ASP:OD1	1:A:14:ASP:O	2.29	0.51
1:A:129:THR:HA	1:A:165:LEU:O	2.11	0.51
1:A:4:ILE:HG13	1:A:20:LEU:O	2.10	0.51
1:A:18:LEU:HD12	1:A:73:LEU:O	2.11	0.51
1:A:49:VAL:HG21	1:A:56:PHE:CE1	2.46	0.51
1:A:91:THR:HG23	1:A:96:ARG:CB	2.39	0.51
1:A:122:VAL:HG12	1:A:123:LYS:H	1.76	0.51
1:A:29:GLY:O	1:A:49:VAL:HG13	2.12	0.50
1:A:180:CYS:SG	1:A:191:SER:HB3	2.51	0.50
1:A:23:ASN:O	1:A:25:PRO:HD3	2.11	0.50
1:A:123:LYS:O	1:A:126:ASP:HB2	2.12	0.50
1:A:66:ILE:HG22	1:A:68:TYR:CE2	2.47	0.50
1:A:29:GLY:O	1:A:49:VAL:CG1	2.60	0.50
1:A:58:GLY:O	1:A:60:ALA:N	2.41	0.50
1:A:58:GLY:C	1:A:60:ALA:H	2.13	0.50
1:A:145:PHE:CE1	1:A:176:GLY:HA3	2.46	0.50
1:A:113:PRO:O	1:A:114:PHE:CB	2.60	0.49
1:A:38:THR:C	1:A:40:ALA:H	2.15	0.49
1:A:92:ASP:OD1	1:A:95:TYR:O	2.29	0.49
1:A:8:PRO:HD2	1:A:17:VAL:HG13	1.93	0.49
1:A:31:PHE:CD2	1:A:48:PHE:HB3	2.48	0.49
1:A:67:ILE:HA	1:A:72:SER:O	2.13	0.49
1:A:201:ASP:HB3	1:A:202:PRO:HD3	1.93	0.49
1:A:83:MET:HE2	1:A:105:HIS:ND1	2.27	0.49
1:A:129:THR:HG22	1:A:129:THR:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:76:GLN:O	1:A:77:MET:C	2.51	0.49
1:A:40:ALA:C	1:A:42:ASP:N	2.67	0.48
1:A:54:MET:HG3	1:A:55:ASN:N	2.27	0.48
1:A:45:ILE:HG23	1:A:60:ALA:CB	2.44	0.48
1:A:126:ASP:O	1:A:170:ILE:HG12	2.14	0.48
1:A:69:SER:C	1:A:71:GLY:H	2.16	0.48
1:A:102:VAL:CG1	1:A:102:VAL:O	2.61	0.48
1:A:29:GLY:C	1:A:50:PRO:HD2	2.34	0.47
1:A:114:PHE:CZ	1:A:116:GLN:HG3	2.49	0.47
1:A:144:LEU:HD13	1:A:144:LEU:N	2.29	0.47
1:A:155:ARG:NH1	1:A:174:ASP:OD1	2.48	0.47
1:A:78:ILE:HG22	1:A:79:THR:N	2.29	0.47
1:A:22:HIS:O	1:A:23:ASN:C	2.53	0.47
1:A:24:LEU:HD12	1:A:70:ASN:O	2.15	0.47
1:A:79:THR:O	1:A:80:MET:C	2.52	0.47
1:A:177:GLU:HA	1:A:195:LYS:HA	1.97	0.47
1:A:44:GLU:O	1:A:58:GLY:HA3	2.15	0.46
1:A:123:LYS:NZ	1:A:201:ASP:CG	2.68	0.46
1:A:151:GLN:O	1:A:152:LEU:HB2	2.14	0.46
1:A:17:VAL:HG23	1:A:78:ILE:HD11	1.98	0.46
1:A:37:ASN:OD1	1:A:37:ASN:O	2.32	0.46
1:A:45:ILE:HG23	1:A:60:ALA:HB1	1.96	0.46
1:A:110:VAL:CG1	1:A:111:THR:N	2.76	0.46
1:A:6:ALA:O	1:A:9:PRO:HD3	2.16	0.46
1:A:6:ALA:O	1:A:9:PRO:CD	2.64	0.46
1:A:143:TRP:C	1:A:144:LEU:HD13	2.36	0.46
1:A:64:ARG:C	1:A:65:GLU:HG3	2.36	0.45
1:A:28:LEU:HB3	1:A:91:THR:O	2.17	0.45
1:A:4:ILE:HD13	1:A:102:VAL:HB	1.98	0.45
1:A:11:VAL:N	1:A:105:HIS:O	2.49	0.45
1:A:114:PHE:HA	1:A:192:ASN:ND2	2.27	0.45
1:A:68:TYR:CD1	4:A:370:NAG:H61	2.51	0.45
1:A:134:SER:CB	1:A:182:ILE:HD11	2.46	0.45
1:A:33:TRP:CD1	1:A:73:LEU:HB2	2.52	0.45
1:A:159:SER:O	1:A:160:GLN:C	2.55	0.45
1:A:45:ILE:CA	1:A:60:ALA:CB	2.85	0.45
1:A:151:GLN:O	1:A:151:GLN:HG2	2.17	0.45
1:A:85:VAL:CG2	1:A:86:TYR:N	2.79	0.44
1:A:68:TYR:CE1	4:A:370:NAG:H61	2.51	0.44
1:A:11:VAL:HG21	1:A:17:VAL:CG2	2.47	0.44
1:A:44:GLU:HG2	1:A:58:GLY:HA3	1.98	0.44
1:A:111:THR:OG1	1:A:136:ASP:OD1	2.22	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:145:PHE:CD1	1:A:145:PHE:C	2.90	0.44
1:A:68:TYR:CE1	4:A:370:NAG:C6	3.01	0.44
1:A:25:PRO:O	1:A:26:LEU:O	2.35	0.44
1:A:140:ASN:ND2	1:A:183:SER:HB2	2.32	0.44
1:A:155:ARG:HH12	1:A:171:LYS:HG2	1.83	0.44
1:A:113:PRO:O	1:A:114:PHE:HB3	2.17	0.44
1:A:9:PRO:O	1:A:10:GLN:CB	2.61	0.43
1:A:34:TYR:CE2	1:A:44:GLU:HA	2.53	0.43
1:A:81:LYS:H	1:A:81:LYS:HG2	1.48	0.43
1:A:115:LEU:HD12	1:A:191:SER:HB2	2.00	0.43
1:A:118:THR:O	1:A:118:THR:HG22	2.18	0.43
1:A:68:TYR:HE1	4:A:370:NAG:HO6	1.65	0.43
1:A:45:ILE:HG12	1:A:60:ALA:CB	2.49	0.43
1:A:123:LYS:NZ	1:A:201:ASP:OD2	2.52	0.43
1:A:64:ARG:CB	1:A:76:GLN:HB2	2.48	0.43
1:A:193:SER:O	1:A:194:ILE:C	2.58	0.43
1:A:110:VAL:CG1	1:A:111:THR:H	2.30	0.43
1:A:80:MET:HA	1:A:106:VAL:HG11	2.01	0.42
1:A:51:ASN:ND2	1:A:51:ASN:H	2.13	0.42
1:A:150:LEU:O	1:A:152:LEU:HD12	2.19	0.42
1:A:172:ARG:O	1:A:175:ALA:N	2.47	0.42
1:A:16:ASN:HD21	1:A:76:GLN:HA	1.80	0.42
1:A:7:VAL:HA	1:A:8:PRO:HA	1.62	0.42
1:A:19:LEU:HD22	1:A:19:LEU:N	2.34	0.42
1:A:123:LYS:HZ3	1:A:201:ASP:CG	2.21	0.42
1:A:134:SER:HB2	1:A:182:ILE:HD11	2.00	0.42
1:A:7:VAL:O	1:A:7:VAL:HG12	2.19	0.42
1:A:122:VAL:CG1	1:A:170:ILE:CD1	2.98	0.42
1:A:89:ASP:OD1	1:A:97:ARG:O	2.38	0.42
1:A:79:THR:O	1:A:81:LYS:N	2.52	0.42
1:A:88:LEU:HG	1:A:89:ASP:N	2.35	0.41
1:A:128:VAL:HG12	1:A:129:THR:N	2.35	0.41
1:A:93:GLU:OE2	1:A:93:GLU:HA	2.17	0.41
1:A:69:SER:C	1:A:71:GLY:N	2.72	0.41
1:A:40:ALA:C	1:A:42:ASP:H	2.22	0.41
1:A:49:VAL:CG2	1:A:56:PHE:CE1	3.04	0.41
1:A:3:THR:CB	1:A:22:HIS:HD2	2.23	0.41
1:A:151:GLN:O	1:A:152:LEU:O	2.38	0.41
1:A:11:VAL:HG12	1:A:12:ALA:H	1.85	0.41
1:A:58:GLY:C	1:A:60:ALA:N	2.73	0.41
1:A:74:LEU:HD21	1:A:76:GLN:HG2	2.02	0.41
1:A:161:ASN:HA	1:A:161:ASN:HD22	1.72	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:101:THR:O	1:A:102:VAL:HG23	2.21	0.41
1:A:11:VAL:HG12	1:A:12:ALA:N	2.36	0.41
1:A:122:VAL:CG1	1:A:170:ILE:HD12	2.51	0.41
1:A:18:LEU:HD12	1:A:73:LEU:C	2.41	0.41
1:A:78:ILE:CD1	1:A:78:ILE:N	2.81	0.41
1:A:29:GLY:N	1:A:91:THR:O	2.43	0.41
1:A:143:TRP:CZ3	1:A:180:CYS:HB3	2.56	0.41
1:A:199:ILE:HG22	1:A:200:PHE:N	2.35	0.41
1:A:155:ARG:NH2	1:A:174:ASP:OD2	2.54	0.41
1:A:52:SER:O	1:A:53:ASN:C	2.60	0.40
1:A:89:ASP:C	1:A:90:MET:HG3	2.41	0.40
1:A:26:LEU:HG	1:A:26:LEU:H	1.58	0.40
1:A:24:LEU:CD2	1:A:24:LEU:C	2.90	0.40
1:A:88:LEU:N	1:A:100:ALA:CB	2.62	0.40
1:A:110:VAL:HG23	1:A:187:SER:O	2.20	0.40
1:A:145:PHE:HD1	1:A:145:PHE:C	2.24	0.40
1:A:186:VAL:HG23	1:A:186:VAL:H	1.67	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	201/216 (93%)	142 (71%)	37 (18%)	22 (11%)	<b>1</b> <b>6</b>

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	28	LEU
1	A	51	ASN
1	A	61	TYR
1	A	94	ASN
1	A	114	PHE

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Mol	Chain	Res	Type
1	A	186	VAL
1	A	192	ASN
1	A	23	ASN
1	A	27	ALA
1	A	50	PRO
1	A	77	MET
1	A	99	GLN
1	A	102	VAL
1	A	53	ASN
1	A	113	PRO
1	A	152	LEU
1	A	59	GLN
1	A	119	ASN
1	A	80	MET
1	A	172	ARG
1	A	13	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	184/196 (94%)	113 (61%)	71 (39%)	<b>0</b> <b>0</b>

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	3	THR
1	A	5	GLU
1	A	7	VAL
1	A	14	ASP
1	A	16	ASN
1	A	17	VAL
1	A	24	LEU
1	A	31	PHE
1	A	38	THR
1	A	39	THR
1	A	41	ILE

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Mol	Chain	Res	Type
1	A	45	ILE
1	A	47	ARG
1	A	49	VAL
1	A	51	ASN
1	A	54	MET
1	A	56	PHE
1	A	57	THR
1	A	61	TYR
1	A	64	ARG
1	A	67	ILE
1	A	69	SER
1	A	73	LEU
1	A	74	LEU
1	A	75	PHE
1	A	77	MET
1	A	80	MET
1	A	81	LYS
1	A	85	VAL
1	A	88	LEU
1	A	90	MET
1	A	92	ASP
1	A	93	GLU
1	A	94	ASN
1	A	95	TYR
1	A	98	THR
1	A	99	GLN
1	A	106	VAL
1	A	114	PHE
1	A	118	THR
1	A	119	ASN
1	A	120	THR
1	A	127	SER
1	A	130	LEU
1	A	133	LEU
1	A	142	GLN
1	A	144	LEU
1	A	145	PHE
1	A	147	SER
1	A	150	LEU
1	A	152	LEU
1	A	153	THR
1	A	155	ARG

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Mol	Chain	Res	Type
1	A	163	SER
1	A	165	LEU
1	A	168	ASP
1	A	170	ILE
1	A	171	LYS
1	A	178	TYR
1	A	183	SER
1	A	187	SER
1	A	188	VAL
1	A	192	ASN
1	A	193	SER
1	A	194	ILE
1	A	195	LYS
1	A	196	LEU
1	A	198	ILE
1	A	200	PHE
1	A	203	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	51	ASN
1	A	59	GLN
1	A	135	ASN
1	A	140	ASN
1	A	161	ASN
1	A	179	GLN
1	A	192	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 ⓘ

3 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	A	370	1,4	12,14,15	0.63	0	15,19,21	1.32	3 (20%)
4	NAG	A	371	4	12,14,15	0.49	0	15,19,21	1.57	5 (33%)
4	BMA	A	372	4	10,11,12	0.78	0	11,15,17	1.38	1 (9%)

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	370	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	371	4	-	0/6/23/26	0/1/1/1
4	BMA	A	372	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	372	BMA	O5-C5-C6	-3.93	102.86	106.98
4	A	370	NAG	C3-C4-C5	3.47	116.39	110.20
4	A	371	NAG	C4-C3-C2	-3.43	102.93	111.32
4	A	371	NAG	O5-C5-C6	-2.64	104.21	106.98
4	A	371	NAG	O5-C5-C4	2.36	113.65	110.65
4	A	371	NAG	C3-C2-N2	2.18	115.08	111.76
4	A	370	NAG	C2-N2-C7	-2.13	119.51	123.09
4	A	370	NAG	O5-C5-C4	2.05	113.25	110.65
4	A	371	NAG	C3-C4-C5	2.02	113.81	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

3 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	$\# Z  > 2$
2	NDG	A	337	1	12,14,15	0.48	0	15,19,21	0.67	0
3	NAG	A	355	1	12,14,15	0.52	0	15,19,21	1.01	1 (6%)
3	NAG	A	419	1	12,14,15	0.50	0	15,19,21	0.62	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
2	NDG	A	337	1	-	1/6/23/26	0/1/1/1
3	NAG	A	355	1	-	0/6/23/26	0/1/1/1
3	NAG	A	419	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	355	NAG	C3-C2-N2	-2.11	108.54	111.76

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	337	NDG	C3-C2-N2-C7

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, 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(Å <sup>2</sup> )	Q<0.9
1	A	203/216 (93%)	-0.12	0 100 100	16, 58, 97, 100	0

There are no RSRZ outliers to report.

### 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	371	14/15	0.23	0.33	63,83,92,93	0
4	NAG	A	370	14/15	0.16	-0.92	14,38,50,60	0
4	BMA	A	372	11/12	0.17	-	97,100,100,100	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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	419	14/15	0.35	1.92	97,100,100,100	0
3	NAG	A	355	14/15	0.28	1.84	90,99,100,100	0
2	NDG	A	337	14/15	0.18	-0.33	94,100,100,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.