



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:59 PM GMT

PDB ID : 5ESZ
Title : Crystal Structure of Broadly Neutralizing Antibody CH04, Isolated from Donor CH0219, in Complex with Scaffolded Trimeric HIV-1 Env V1V2 Domain from the Clade AE Strain A244
Authors : Gorman, J.; Yang, M.; Kwong, P.D.
Deposited on : 2015-11-17
Resolution : 4.19 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20026982

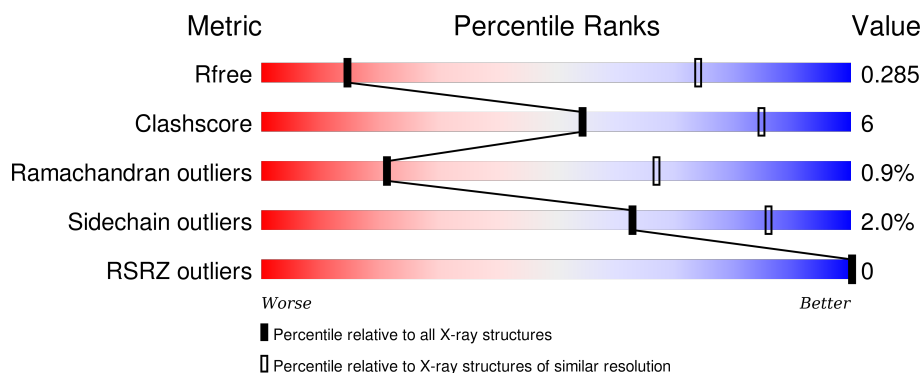
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.19 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.



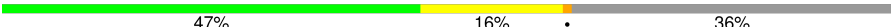
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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. 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	244	<div> <div>77%</div> <div>10%</div> <div>13%</div> </div>
1	H	244	<div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
2	B	215	<div> <div>82%</div> <div>15%</div> <div>••</div> </div>
2	L	215	<div> <div>86%</div> <div>13%</div> <div>•</div> </div>
3	C	222	<div> <div>55%</div> <div>17%</div> <div>•</div> <div>27%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	222	

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	G	402	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9244 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 CH04 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	229	Total	C	N	O	S	0	0	0
			1735	1097	296	337	5			
1	A	212	Total	C	N	O	S	0	0	0
			1620	1026	276	313	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	219	GLY	-	expression tag	UNP A0A087WYE1
H	220	LEU	-	expression tag	UNP A0A087WYE1
H	221	GLU	-	expression tag	UNP A0A087WYE1
H	222	VAL	-	expression tag	UNP A0A087WYE1
H	223	LEU	-	expression tag	UNP A0A087WYE1
H	224	PHE	-	expression tag	UNP A0A087WYE1
A	219	GLY	-	expression tag	UNP A0A087WYE1
A	220	LEU	-	expression tag	UNP A0A087WYE1
A	221	GLU	-	expression tag	UNP A0A087WYE1
A	222	VAL	-	expression tag	UNP A0A087WYE1
A	223	LEU	-	expression tag	UNP A0A087WYE1
A	224	PHE	-	expression tag	UNP A0A087WYE1

- Molecule 2 is a protein called CH04 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1660	1039	288	329	4			
2	B	211	Total	C	N	O	S	0	0	0
			1636	1023	284	325	4			

- Molecule 3 is a protein called 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	163	Total 1199	C 749	N 217	O 225	S 8	0	0	0
3	G	142	Total 1072	C 665	N 197	O 203	S 7	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

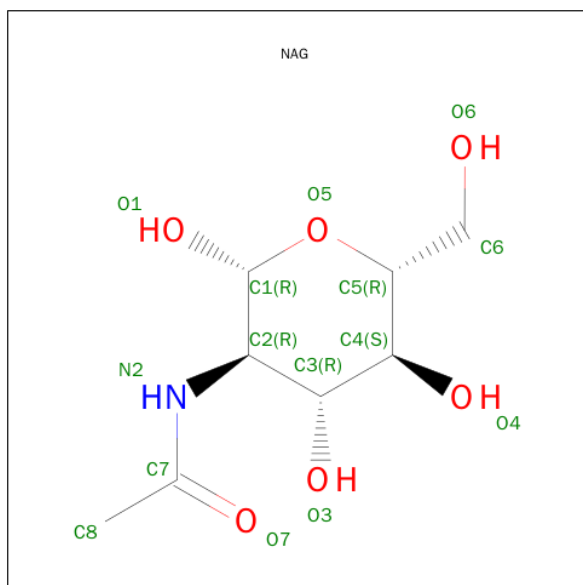
Chain	Residue	Modelled	Actual	Comment	Reference
C	111	SER	-	expression tag	UNP P44815
C	112	LEU	MET	conflict	UNP P44815
C	198	GLY	-	linker	UNP Q4QX31
C	199	GLY	-	linker	UNP Q4QX31
C	200	SER	-	linker	UNP Q4QX31
C	201	GLY	-	linker	UNP Q4QX31
C	?	-	ASP	deletion	UNP P44815
C	?	-	THR	deletion	UNP P44815
C	?	-	ASP	deletion	UNP P44815
C	?	-	MET	deletion	UNP P44815
C	?	-	GLN	deletion	UNP P44815
C	?	-	TYR	deletion	UNP P44815
C	317	GLY	-	expression tag	UNP P44815
C	318	LEU	-	expression tag	UNP P44815
C	319	GLU	-	expression tag	UNP P44815
C	320	VAL	-	expression tag	UNP P44815
C	321	LEU	-	expression tag	UNP P44815
C	322	PHE	-	expression tag	UNP P44815
C	323	GLN	-	expression tag	UNP P44815
G	111	SER	-	expression tag	UNP P44815
G	112	LEU	MET	conflict	UNP P44815
G	198	GLY	-	linker	UNP Q4QX31
G	199	GLY	-	linker	UNP Q4QX31
G	200	SER	-	linker	UNP Q4QX31
G	201	GLY	-	linker	UNP Q4QX31
G	?	-	ASP	deletion	UNP P44815
G	?	-	THR	deletion	UNP P44815
G	?	-	ASP	deletion	UNP P44815
G	?	-	MET	deletion	UNP P44815
G	?	-	GLN	deletion	UNP P44815
G	?	-	TYR	deletion	UNP P44815
G	317	GLY	-	expression tag	UNP P44815
G	318	LEU	-	expression tag	UNP P44815
G	319	GLU	-	expression tag	UNP P44815
G	320	VAL	-	expression tag	UNP P44815

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	321	LEU	-	expression tag	UNP P44815
G	322	PHE	-	expression tag	UNP P44815
G	323	GLN	-	expression tag	UNP P44815

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



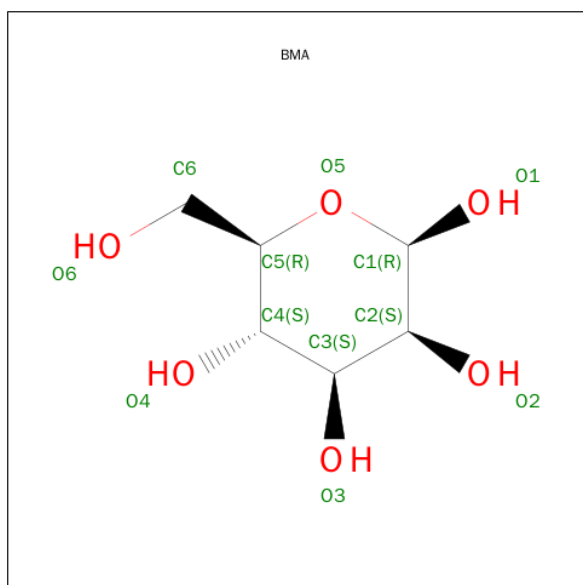
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1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

Continued on next page...

Continued from previous page...

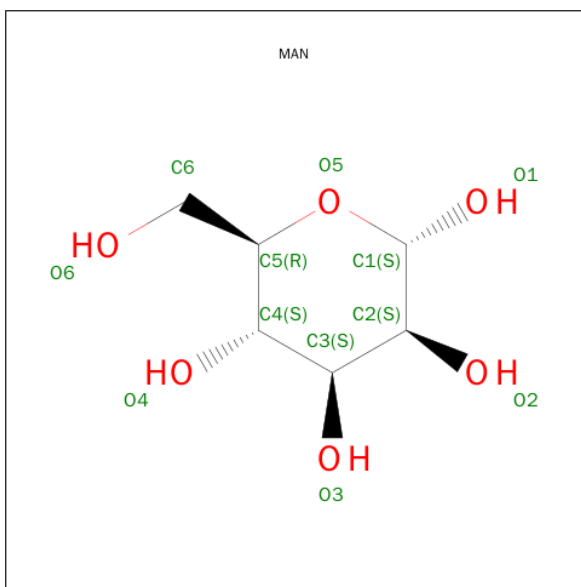
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

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

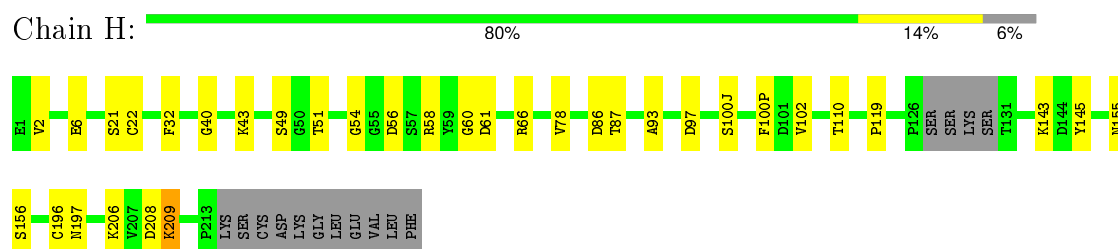


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			11	6	5		
6	L	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6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

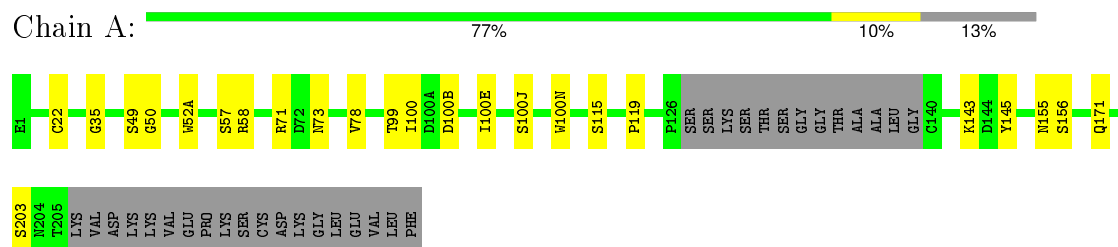
3 Residue-property plots

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.

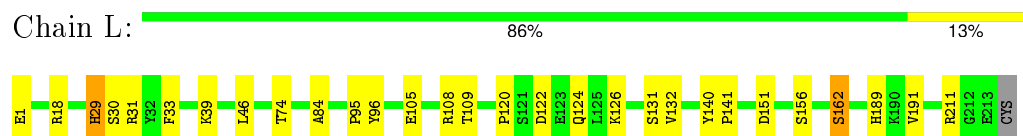
- Molecule 1: CH04 Heavy Chain



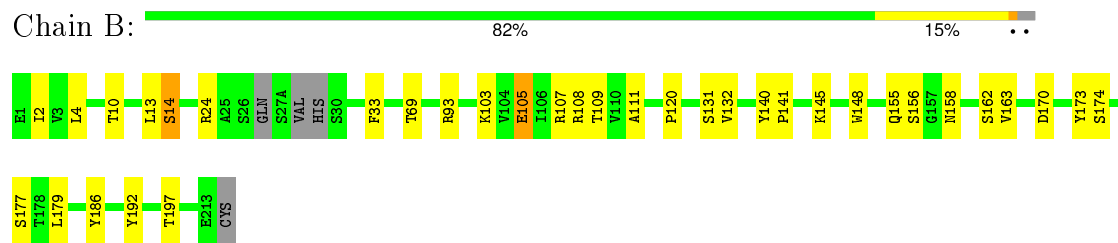
- Molecule 1: CH04 Heavy Chain



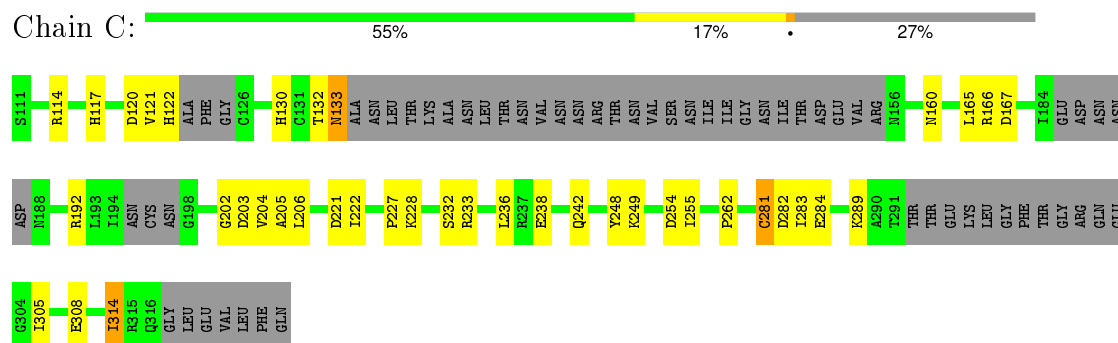
- Molecule 2: CH04 Light Chain



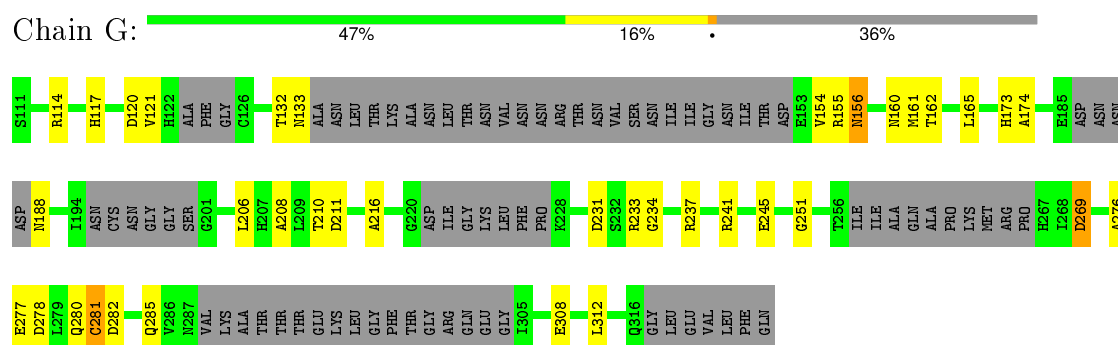
- Molecule 2: CH04 Light Chain



- Molecule 3: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160



- Molecule 3: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase,Envelope glycoprotein gp160



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	116.72Å 116.72Å 249.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.77 – 4.19 47.77 – 4.19	Depositor EDS
% Data completeness (in resolution range)	92.3 (47.77-4.19) 92.3 (47.77-4.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 4.14Å)	Xtriage
Refinement program	PHENIX (dev_2243: ???)	Depositor
R, R_{free}	0.252 , 0.282 0.262 , 0.285	Depositor DCC
R_{free} test set	667 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , -62.9	EDS
Estimated twinning fraction	0.299 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 13061 reflections	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	9244	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.28	0/1664	0.50	0/2264
1	H	0.28	0/1780	0.51	0/2420
2	B	0.27	0/1672	0.52	0/2268
2	L	0.27	0/1699	0.50	0/2308
3	C	0.29	0/1208	0.50	0/1628
3	G	0.29	0/1076	0.47	0/1443
All	All	0.28	0/9099	0.50	0/12331

There are no bond length outliers.

There are no bond angle outliers.

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	1620	0	1542	18	0
1	H	1735	0	1665	20	0
2	B	1636	0	1575	19	0
2	L	1660	0	1601	16	0
3	C	1199	0	1179	23	1
3	G	1072	0	1050	22	0
4	A	28	0	24	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	56	0	49	4	0
4	G	56	0	49	7	0
4	L	28	0	24	0	0
5	A	11	0	9	1	0
5	C	11	0	8	1	0
5	G	11	0	8	0	0
5	L	11	0	8	0	0
6	A	11	0	10	2	0
6	C	33	0	29	0	0
6	G	44	0	38	0	0
6	L	22	0	20	1	0
All	All	9244	0	8888	116	1

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 6.

All (116) 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)
4:G:401:NAG:O3	4:G:401:NAG:O7	1.99	0.79
3:G:117:HIS:NE2	3:G:308:GLU:OE1	2.18	0.77
3:C:281:CYS:SG	3:C:282:ASP:N	2.56	0.76
3:C:282:ASP:OD2	3:C:283:ILE:N	2.22	0.72
1:A:143:LYS:NZ	1:A:171:GLN:OE1	2.23	0.71
3:C:203:ASP:OD2	3:C:204:VAL:N	2.24	0.70
1:A:100(N):TRP:HE1	6:A:304:MAN:HO6	1.40	0.67
1:A:71:ARG:NE	1:A:73:ASN:OD1	2.28	0.67
3:G:233:ARG:NH2	3:G:277:GLU:OE2	2.27	0.67
3:G:231:ASP:OD2	3:G:234:GLY:N	2.26	0.66
3:C:160:ASN:OD1	4:C:403:NAG:H2	1.96	0.66
1:A:100(N):TRP:NE1	6:A:304:MAN:O6	2.30	0.64
2:L:29:HIS:O	2:L:31:ARG:N	2.32	0.63
3:G:251:GLY:O	3:G:285:GLN:NE2	2.32	0.62
3:C:238:GLU:OE2	3:C:242:GLN:NE2	2.25	0.62
3:G:156:ASN:OD1	4:G:401:NAG:N2	2.33	0.61
1:A:49:SER:OG	1:A:50:GLY:N	2.34	0.61
3:C:254:ASP:OD2	3:C:289:LYS:NZ	2.34	0.60
1:H:209:LYS:NZ	1:A:203:SER:O	2.34	0.60
3:C:165:LEU:O	3:C:167:ASP:N	2.35	0.60
2:L:96:TYR:HH	6:L:304:MAN:HO3	1.51	0.58
3:C:132:THR:OG1	3:C:133:ASN:N	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:114:ARG:NH2	3:G:216:ALA:O	2.36	0.58
4:G:401:NAG:HO3	4:G:401:NAG:C7	2.13	0.57
3:C:203:ASP:OD2	3:C:205:ALA:N	2.34	0.57
2:L:189:HIS:O	2:L:211:ARG:NE	2.37	0.57
2:L:124:GLN:NE2	2:L:131:SER:OG	2.37	0.57
3:G:132:THR:OG1	3:G:133:ASN:N	2.34	0.55
2:B:108:ARG:NE	2:B:109:THR:O	2.35	0.55
2:L:151:ASP:HA	2:L:191:VAL:HB	1.89	0.55
4:G:404:NAG:O7	4:G:404:NAG:O3	2.21	0.54
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.90	0.54
3:C:117:HIS:NE2	3:C:308:GLU:OE1	2.30	0.53
1:H:100(J):SER:OG	4:G:403:NAG:O7	2.24	0.52
3:G:237:ARG:NE	3:G:278:ASP:OD1	2.42	0.52
2:L:126:LYS:HB3	1:A:115:SER:HB3	1.92	0.52
3:C:282:ASP:OD2	3:C:283:ILE:HG22	2.11	0.50
2:B:131:SER:HA	2:B:179:LEU:O	2.12	0.50
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.94	0.50
3:G:206:LEU:O	3:G:210:THR:OG1	2.25	0.50
2:L:108:ARG:NE	2:L:109:THR:O	2.33	0.50
2:B:140:TYR:CG	2:B:141:PRO:HA	2.48	0.49
4:A:302:NAG:O3	5:A:303:BMA:O5	2.13	0.49
1:H:143:LYS:HE2	2:L:131:SER:OG	2.12	0.49
4:C:402:NAG:O7	4:C:402:NAG:O3	2.25	0.49
1:H:93:ALA:HB1	1:H:100(P):PHE:HB3	1.95	0.49
3:G:281:CYS:SG	3:G:282:ASP:N	2.85	0.49
3:G:154:VAL:HG22	3:G:155:ARG:H	1.78	0.48
3:G:269:ASP:N	3:G:269:ASP:OD2	2.45	0.48
2:B:108:ARG:NH2	2:B:109:THR:O	2.46	0.48
3:C:167:ASP:HA	1:A:100(E):ILE:HG23	1.96	0.47
2:B:145:LYS:HB3	2:B:197:THR:HB	1.96	0.47
1:H:61:ASP:HB2	2:L:1:GLU:OE2	2.14	0.47
1:H:155:ASN:O	1:H:156:SER:HB2	2.14	0.47
3:C:167:ASP:CA	1:A:100(E):ILE:HG23	2.45	0.46
3:C:120:ASP:OD2	3:C:121:VAL:N	2.49	0.46
1:H:32:PHE:CE1	1:H:97:ASP:HB3	2.50	0.46
1:H:51:THR:OG1	1:H:54:GLY:HA2	2.16	0.46
1:H:56:ASP:OD1	1:H:58:ARG:NH1	2.49	0.46
1:H:196:CYS:O	1:H:208:ASP:HA	2.16	0.46
2:B:148:TRP:HE1	2:B:177:SER:HG	1.62	0.46
2:B:13:LEU:HA	2:B:107:ARG:HH11	1.81	0.46
3:C:132:THR:O	3:C:133:ASN:ND2	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:165:LEU:H	3:G:165:LEU:HD23	1.80	0.45
3:C:130:HIS:NE2	4:C:403:NAG:O6	2.28	0.45
2:B:4:LEU:HA	2:B:24:ARG:O	2.16	0.45
2:B:186:TYR:O	2:B:192:TYR:OH	2.33	0.45
2:B:105:GLU:OE2	2:B:173:TYR:OH	2.26	0.45
3:G:241:ARG:NH1	3:G:245:GLU:OE1	2.50	0.45
1:H:60:GLY:HA2	2:L:95:PRO:HB3	1.98	0.45
2:L:18:ARG:HD2	2:L:74:THR:HG23	1.98	0.44
3:G:156:ASN:OD1	4:G:401:NAG:C2	2.64	0.44
3:G:208:ALA:O	3:G:211:ASP:N	2.51	0.44
1:H:2:VAL:HG11	1:H:102:VAL:HG21	1.99	0.44
1:A:155:ASN:O	1:A:156:SER:HB2	2.18	0.44
2:B:155:GLN:OE1	2:B:158:ASN:ND2	2.49	0.44
2:L:120:PRO:HD3	2:L:132:VAL:HG22	2.00	0.43
1:H:66:ARG:NH1	1:H:86:ASP:OD1	2.40	0.43
2:B:2:ILE:HD11	2:B:93:ARG:HB3	1.99	0.43
3:C:255:ILE:O	3:C:289:LYS:HG2	2.19	0.43
3:G:120:ASP:OD1	3:G:121:VAL:N	2.52	0.42
1:A:100:ILE:HA	1:A:100(E):ILE:O	2.18	0.42
1:A:22:CYS:HB3	1:A:78:VAL:HG13	2.00	0.42
2:B:10:THR:HA	2:B:103:LYS:O	2.19	0.42
3:G:276:ALA:O	3:G:280:GLN:N	2.52	0.42
3:G:251:GLY:N	3:G:312:LEU:O	2.46	0.42
2:L:122:ASP:O	2:L:126:LYS:HG3	2.20	0.42
1:H:100(P):PHE:O	2:L:46:LEU:HB2	2.20	0.42
3:C:249:LYS:N	3:C:314:ILE:O	2.50	0.42
1:H:87:THR:HG23	1:H:110:THR:HA	2.02	0.42
1:H:197:ASN:HB3	1:H:206:LYS:NZ	2.35	0.42
1:H:40:GLY:HA3	1:H:43:LYS:HE2	2.01	0.42
3:C:114:ARG:HG3	3:C:248:TYR:CZ	2.55	0.41
1:A:52(A):TRP:O	1:A:71:ARG:CZ	2.68	0.41
2:B:14:SER:OG	2:B:107:ARG:O	2.39	0.41
2:L:39:LYS:HG2	2:L:84:ALA:HB2	2.02	0.41
1:A:35:GLY:HA2	1:A:50:GLY:HA2	2.02	0.41
2:B:108:ARG:NH2	2:B:111:ALA:HB2	2.36	0.41
2:B:163:VAL:HG23	2:B:174:SER:O	2.21	0.41
3:C:206:LEU:HB2	3:C:232:SER:HB3	2.03	0.41
4:C:404:NAG:H3	5:C:405:BMA:H2	2.03	0.41
1:A:99:THR:HB	1:A:100(J):SER:O	2.20	0.41
2:B:120:PRO:HD3	2:B:132:VAL:HG22	2.02	0.41
2:L:140:TYR:CG	2:L:141:PRO:HA	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:C	1:A:58:ARG:HG3	2.41	0.41
2:B:24:ARG:HA	2:B:69:THR:O	2.21	0.41
1:H:6:GLU:HA	1:H:21:SER:O	2.21	0.41
2:B:170:ASP:C	2:B:170:ASP:OD1	2.59	0.41
3:G:173:HIS:CE1	4:G:401:NAG:O6	2.74	0.41
3:C:122:HIS:O	3:C:305:ILE:HG12	2.22	0.40
1:H:22:CYS:HB3	1:H:78:VAL:HG13	2.02	0.40
1:A:100(B):ASP:O	4:A:302:NAG:H3	2.21	0.40
3:C:233:ARG:O	3:C:236:LEU:N	2.53	0.40
3:G:165:LEU:O	3:G:165:LEU:HG	2.22	0.40
3:C:227:PRO:HA	3:C:228:LYS:HA	1.86	0.40
3:G:161:MET:SD	3:G:162:THR:N	2.91	0.40

All (1) 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)
3:C:114:ARG:NH2	3:C:284:GLU:O[3_475]	2.17	0.03

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	208/244 (85%)	201 (97%)	7 (3%)	0	100	100
1	H	225/244 (92%)	220 (98%)	5 (2%)	0	100	100
2	B	206/215 (96%)	197 (96%)	8 (4%)	1 (0%)	34	77
2	L	212/215 (99%)	202 (95%)	8 (4%)	2 (1%)	21	67
3	C	151/222 (68%)	117 (78%)	29 (19%)	5 (3%)	5	43
3	G	126/222 (57%)	103 (82%)	21 (17%)	2 (2%)	12	57
All	All	1128/1362 (83%)	1040 (92%)	78 (7%)	10 (1%)	21	67

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	30	SER
3	C	166	ARG
3	C	221	ASP
3	C	222	ILE
3	C	262	PRO
3	G	174	ALA
2	B	156	SER
2	L	162	SER
3	G	281	CYS
3	C	202	GLY

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	178/204 (87%)	178 (100%)	0	100	100
1	H	190/204 (93%)	188 (99%)	2 (1%)	80	91
2	B	181/186 (97%)	177 (98%)	4 (2%)	60	84
2	L	184/186 (99%)	179 (97%)	5 (3%)	52	80
3	C	121/183 (66%)	117 (97%)	4 (3%)	45	78
3	G	111/183 (61%)	107 (96%)	4 (4%)	42	76
All	All	965/1146 (84%)	946 (98%)	19 (2%)	63	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	49	SER
1	H	209	LYS
2	L	29	HIS
2	L	33	PHE
2	L	105	GLU
2	L	156	SER
2	L	162	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	133	ASN
3	C	192	ARG
3	C	281	CYS
3	C	314	ILE
3	G	156	ASN
3	G	160	ASN
3	G	188	ASN
3	G	269	ASP
2	B	14	SER
2	B	33	PHE
2	B	105	GLU
2	B	162	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	70	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

26 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	301	4	14,14,15	0.32	0	15,19,21	0.26	0
4	NAG	A	302	5,4	14,14,15	0.32	0	15,19,21	0.49	0
5	BMA	A	303	4,6	11,11,12	1.06	0	15,15,17	1.15	2 (13%)
6	MAN	A	304	5	11,11,12	0.99	1 (9%)	15,15,17	1.29	1 (6%)
4	NAG	C	401	3,4	14,14,15	0.54	0	15,19,21	0.85	0
4	NAG	C	402	4	14,14,15	0.32	0	15,19,21	0.26	0
4	NAG	C	403	3,4	14,14,15	0.87	1 (7%)	15,19,21	0.58	0
4	NAG	C	404	5,4	14,14,15	0.21	0	15,19,21	0.44	0
5	BMA	C	405	4,6	11,11,12	0.93	0	15,15,17	1.40	1 (6%)
6	MAN	C	406	5	11,11,12	1.09	1 (9%)	15,15,17	1.44	3 (20%)
6	MAN	C	407	5,6	11,11,12	0.93	1 (9%)	15,15,17	1.39	4 (26%)
6	MAN	C	408	6	11,11,12	0.64	0	15,15,17	1.08	2 (13%)
4	NAG	G	401	3,4	14,14,15	1.03	1 (7%)	15,19,21	1.31	1 (6%)
4	NAG	G	402	4	14,14,15	0.18	0	15,19,21	0.61	1 (6%)
4	NAG	G	403	3,4	14,14,15	0.49	0	15,19,21	0.76	0
4	NAG	G	404	5,4	14,14,15	0.30	0	15,19,21	0.52	0
5	BMA	G	405	4,6	11,11,12	1.07	1 (9%)	15,15,17	1.50	3 (20%)
6	MAN	G	406	5	11,11,12	1.10	1 (9%)	15,15,17	0.98	1 (6%)
6	MAN	G	407	5,6	11,11,12	0.63	0	15,15,17	1.12	1 (6%)
6	MAN	G	408	6	11,11,12	0.63	0	15,15,17	0.99	1 (6%)
6	MAN	G	409	6	11,11,12	0.88	1 (9%)	15,15,17	1.43	3 (20%)
4	NAG	L	301	4	14,14,15	0.21	0	15,19,21	0.42	0
4	NAG	L	302	5,4	14,14,15	0.19	0	15,19,21	0.35	0
5	BMA	L	303	4,6	11,11,12	0.63	0	15,15,17	0.70	0
6	MAN	L	304	5	11,11,12	1.05	1 (9%)	15,15,17	1.75	5 (33%)
6	MAN	L	305	5	11,11,12	0.50	0	15,15,17	0.97	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
4	NAG	A	301	4	-	0/6/23/26	0/1/1/1
4	NAG	A	302	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	303	4,6	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	304	5	-	0/2/19/22	0/1/1/1
4	NAG	C	401	3,4	-	0/6/23/26	0/1/1/1
4	NAG	C	402	4	-	0/6/23/26	0/1/1/1
4	NAG	C	403	3,4	-	0/6/23/26	0/1/1/1
4	NAG	C	404	5,4	-	0/6/23/26	0/1/1/1
5	BMA	C	405	4,6	-	0/2/19/22	0/1/1/1
6	MAN	C	406	5	-	0/2/19/22	0/1/1/1
6	MAN	C	407	5,6	-	0/2/19/22	0/1/1/1
6	MAN	C	408	6	-	0/2/19/22	0/1/1/1
4	NAG	G	401	3,4	-	0/6/23/26	0/1/1/1
4	NAG	G	402	4	-	0/6/23/26	0/1/1/1
4	NAG	G	403	3,4	-	0/6/23/26	0/1/1/1
4	NAG	G	404	5,4	-	0/6/23/26	0/1/1/1
5	BMA	G	405	4,6	-	0/2/19/22	0/1/1/1
6	MAN	G	406	5	-	0/2/19/22	1/1/1/1
6	MAN	G	407	5,6	-	0/2/19/22	0/1/1/1
6	MAN	G	408	6	-	0/2/19/22	0/1/1/1
6	MAN	G	409	6	-	0/2/19/22	0/1/1/1
4	NAG	L	301	4	-	0/6/23/26	0/1/1/1
4	NAG	L	302	5,4	-	0/6/23/26	0/1/1/1
5	BMA	L	303	4,6	-	0/2/19/22	0/1/1/1
6	MAN	L	304	5	-	0/2/19/22	0/1/1/1
6	MAN	L	305	5	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	NAG	O5-C1	-2.52	1.39	1.43
6	A	304	MAN	C1-C2	2.33	1.57	1.52
6	C	406	MAN	C1-C2	2.47	1.58	1.52
6	C	407	MAN	C1-C2	2.58	1.58	1.52
6	G	409	MAN	C1-C2	2.63	1.58	1.52
6	L	304	MAN	C1-C2	2.71	1.58	1.52
5	G	405	BMA	C2-C3	2.73	1.56	1.52
6	G	406	MAN	C1-C2	3.27	1.60	1.52
4	G	401	NAG	C1-C2	3.54	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	304	MAN	O5-C5-C4	-2.63	105.78	110.13
6	C	408	MAN	O2-C2-C3	-2.61	104.93	110.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	408	MAN	O2-C2-C3	-2.39	105.36	110.19
6	G	409	MAN	O2-C2-C3	-2.27	105.61	110.19
6	C	406	MAN	O2-C2-C3	-2.23	105.70	110.19
6	C	407	MAN	O2-C2-C3	-2.21	105.73	110.19
6	L	305	MAN	O2-C2-C3	-2.14	105.86	110.19
6	L	304	MAN	O2-C2-C3	-2.14	105.87	110.19
5	G	405	BMA	O2-C2-C3	-2.13	105.90	110.19
6	C	406	MAN	O5-C5-C4	-2.05	106.74	110.13
5	A	303	BMA	O2-C2-C3	-2.03	106.09	110.19
6	G	406	MAN	O2-C2-C3	-2.03	106.09	110.19
6	C	408	MAN	C1-O5-C5	2.04	115.13	112.14
4	G	402	NAG	C1-O5-C5	2.04	115.14	112.14
6	C	407	MAN	O5-C1-C2	2.09	114.24	110.89
6	G	409	MAN	C1-C2-C3	2.32	112.36	109.55
6	C	407	MAN	C1-C2-C3	2.34	112.39	109.55
6	L	305	MAN	C1-O5-C5	2.50	115.81	112.14
6	L	304	MAN	C1-C2-C3	2.53	112.61	109.55
6	G	407	MAN	C1-O5-C5	2.58	115.93	112.14
6	C	407	MAN	C1-O5-C5	2.62	115.99	112.14
5	G	405	BMA	C2-C3-C4	2.69	115.74	111.05
5	A	303	BMA	C1-C2-C3	2.85	113.00	109.55
5	C	405	BMA	C1-O5-C5	2.88	116.38	112.14
6	L	304	MAN	C1-O5-C5	3.04	116.61	112.14
6	L	304	MAN	O5-C1-C2	3.29	116.16	110.89
6	C	406	MAN	C1-C2-C3	3.43	113.70	109.55
6	A	304	MAN	C1-O5-C5	3.63	117.47	112.14
6	G	409	MAN	C1-O5-C5	3.71	117.59	112.14
5	G	405	BMA	C1-C2-C3	3.99	114.38	109.55
4	G	401	NAG	C1-O5-C5	4.75	119.13	112.14

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	406	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	NAG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	303	BMA	1	0
6	A	304	MAN	2	0
4	C	402	NAG	1	0
4	C	403	NAG	2	0
4	C	404	NAG	1	0
5	C	405	BMA	1	0
4	G	401	NAG	5	0
4	G	403	NAG	1	0
4	G	404	NAG	1	0
6	L	304	MAN	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	212/244 (86%)	-0.37	0 100 100	68, 86, 109, 122	0
1	H	229/244 (93%)	-0.59	0 100 100	15, 57, 89, 124	0
2	B	211/215 (98%)	-0.37	0 100 100	67, 95, 122, 148	0
2	L	214/215 (99%)	-0.57	0 100 100	49, 65, 96, 120	0
3	C	163/222 (73%)	-0.41	0 100 100	7, 39, 114, 152	0
3	G	142/222 (63%)	-0.22	0 100 100	65, 93, 115, 130	0
All	All	1171/1362 (85%)	-0.44	0 100 100	7, 78, 113, 152	0

There are no RSRZ outliers to report.

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	G	402	14/15	0.84	0.30	2.50	63,66,70,70	0
4	NAG	A	302	14/15	0.80	0.34	0.81	69,72,75,75	0
4	NAG	L	302	14/15	0.90	0.27	-0.23	60,61,62,62	0
4	NAG	G	403	14/15	0.96	0.19	-0.33	60,64,74,75	0
4	NAG	G	404	14/15	0.91	0.20	-0.36	60,60,60,60	0
6	MAN	L	304	11/12	0.90	0.19	-0.57	63,63,66,68	0
6	MAN	A	304	11/12	0.92	0.17	-1.41	60,60,61,62	0
6	MAN	L	305	11/12	0.75	0.38	-	60,60,60,61	0
4	NAG	A	301	14/15	0.85	0.38	-	66,69,76,77	0
5	BMA	C	405	11/12	0.80	0.26	-	65,69,72,72	0
4	NAG	C	401	14/15	0.88	0.38	-	60,60,62,63	0
5	BMA	L	303	11/12	0.90	0.17	-	60,60,60,61	0
6	MAN	C	407	11/12	0.83	0.25	-	62,63,64,64	0
4	NAG	C	404	14/15	0.76	0.51	-	63,71,77,80	0
6	MAN	G	407	11/12	0.88	0.18	-	60,60,61,62	0
6	MAN	C	406	11/12	0.90	0.22	-	72,72,73,73	0
5	BMA	G	405	11/12	0.91	0.19	-	60,61,63,65	0
6	MAN	G	408	11/12	0.86	0.32	-	60,60,60,60	0
4	NAG	C	403	14/15	0.71	0.42	-	60,60,63,65	0
4	NAG	C	402	14/15	0.67	0.45	-	66,68,72,72	0
4	NAG	L	301	14/15	0.90	0.30	-	60,61,66,67	0
4	NAG	G	401	14/15	0.90	0.17	-	60,60,65,70	0
5	BMA	A	303	11/12	0.90	0.18	-	65,69,71,72	0
6	MAN	C	408	11/12	0.85	0.29	-	63,64,64,65	0
6	MAN	G	409	11/12	0.91	0.22	-	63,64,65,65	0
6	MAN	G	406	11/12	0.87	0.23	-	66,66,69,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.