



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:59 PM EDT

PDB ID : 7MMN  
Title : Crystal Structure of the Prefusion RSV F Glycoprotein bound by human antibody AM14  
Authors : Harshbarger, W.; Malito, E.  
Deposited on : 2021-04-29  
Resolution : 3.57 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

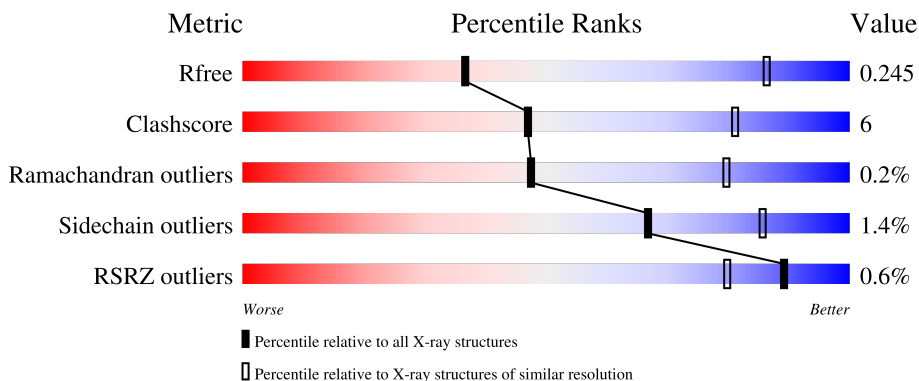
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.57 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))
$R_{free}$	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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  $\geq 3$ , 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	E	219	 86% 12% ..
1	G	219	 84% 14% .
1	L	219	 83% 15% .
2	A	72	 3% 83% 17%
2	C	72	 3% 79% 19% .

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Mol	Chain	Length	Quality of chain
2	J	72	<p>3% 85% 15%</p>
3	B	414	<p>73% 17% 10%</p>
3	I	414	<p>73% 16% 10%</p>
3	K	414	<p>3% 73% 16% 10%</p>
4	D	244	<p>78% 12% 9%</p>
4	H	244	<p>2% 76% 15% 9%</p>
4	M	244	<p>78% 13% 9%</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 20390 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 AM14 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	216	Total 1667	C 1040	N 283	O 338	S 6	0	0	0
1	E	216	Total 1667	C 1040	N 283	O 338	S 6	0	0	0
1	G	216	Total 1667	C 1040	N 283	O 338	S 6	0	0	0

- Molecule 2 is a protein called Fusion glycoprotein F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	72	Total 571	C 361	N 93	O 114	S 3	0	0	0
2	C	72	Total 571	C 361	N 93	O 114	S 3	0	0	0
2	J	72	Total 571	C 361	N 93	O 114	S 3	7	0	0

- Molecule 3 is a protein called Fusion glycoprotein F1,Fibritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	373	Total 2878	C 1820	N 476	O 562	S 20	0	0	0
3	I	373	Total 2878	C 1820	N 476	O 562	S 20	0	0	0
3	K	373	Total 2878	C 1820	N 476	O 562	S 20	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	155	CYS	SER	engineered mutation	UNP P03420
B	190	PHE	SER	engineered mutation	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
B	207	LEU	VAL	engineered mutation	UNP P03420
B	290	CYS	SER	engineered mutation	UNP P03420
B	379	VAL	ILE	variant	UNP P03420
B	447	VAL	MET	variant	UNP P03420
I	155	CYS	SER	engineered mutation	UNP P03420
I	190	PHE	SER	engineered mutation	UNP P03420
I	207	LEU	VAL	engineered mutation	UNP P03420
I	290	CYS	SER	engineered mutation	UNP P03420
I	379	VAL	ILE	variant	UNP P03420
I	447	VAL	MET	variant	UNP P03420
K	155	CYS	SER	engineered mutation	UNP P03420
K	190	PHE	SER	engineered mutation	UNP P03420
K	207	LEU	VAL	engineered mutation	UNP P03420
K	290	CYS	SER	engineered mutation	UNP P03420
K	379	VAL	ILE	variant	UNP P03420
K	447	VAL	MET	variant	UNP P03420

- Molecule 4 is a protein called AM14 Fab Heavy Chain.

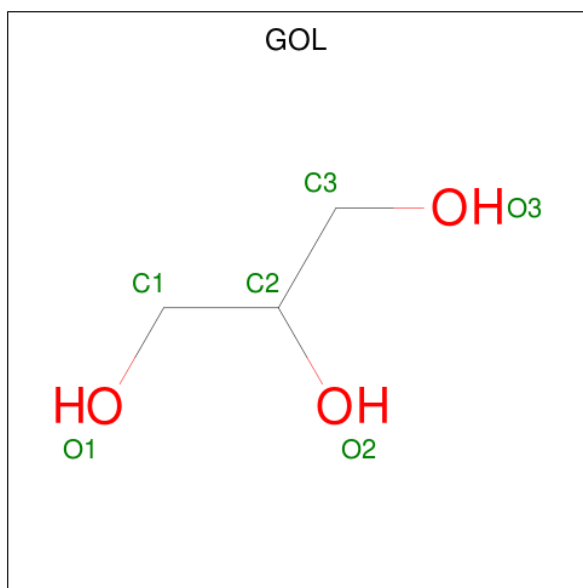
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	222	Total	C	N	O	S	0	0	0
			1674	1054	283	330	7			
4	H	222	Total	C	N	O	S	0	0	0
			1674	1054	283	330	7			
4	D	222	Total	C	N	O	S	0	0	0
			1674	1054	283	330	7			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

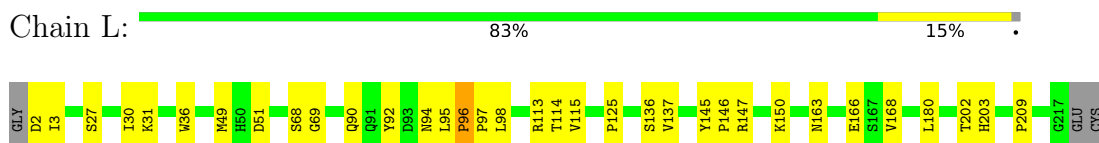


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	M	1	6	3	3	0	0

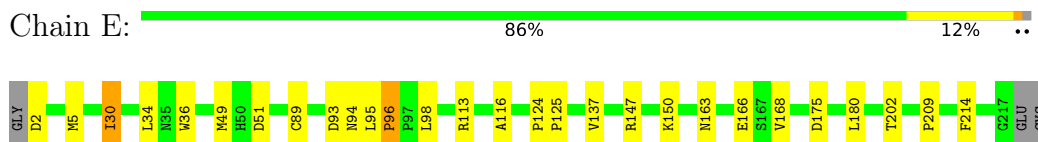
### 3 Residue-property plots [i](#)

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.

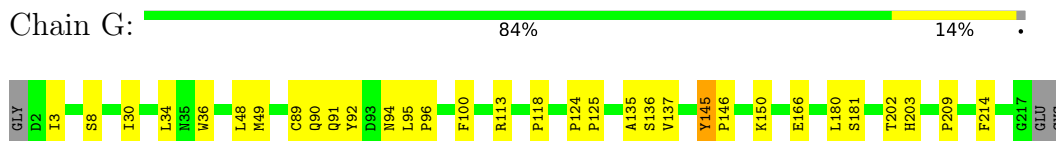
- Molecule 1: AM14 Fab Light Chain



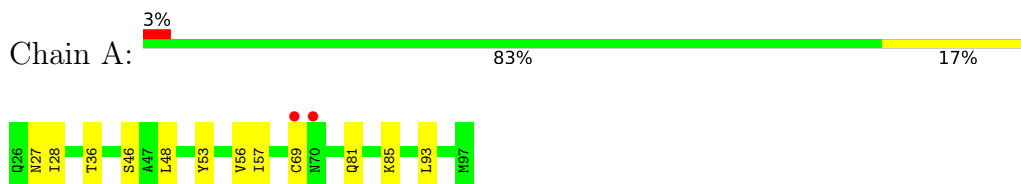
- Molecule 1: AM14 Fab Light Chain



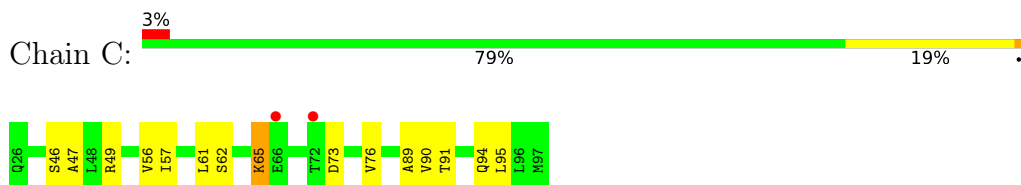
- Molecule 1: AM14 Fab Light Chain



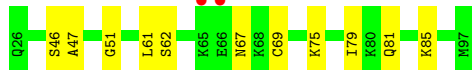
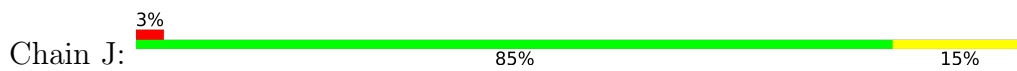
- Molecule 2: Fusion glycoprotein F2



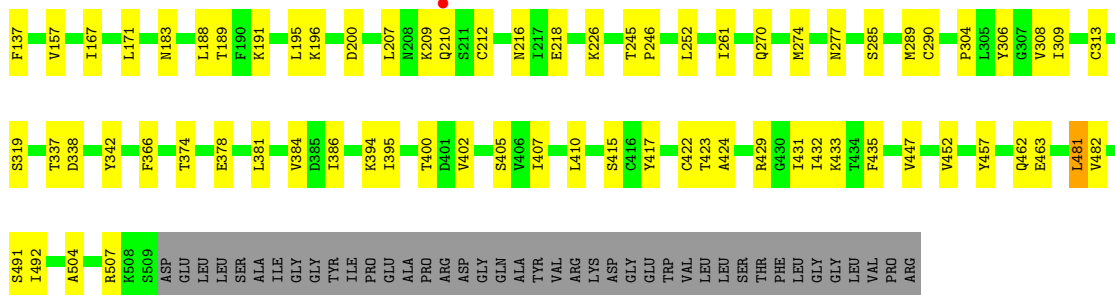
- Molecule 2: Fusion glycoprotein F2



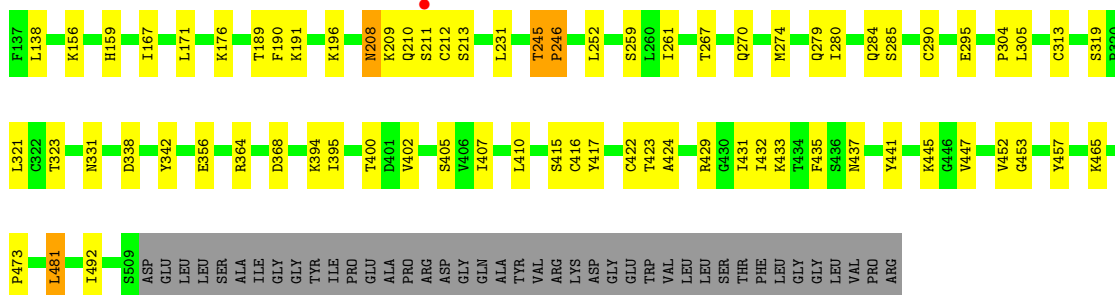
- Molecule 2: Fusion glycoprotein F2



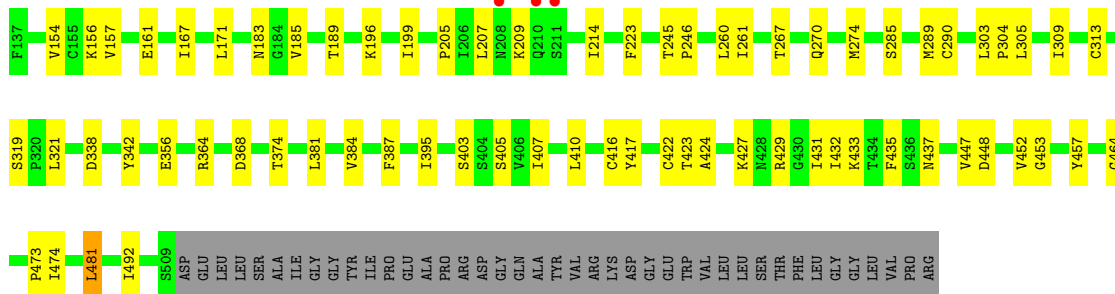
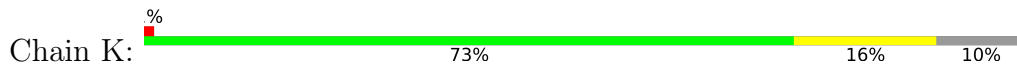
• Molecule 3: Fusion glycoprotein F1,Fibrin



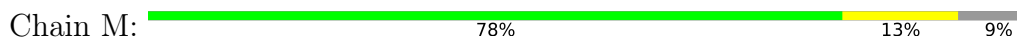
• Molecule 3: Fusion glycoprotein F1,Fibrin



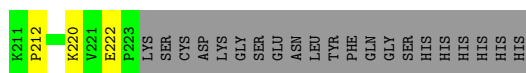
• Molecule 3: Fusion glycoprotein F1,Fibrin



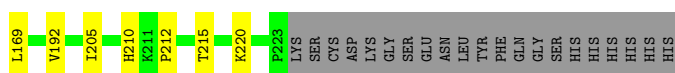
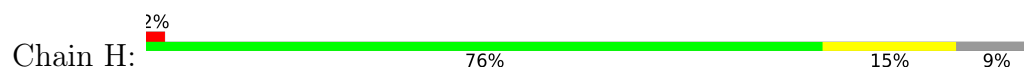
• Molecule 4: AM14 Fab Heavy Chain



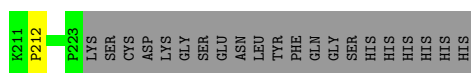
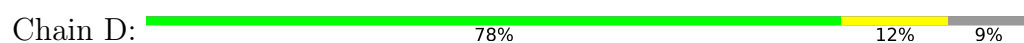




- Molecule 4: AM14 Fab Heavy Chain



- Molecule 4: AM14 Fab Heavy Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.42Å 183.00Å 135.78Å 90.00° 103.14° 90.00°	Depositor
Resolution (Å)	42.33 – 3.57 45.31 – 3.57	Depositor EDS
% Data completeness (in resolution range)	87.9 (42.33-3.57) 82.3 (45.31-3.57)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 3.57Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.202 , 0.245 0.202 , 0.245	Depositor DCC
$R_{free}$ test set	1984 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 13.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	20390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL

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	E	0.25	0/1702	0.50	0/2311
1	G	0.26	0/1702	0.49	0/2311
1	L	0.26	0/1702	0.49	0/2311
2	A	0.26	0/577	0.53	0/777
2	C	0.24	0/577	0.49	0/777
2	J	0.24	0/577	0.47	0/777
3	B	0.26	0/2922	0.46	0/3962
3	I	0.26	0/2922	0.45	0/3962
3	K	0.26	0/2922	0.45	0/3962
4	D	0.25	0/1716	0.48	0/2339
4	H	0.26	0/1716	0.48	0/2339
4	M	0.25	0/1716	0.47	0/2339
All	All	0.26	0/20751	0.47	0/28167

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	3
1	L	0	3
3	I	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	30	ILE	Peptide
1	G	145	TYR	Peptide
1	G	30	ILE	Peptide
1	G	8	SER	Peptide
3	I	245	THR	Peptide
1	L	145	TYR	Peptide
1	L	30	ILE	Peptide
1	L	96	PRO	Peptide

## 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	E	1667	0	1623	16	0
1	G	1667	0	1623	21	0
1	L	1667	0	1623	25	0
2	A	571	0	581	12	0
2	C	571	0	581	13	0
2	J	571	0	581	9	0
3	B	2878	0	2912	48	0
3	I	2878	0	2913	46	0
3	K	2878	0	2913	45	0
4	D	1674	0	1618	16	0
4	H	1674	0	1618	22	0
4	M	1674	0	1618	18	0
5	B	14	0	13	0	0
6	M	6	0	8	0	0
All	All	20390	0	20225	252	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 6.

All (252) 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)
1:L:96:PRO:HB3	1:L:98:LEU:HD13	1.27	1.08
3:K:245:THR:HG23	3:K:246:PRO:HD3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:245:THR:HG23	3:B:246:PRO:HD3	1.51	0.90
1:L:96:PRO:HB3	1:L:98:LEU:CD1	2.09	0.82
3:I:407:ILE:HD11	3:I:457:TYR:HB3	1.63	0.79
3:K:183:ASN:HD21	3:K:185:VAL:HG22	1.49	0.78
3:K:407:ILE:HD11	3:K:457:TYR:HB3	1.69	0.73
1:G:94:ASN:HB3	1:G:96:PRO:HD2	1.71	0.73
3:B:407:ILE:HD11	3:B:457:TYR:HB3	1.72	0.71
1:L:90:GLN:NE2	1:L:98:LEU:HD23	2.04	0.70
4:H:169:LEU:HD21	4:H:192:VAL:HG11	1.74	0.70
4:D:169:LEU:HD21	4:D:192:VAL:HG11	1.74	0.70
1:L:146:PRO:HD2	1:L:203:HIS:CE1	2.26	0.70
1:G:92:TYR:O	3:K:429:ARG:NH1	2.24	0.70
4:H:52:SER:O	4:H:72:ARG:NH1	2.25	0.70
3:K:285:SER:HB3	3:K:304:PRO:HD3	1.75	0.69
1:G:125:PRO:HD3	1:G:137:VAL:HG22	1.75	0.69
2:J:75:LYS:HE2	3:K:214:ILE:HG13	1.76	0.67
1:L:96:PRO:CB	1:L:98:LEU:HD13	2.16	0.67
1:G:95:LEU:HD12	1:G:95:LEU:H	1.59	0.67
3:B:137:PHE:HD2	3:B:337:THR:HG22	1.59	0.66
4:M:169:LEU:HD21	4:M:192:VAL:HG11	1.78	0.66
3:I:209:LYS:HG3	3:I:210:GLN:H	1.61	0.66
3:B:167:ILE:HG23	3:B:189:THR:HG21	1.77	0.65
3:K:321:LEU:HD11	3:K:473:PRO:HB3	1.78	0.65
1:L:115:VAL:HG13	1:L:146:PRO:HD3	1.79	0.64
4:M:52:SER:O	4:M:72:ARG:NH1	2.29	0.64
1:L:113:ARG:NH1	1:L:114:THR:O	2.31	0.63
1:G:36:TRP:HB2	1:G:49:MET:HG2	1.82	0.62
3:I:167:ILE:HG23	3:I:189:THR:HG21	1.81	0.62
2:J:79:ILE:HG21	3:K:207:LEU:HD11	1.82	0.61
3:B:277:ASN:HD22	3:B:366:PHE:HZ	1.47	0.61
3:B:424:ALA:HB3	3:B:433:LYS:HB3	1.80	0.61
2:C:62:SER:HB2	3:I:196:LYS:HA	1.82	0.61
2:C:49:ARG:NH1	3:I:368:ASP:OD1	2.35	0.60
3:B:171:LEU:HD11	3:B:189:THR:HG22	1.83	0.60
3:I:171:LEU:HD11	3:I:189:THR:HG22	1.84	0.60
2:A:48:LEU:O	3:B:306:TYR:HA	2.01	0.59
3:K:423:THR:HG23	3:K:431:ILE:HG23	1.84	0.59
1:L:51:ASP:OD1	1:L:92:TYR:OH	2.22	0.58
3:K:429:ARG:HH21	4:M:106:TYR:HB3	1.67	0.58
1:E:94:ASN:H	3:B:429:ARG:NH1	2.02	0.58
3:B:422:CYS:HB2	3:B:435:PHE:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:424:ALA:HB3	3:I:433:LYS:HB3	1.86	0.58
1:E:113:ARG:HH21	1:E:116:ALA:HB2	1.69	0.57
3:K:427:LYS:NZ	3:K:448:ASP:OD2	2.30	0.56
3:B:207:LEU:O	3:B:212:CYS:HA	2.04	0.56
3:B:157:VAL:HG21	3:B:183:ASN:HB2	1.86	0.56
4:D:52:SER:O	4:D:72:ARG:NH1	2.34	0.56
1:E:2:ASP:N	1:E:2:ASP:OD1	2.39	0.56
1:E:202:THR:HG22	1:E:209:PRO:HB3	1.88	0.55
4:M:129:PRO:HB3	4:M:155:TYR:HB3	1.87	0.55
1:L:2:ASP:N	1:L:2:ASP:OD1	2.38	0.55
1:L:147:ARG:HH22	1:L:168:VAL:HG11	1.72	0.55
4:D:34:MET:HG3	4:D:79:VAL:HG21	1.89	0.55
4:H:83:MET:HB3	4:H:86:LEU:HD11	1.88	0.55
2:C:65:LYS:NZ	3:I:208:ASN:OD1	2.38	0.55
3:I:323:THR:OG1	3:I:331:ASN:OD1	2.14	0.55
1:L:202:THR:HG22	1:L:209:PRO:HB3	1.88	0.54
3:K:403:SER:OG	3:K:417:TYR:O	2.26	0.54
3:K:424:ALA:HB3	3:K:433:LYS:HB3	1.87	0.54
4:H:129:PRO:HB3	4:H:155:TYR:HB3	1.88	0.54
3:B:423:THR:HG23	3:B:431:ILE:HG23	1.89	0.54
3:K:270:GLN:HG2	3:K:309:ILE:HD12	1.90	0.54
1:L:90:GLN:HE22	1:L:98:LEU:HD23	1.70	0.54
4:D:136:PRO:HD3	4:D:148:LEU:HB3	1.88	0.54
3:I:338:ASP:HB2	3:I:342:TYR:OH	2.08	0.53
1:E:96:PRO:HG3	1:E:98:LEU:HD13	1.89	0.53
1:E:34:LEU:HD11	1:E:89:CYS:HB2	1.89	0.53
3:I:321:LEU:HD11	3:I:473:PRO:HB3	1.91	0.53
3:I:453:GLY:HA3	3:K:374:THR:HG21	1.90	0.53
3:B:338:ASP:HB2	3:B:342:TYR:OH	2.09	0.53
3:I:285:SER:HB3	3:I:304:PRO:HD3	1.91	0.53
3:K:405:SER:HB2	3:K:452:VAL:HG21	1.90	0.52
1:G:113:ARG:H	1:G:145:TYR:HE2	1.57	0.52
3:I:171:LEU:HD13	3:I:191:LYS:HB2	1.91	0.52
3:K:161:GLU:HB3	4:H:27:PHE:HA	1.91	0.52
1:L:36:TRP:HB2	1:L:49:MET:HG2	1.92	0.52
2:A:93:LEU:HD22	3:B:289:MET:CE	2.39	0.52
4:H:136:PRO:HD3	4:H:148:LEU:HB3	1.92	0.52
3:B:261:ILE:HD13	3:B:274:MET:HB3	1.91	0.52
3:B:209:LYS:HE2	3:B:210:GLN:HG2	1.91	0.52
3:I:423:THR:HG23	3:I:431:ILE:HG23	1.92	0.52
1:L:146:PRO:HD2	1:L:203:HIS:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:125:PRO:HD3	1:L:137:VAL:HG22	1.90	0.51
1:G:150:LYS:HB2	1:G:202:THR:OG1	2.10	0.51
3:B:209:LYS:HG3	3:B:210:GLN:H	1.75	0.51
2:A:28:ILE:HG22	3:B:410:LEU:HD11	1.93	0.51
4:M:136:PRO:HD3	4:M:148:LEU:HB3	1.92	0.51
3:I:138:LEU:HD21	3:I:394:LYS:HD2	1.92	0.51
3:I:395:ILE:HD13	3:I:492:ILE:HD13	1.92	0.51
4:D:50:VAL:HG12	4:D:59:TYR:HB2	1.93	0.51
3:B:432:ILE:HD11	3:B:447:VAL:HG22	1.92	0.51
3:B:285:SER:HB3	3:B:304:PRO:HD3	1.92	0.50
2:C:73:ASP:HB3	2:C:76:VAL:HB	1.94	0.50
3:K:338:ASP:HB2	3:K:342:TYR:OH	2.11	0.50
4:D:40:ALA:HB3	4:D:43:LYS:HB2	1.94	0.50
1:E:150:LYS:HB2	1:E:202:THR:OG1	2.12	0.50
2:A:53:TYR:OH	3:B:188:LEU:HD12	2.11	0.50
3:K:432:ILE:HD11	3:K:447:VAL:HG22	1.92	0.49
4:D:129:PRO:HB3	4:D:155:TYR:HB3	1.93	0.49
1:G:146:PRO:HD2	1:G:203:HIS:CE1	2.47	0.49
3:B:338:ASP:OD1	3:B:338:ASP:N	2.39	0.49
1:G:125:PRO:HB3	1:G:136:SER:H	1.77	0.49
4:H:98:ARG:NH2	4:H:111:ASP:OD2	2.46	0.49
4:H:34:MET:HG3	4:H:79:VAL:HG21	1.94	0.49
3:B:270:GLN:HG2	3:B:309:ILE:HD12	1.94	0.48
1:E:125:PRO:HD3	1:E:137:VAL:HG22	1.95	0.48
1:G:34:LEU:HD11	1:G:89:CYS:HB2	1.95	0.48
1:E:147:ARG:NH2	1:E:168:VAL:HG11	2.28	0.48
4:H:17:SER:OG	4:H:82:GLN:NE2	2.47	0.48
2:J:51:GLY:C	3:K:305:LEU:HB2	2.34	0.48
2:A:48:LEU:HB2	3:B:308:VAL:HB	1.96	0.47
3:I:211:SER:O	3:I:213:SER:N	2.47	0.47
3:I:415:SER:HB3	3:I:417:TYR:CE2	2.49	0.47
4:M:210:HIS:CD2	4:M:212:PRO:HD2	2.49	0.47
3:I:305:LEU:HD23	3:I:305:LEU:HA	1.72	0.47
3:B:415:SER:HB3	3:B:417:TYR:CE2	2.48	0.47
1:G:145:TYR:CG	1:G:145:TYR:O	2.67	0.47
3:I:410:LEU:O	3:I:441:TYR:OH	2.32	0.47
3:I:422:CYS:HB2	3:I:435:PHE:HB2	1.96	0.47
4:M:34:MET:HG3	4:M:79:VAL:HG21	1.97	0.47
2:J:46:SER:HB3	3:K:313:CYS:SG	2.54	0.47
1:G:3:ILE:HB	1:G:91:GLN:NE2	2.29	0.47
2:J:81:GLN:O	2:J:85:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:PRO:HD2	1:G:203:HIS:NE2	2.30	0.47
1:G:202:THR:HG22	1:G:209:PRO:HB3	1.96	0.47
2:A:93:LEU:HD22	3:B:289:MET:HE1	1.97	0.47
3:K:171:LEU:HD11	3:K:189:THR:HG22	1.97	0.47
4:H:98:ARG:O	4:H:110:MET:HA	2.14	0.47
3:B:216:ASN:HB2	3:B:218:GLU:OE1	2.15	0.46
4:H:210:HIS:CD2	4:H:212:PRO:HD2	2.50	0.46
3:I:400:THR:HG22	3:I:402:VAL:HG23	1.97	0.46
2:A:36:THR:HG21	3:B:386:ILE:HG12	1.97	0.46
3:I:416:CYS:O	3:I:437:ASN:HA	2.15	0.46
3:K:260:LEU:HD23	3:K:303:LEU:HD11	1.97	0.46
1:L:150:LYS:HB2	1:L:202:THR:OG1	2.16	0.46
2:J:61:LEU:O	3:K:196:LYS:HB2	2.15	0.46
3:B:405:SER:HB2	3:B:452:VAL:HG21	1.97	0.46
2:C:91:THR:O	2:C:95:LEU:HD13	2.16	0.46
1:E:5:MET:HE3	1:E:5:MET:HB3	1.85	0.46
1:L:92:TYR:O	3:I:429:ARG:NH2	2.48	0.45
3:B:462:GLN:OE1	3:B:463:GLU:N	2.50	0.45
3:K:267:THR:OG1	3:K:270:GLN:HG3	2.15	0.45
4:H:50:VAL:HG12	4:H:59:TYR:HB2	1.98	0.45
1:E:124:PRO:HB3	1:E:214:PHE:CE2	2.50	0.45
4:M:29:PHE:CD1	4:M:77:ASN:HA	2.52	0.45
2:A:27:ASN:O	2:A:28:ILE:HG13	2.16	0.45
3:I:445:LYS:HE3	4:H:54:ASP:OD2	2.16	0.45
1:L:95:LEU:HD23	1:L:95:LEU:HA	1.71	0.45
1:E:36:TRP:HB2	1:E:49:MET:HG2	1.99	0.45
3:K:261:ILE:HD13	3:K:274:MET:HB3	1.98	0.45
3:B:405:SER:HB3	3:B:457:TYR:CE2	2.51	0.45
3:I:245:THR:OG1	3:I:246:PRO:HD3	2.17	0.45
3:K:410:LEU:HD12	3:K:410:LEU:O	2.16	0.45
2:A:81:GLN:O	2:A:85:LYS:HG3	2.17	0.44
4:H:205:ILE:HG12	4:H:220:LYS:HA	1.98	0.44
3:B:171:LEU:HD13	3:B:191:LYS:HB2	1.98	0.44
3:B:381:LEU:HA	3:B:384:VAL:HG22	2.00	0.44
3:I:261:ILE:HD13	3:I:274:MET:HB3	1.98	0.44
4:D:210:HIS:CD2	4:D:212:PRO:HD2	2.53	0.44
1:G:124:PRO:HB3	1:G:214:PHE:CE1	2.53	0.44
1:G:181:SER:HB3	4:M:176:PHE:CZ	2.53	0.44
4:D:97:ALA:HB1	4:D:110:MET:HB3	2.00	0.44
4:H:129:PRO:HD2	4:H:215:THR:HG21	2.00	0.44
3:I:481:LEU:HD23	3:I:481:LEU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:203:THR:HG23	4:M:220:LYS:HZ2	1.83	0.44
4:D:98:ARG:O	4:D:110:MET:HA	2.16	0.44
2:A:46:SER:HB3	3:B:313:CYS:SG	2.58	0.43
2:A:57:ILE:HD13	3:B:252:LEU:HD13	2.00	0.43
3:B:481:LEU:HD23	3:B:481:LEU:H	1.82	0.43
3:B:481:LEU:HG	3:B:482:VAL:HG23	1.99	0.43
4:M:98:ARG:O	4:M:110:MET:HA	2.18	0.43
2:C:56:VAL:HG11	3:I:167:ILE:HD13	1.99	0.43
1:L:94:ASN:OD1	1:L:95:LEU:HG	2.18	0.43
3:B:395:ILE:HD13	3:B:492:ILE:HD13	2.00	0.43
1:E:163:ASN:OD1	1:E:163:ASN:N	2.50	0.43
4:M:8:GLY:O	4:M:18:LEU:HD11	2.18	0.43
4:M:220:LYS:HE3	4:M:222:GLU:OE2	2.18	0.43
2:C:56:VAL:O	3:I:189:THR:HA	2.19	0.43
2:C:89:ALA:HB2	3:I:231:LEU:HD23	2.01	0.43
3:I:445:LYS:HG2	4:H:53:TYR:OH	2.18	0.43
1:G:166:GLU:HB3	1:G:180:LEU:HD11	2.00	0.43
3:B:195:LEU:HD21	3:B:226:LYS:O	2.18	0.43
3:B:196:LYS:O	3:B:200:ASP:HB2	2.19	0.43
2:C:46:SER:HB3	3:I:313:CYS:SG	2.58	0.43
1:L:163:ASN:OD1	1:L:163:ASN:N	2.52	0.43
2:J:47:ALA:HB2	3:K:364:ARG:HD2	2.00	0.43
4:D:83:MET:HB3	4:D:86:LEU:HD11	2.01	0.43
3:I:176:LYS:NZ	3:I:259:SER:HB3	2.34	0.42
4:D:91:THR:HG23	4:D:120:THR:HA	2.01	0.42
1:L:166:GLU:HB3	1:L:180:LEU:HD11	2.01	0.42
3:K:205:PRO:O	3:K:209:LYS:HB2	2.19	0.42
3:I:465:LYS:HB3	3:I:465:LYS:HE2	1.77	0.42
3:K:338:ASP:OD1	3:K:338:ASP:N	2.37	0.42
3:K:423:THR:HG21	3:K:431:ILE:HG12	2.01	0.42
2:C:47:ALA:HB2	3:I:364:ARG:HD2	2.00	0.42
4:D:145:THR:HG22	4:D:145:THR:O	2.20	0.42
1:E:166:GLU:HB3	1:E:180:LEU:HD11	2.01	0.42
3:B:400:THR:HG22	3:B:402:VAL:HG23	2.00	0.42
3:I:267:THR:CG2	3:I:270:GLN:HG3	2.49	0.42
3:I:405:SER:HB2	3:I:452:VAL:HG21	2.00	0.42
3:I:156:LYS:HA	3:I:156:LYS:HD2	1.75	0.42
3:B:378:GLU:HA	3:B:381:LEU:HD13	2.02	0.42
3:I:176:LYS:HA	3:I:189:THR:O	2.20	0.42
3:K:395:ILE:HD13	3:K:492:ILE:HD13	2.01	0.42
3:K:422:CYS:HB2	3:K:435:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:481:LEU:H	3:K:481:LEU:HD23	1.85	0.42
2:J:62:SER:HB2	3:K:196:LYS:HA	2.01	0.42
3:K:387:PHE:HE2	3:K:474:ILE:HD12	1.85	0.42
4:M:91:THR:HG23	4:M:120:THR:HA	2.01	0.42
1:L:3:ILE:HG23	1:L:27:SER:HB3	2.02	0.42
1:E:113:ARG:HD2	1:E:175:ASP:O	2.19	0.42
4:D:29:PHE:CD1	4:D:77:ASN:HA	2.55	0.42
3:I:432:ILE:HD11	3:I:447:VAL:HG22	2.02	0.41
1:L:68:SER:OG	1:L:69:GLY:N	2.53	0.41
2:C:90:VAL:O	2:C:94:GLN:HG3	2.20	0.41
3:I:279:GLN:HG2	3:I:280:ILE:N	2.36	0.41
3:K:167:ILE:HG23	3:K:189:THR:HG21	2.02	0.41
4:H:145:THR:HG22	4:H:145:THR:O	2.20	0.41
2:J:79:ILE:HD11	3:K:214:ILE:HD13	2.00	0.41
3:K:154:VAL:O	3:K:157:VAL:HG12	2.20	0.41
4:M:205:ILE:HG12	4:M:220:LYS:HA	2.02	0.41
4:H:43:LYS:HD3	4:H:43:LYS:HA	1.92	0.41
4:H:97:ALA:HB1	4:H:110:MET:HB3	2.01	0.41
1:G:118:PRO:HD3	1:G:203:HIS:CE1	2.56	0.41
3:I:356:GLU:H	3:I:356:GLU:CD	2.23	0.41
3:K:199:ILE:HD11	3:K:223:PHE:CE1	2.55	0.41
4:M:40:ALA:HB3	4:M:43:LYS:HB2	2.03	0.41
4:D:98:ARG:NH2	4:D:111:ASP:OD2	2.53	0.41
2:C:61:LEU:O	3:I:295:GLU:HB3	2.20	0.41
3:K:410:LEU:HD22	3:K:464:GLY:HA3	2.02	0.41
2:A:56:VAL:HG11	3:B:167:ILE:HD13	2.02	0.41
3:K:356:GLU:H	3:K:356:GLU:CD	2.24	0.41
3:K:416:CYS:O	3:K:437:ASN:HA	2.20	0.41
1:E:30:ILE:HA	1:E:93:ASP:OD2	2.21	0.41
1:G:125:PRO:HG3	1:G:135:ALA:HB1	2.03	0.41
3:B:504:ALA:HA	3:B:507:ARG:HG2	2.03	0.41
4:M:145:THR:HG22	4:M:145:THR:O	2.20	0.41
4:D:8:GLY:O	4:D:18:LEU:HD11	2.21	0.41
3:B:252:LEU:HD12	3:B:252:LEU:HA	1.92	0.41
1:G:48:LEU:HD23	1:G:48:LEU:HA	1.89	0.40
2:C:57:ILE:HD13	3:I:252:LEU:HD13	2.02	0.40
4:M:43:LYS:HD3	4:M:43:LYS:HA	1.91	0.40
1:G:90:GLN:HB2	1:G:100:PHE:CD2	2.57	0.40
1:L:96:PRO:HG3	4:H:107:TYR:CD2	2.56	0.40
3:B:374:THR:HG21	3:K:453:GLY:HA3	2.04	0.40
1:L:125:PRO:HB3	1:L:136:SER:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:394:LYS:HA	3:B:491:SER:HA	2.03	0.40
3:K:381:LEU:HA	3:K:384:VAL:HG22	2.03	0.40
4:H:91:THR:HG23	4:H:120:THR:HA	2.04	0.40
4:H:99:ASP:HA	4:H:109:GLY:O	2.21	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	E	214/219 (98%)	200 (94%)	12 (6%)	2 (1%)	17	57
1	G	214/219 (98%)	201 (94%)	13 (6%)	0	100	100
1	L	214/219 (98%)	200 (94%)	13 (6%)	1 (0%)	29	67
2	A	70/72 (97%)	64 (91%)	6 (9%)	0	100	100
2	C	70/72 (97%)	63 (90%)	7 (10%)	0	100	100
2	J	70/72 (97%)	64 (91%)	6 (9%)	0	100	100
3	B	371/414 (90%)	346 (93%)	25 (7%)	0	100	100
3	I	371/414 (90%)	349 (94%)	20 (5%)	2 (0%)	29	67
3	K	371/414 (90%)	352 (95%)	19 (5%)	0	100	100
4	D	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
4	H	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
4	M	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
All	All	2625/2847 (92%)	2478 (94%)	142 (5%)	5 (0%)	47	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	212	CYS
3	I	246	PRO
1	E	95	LEU
1	L	97	PRO
1	E	96	PRO

### 5.3.2 Protein sidechains [i](#)

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	E	192/194 (99%)	191 (100%)	1 (0%)	88	95
1	G	192/194 (99%)	192 (100%)	0	100	100
1	L	192/194 (99%)	191 (100%)	1 (0%)	88	95
2	A	65/65 (100%)	64 (98%)	1 (2%)	65	85
2	C	65/65 (100%)	64 (98%)	1 (2%)	65	85
2	J	65/65 (100%)	63 (97%)	2 (3%)	40	71
3	B	341/373 (91%)	338 (99%)	3 (1%)	78	90
3	I	341/373 (91%)	334 (98%)	7 (2%)	53	79
3	K	341/373 (91%)	335 (98%)	6 (2%)	59	81
4	D	187/207 (90%)	184 (98%)	3 (2%)	62	83
4	H	187/207 (90%)	184 (98%)	3 (2%)	62	83
4	M	187/207 (90%)	183 (98%)	4 (2%)	53	79
All	All	2355/2517 (94%)	2323 (99%)	32 (1%)	67	85

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	31	LYS
1	E	51	ASP
2	A	69	CYS
3	B	290	CYS
3	B	319	SER
3	B	481	LEU

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Mol	Chain	Res	Type
2	C	65	LYS
3	I	159	HIS
3	I	190	PHE
3	I	208	ASN
3	I	284	GLN
3	I	290	CYS
3	I	319	SER
3	I	481	LEU
2	J	67	ASN
2	J	69	CYS
3	K	156	LYS
3	K	289	MET
3	K	290	CYS
3	K	319	SER
3	K	368	ASP
3	K	481	LEU
4	M	22	CYS
4	M	139	LYS
4	M	142	SER
4	M	148	LEU
4	H	22	CYS
4	H	139	LYS
4	H	148	LEU
4	D	139	LYS
4	D	142	SER
4	D	148	LEU

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

Mol	Chain	Res	Type
3	K	183	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
6	GOL	M	301	-	5,5,5	0.90	0	5,5,5	1.07	0
5	NAG	B	601	3	14,14,15	0.96	1 (7%)	17,19,21	1.54	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	M	301	-	-	2/4/4/4	-
5	NAG	B	601	3	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	NAG	O5-C1	3.48	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	NAG	C1-O5-C5	6.06	120.40	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	NAG	O5-C5-C6-O6
5	B	601	NAG	C8-C7-N2-C2
5	B	601	NAG	O7-C7-N2-C2
5	B	601	NAG	C4-C5-C6-O6
6	M	301	GOL	O1-C1-C2-O2
6	M	301	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 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(Å <sup>2</sup> )	Q<0.9
1	E	216/219 (98%)	-0.27	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	31, 55, 80, 107	0
1	G	216/219 (98%)	-0.34	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	12, 47, 81, 92	0
1	L	216/219 (98%)	-0.47	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	17, 39, 65, 91	0
2	A	72/72 (100%)	-0.14	2 (2%) <span style="border: 1px solid gray; padding: 2px;">53</span> <span style="border: 1px solid gray; padding: 2px;">35</span>	18, 44, 120, 163	0
2	C	72/72 (100%)	-0.22	2 (2%) <span style="border: 1px solid gray; padding: 2px;">53</span> <span style="border: 1px solid gray; padding: 2px;">35</span>	21, 51, 132, 151	0
2	J	71/72 (98%)	-0.25	2 (2%) <span style="border: 1px solid gray; padding: 2px;">53</span> <span style="border: 1px solid gray; padding: 2px;">35</span>	20, 49, 118, 136	0
3	B	373/414 (90%)	-0.46	1 (0%) <span style="border: 1px solid blue; padding: 2px;">94</span> <span style="border: 1px solid blue; padding: 2px;">88</span>	18, 43, 98, 136	0
3	I	373/414 (90%)	-0.44	1 (0%) <span style="border: 1px solid blue; padding: 2px;">94</span> <span style="border: 1px solid blue; padding: 2px;">88</span>	22, 49, 107, 138	0
3	K	373/414 (90%)	-0.40	3 (0%) <span style="border: 1px solid blue; padding: 2px;">86</span> <span style="border: 1px solid blue; padding: 2px;">73</span>	17, 47, 108, 152	0
4	D	222/244 (90%)	-0.39	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	25, 50, 76, 100	0
4	H	222/244 (90%)	-0.36	4 (1%) <span style="border: 1px solid gray; padding: 2px;">68</span> <span style="border: 1px solid gray; padding: 2px;">51</span>	13, 35, 83, 142	0
4	M	222/244 (90%)	-0.39	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	16, 43, 70, 86	0
All	All	2648/2847 (93%)	-0.38	15 (0%) <span style="border: 1px solid blue; padding: 2px;">89</span> <span style="border: 1px solid blue; padding: 2px;">80</span>	12, 46, 96, 163	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	70	ASN	3.7
3	K	210	GLN	3.5
2	A	69	CYS	3.3
3	B	210	GLN	2.7
2	C	72	THR	2.5
2	J	65	LYS	2.5
4	H	142	SER	2.2
3	K	208	ASN	2.2
2	J	66	GLU	2.1
2	C	66	GLU	2.1
3	I	211	SER	2.1

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Mol	Chain	Res	Type	RSRZ
4	H	140	SER	2.1
4	H	143	GLY	2.1
3	K	211	SER	2.1
4	H	141	THR	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	601	14/15	0.80	0.25	58,72,81,82	0
6	GOL	M	301	6/6	0.93	0.20	24,35,38,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.