



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:54 PM GMT

PDB ID : 5BV7  
Title : Crystal structure of human LCAT (L4F, N5D) in complex with Fab of an agonistic antibody  
Authors : Piper, D.E.; Romanow, W.G.; Thibault, S.T.; Walker, N.P.C.  
Deposited on : 2015-06-04  
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (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

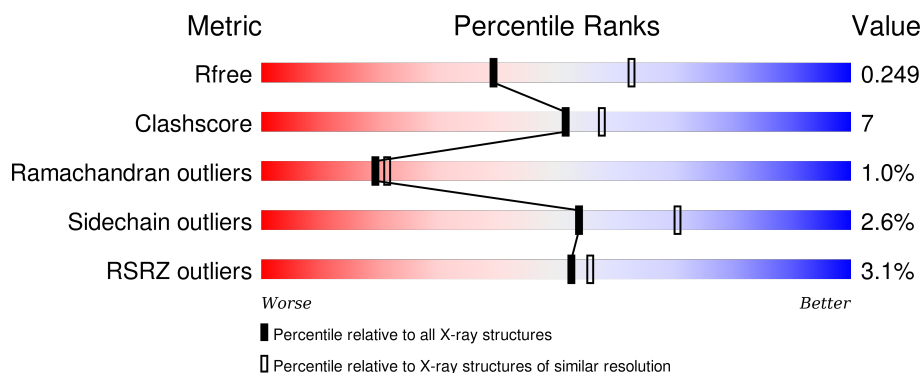
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>• 11%</div> </div> </div>
2	L	214	<div> <div>91%</div> <div>7%</div> <div>•</div> </div>
3	H	233	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>
4	B	213	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>15%</div> </div> </div>
5	C	238	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>21%</div> <div>• 8%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10030 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 Phosphatidylcholine-sterol acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3036	1972	510	539	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	PHE	LEU	engineered mutation	UNP P04180
A	5	ASP	ASN	engineered mutation	UNP P04180
A	417	GLU	-	expression tag	UNP P04180
A	418	ASN	-	expression tag	UNP P04180
A	419	LEU	-	expression tag	UNP P04180
A	420	TYR	-	expression tag	UNP P04180
A	421	PHE	-	expression tag	UNP P04180
A	422	GLN	-	expression tag	UNP P04180

- Molecule 2 is a protein called 27C3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1575	979	270	322	4			

- Molecule 3 is a protein called 27C3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	222	Total	C	N	O	S	0	0	0
			1657	1044	276	330	7			

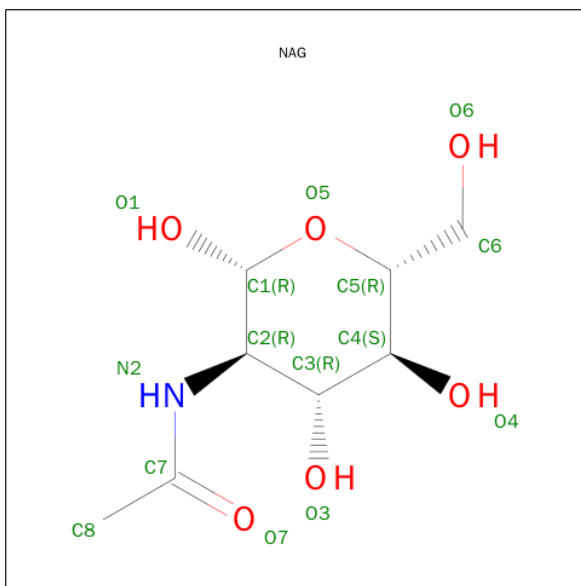
- Molecule 4 is a protein called Fab1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	212	Total	C	N	O	S	0	0	0
			1592	998	261	327	6			

- Molecule 5 is a protein called Fab1 heavy chain.

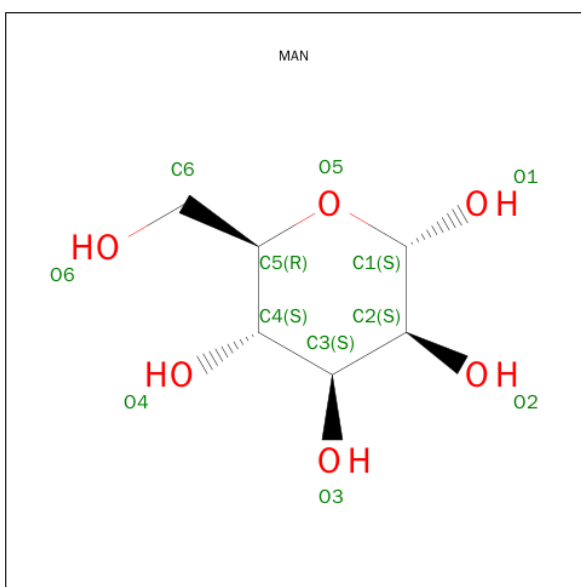
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	220	Total	C	N	O	S	0	0	0
			1671	1059	281	324	7			

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



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

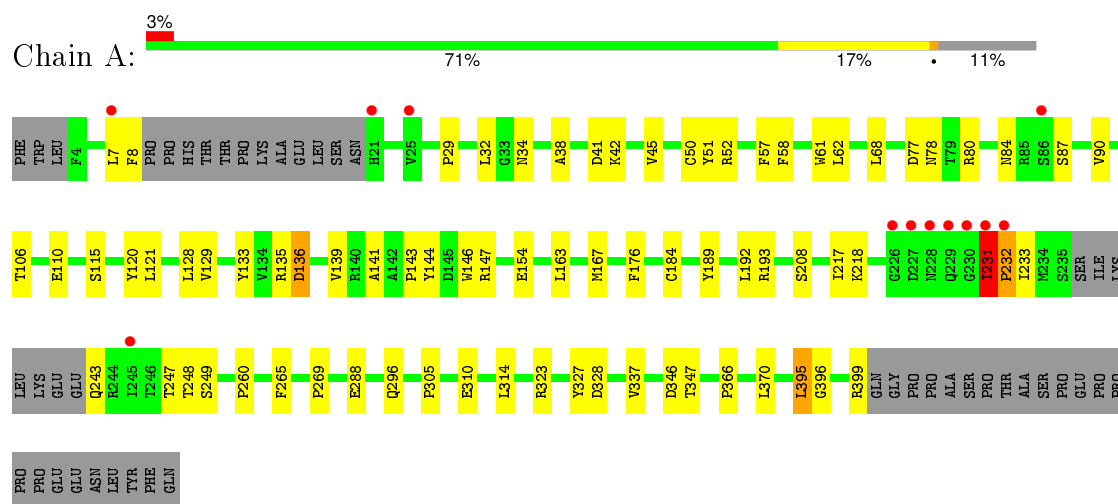
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	118	Total	O	0	0
			118	118		
8	L	107	Total	O	0	0
			107	107		
8	H	98	Total	O	0	0
			98	98		
8	B	52	Total	O	0	0
			52	52		
8	C	13	Total	O	0	0
			13	13		

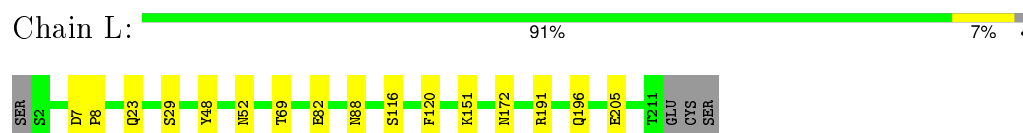
### 3 Residue-property plots [i](#)

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.

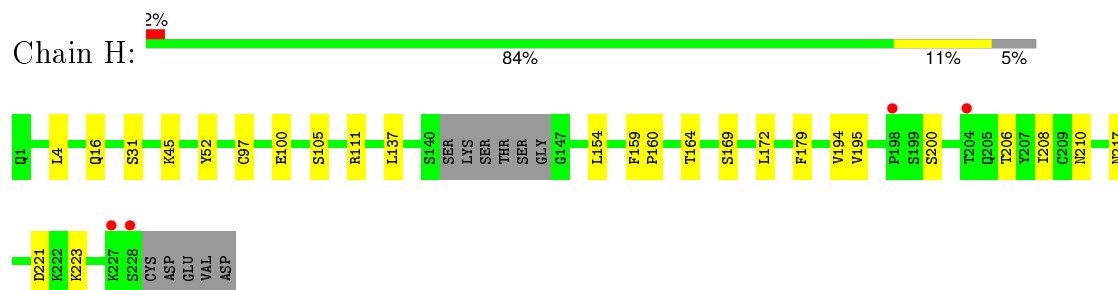
- Molecule 1: Phosphatidylcholine-sterol acyltransferase



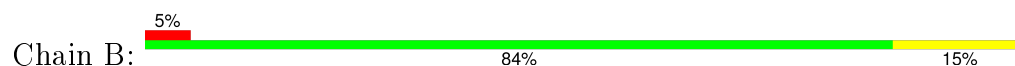
- Molecule 2: 27C3 light chain

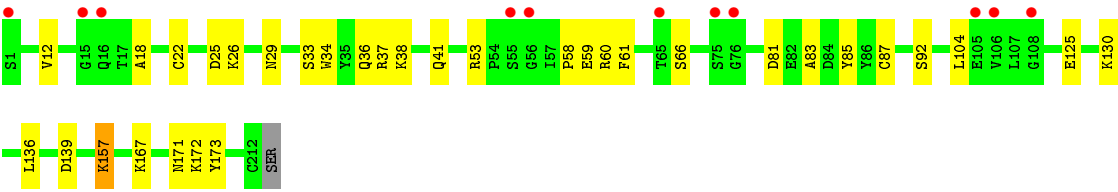


- Molecule 3: 27C3 heavy chain

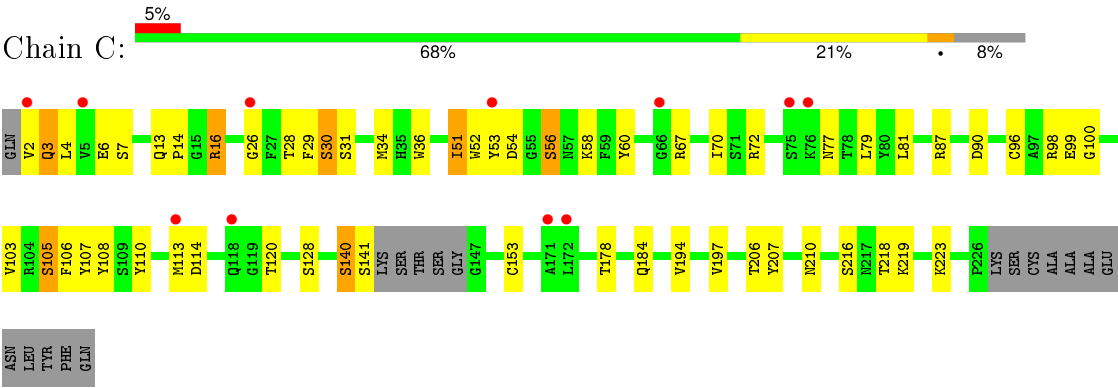


- Molecule 4: Fab1 light chain





● Molecule 5: Fab1 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.94Å 127.59Å 256.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.45 29.88 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.88-2.45) 93.3 (29.88-2.45)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.45Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.189 , 0.241 0.206 , 0.249	Depositor DCC
$R_{free}$ test set	3224 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 66120 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.49	0/3132	0.63	1/4272 (0.0%)
2	L	0.52	0/1611	0.61	0/2199
3	H	0.53	0/1697	0.67	0/2316
4	B	0.47	0/1633	0.62	0/2231
5	C	0.45	0/1715	0.60	0/2335
All	All	0.49	0/9788	0.62	1/13353 (0.0%)

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	A	0	1
5	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ASP	CB-CG-OD1	5.43	123.19	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	ILE	Peptide
5	C	30	SER	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3036	0	2938	52	1
2	L	1575	0	1519	9	1
3	H	1657	0	1628	13	0
4	B	1592	0	1538	21	0
5	C	1671	0	1608	41	0
6	A	56	0	50	2	0
7	A	55	0	46	1	0
8	A	118	0	0	2	0
8	B	52	0	0	0	0
8	C	13	0	0	1	0
8	H	98	0	0	0	0
8	L	107	0	0	0	0
All	All	10030	0	9327	129	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 7.

All (129) 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:B:60:ARG:NH2	4:B:81:ASP:OD2	2.08	0.85
5:C:51:ILE:HG21	5:C:72:ARG:HD2	1.61	0.81
1:A:218:LYS:HG3	1:A:347:THR:HG23	1.64	0.79
5:C:13:GLN:HG3	5:C:14:PRO:HD2	1.67	0.76
1:A:45:VAL:HB	1:A:52:ARG:HE	1.55	0.71
1:A:77:ASP:HA	1:A:80:ARG:HD3	1.77	0.66
1:A:328:ASP:HB3	1:A:337:VAL:HG11	1.77	0.66
5:C:105:SER:OG	5:C:106:PHE:N	2.27	0.66
3:H:210:ASN:ND2	3:H:221:ASP:OD1	2.30	0.64
2:L:82:GLU:OE1	2:L:172:ASN:ND2	2.31	0.63
5:C:51:ILE:CG2	5:C:72:ARG:HD2	2.28	0.63
3:H:172:LEU:HD21	3:H:195:VAL:HG21	1.81	0.63
1:A:87:SER:HB2	6:A:501:NAG:N2	2.15	0.62
1:A:217:ILE:HD13	1:A:265:PHE:HD1	1.66	0.61
5:C:7:SER:HA	5:C:120:THR:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:151:LYS:HE2	2:L:196:GLN:NE2	2.16	0.61
2:L:23:GLN:HG3	2:L:69:THR:HG22	1.83	0.61
1:A:133:TYR:HB3	1:A:139:VAL:CG2	2.32	0.59
1:A:260:PRO:HG2	3:H:31:SER:O	2.02	0.59
2:L:48:TYR:O	2:L:52:ASN:HB2	2.03	0.59
4:B:34:TRP:CZ3	4:B:87:CYS:HB3	2.38	0.58
5:C:140:SER:OG	5:C:141:SER:N	2.36	0.58
4:B:136:LEU:HD13	5:C:194:VAL:HG21	1.86	0.57
5:C:53:TYR:CE1	5:C:103:VAL:HG21	2.41	0.56
5:C:6:GLU:HG2	5:C:120:THR:HG23	1.87	0.56
5:C:54:ASP:HB2	5:C:56:SER:H	1.72	0.55
4:B:59:GLU:H	4:B:59:GLU:CD	2.09	0.55
1:A:314:LEU:HD11	1:A:370:LEU:HD12	1.87	0.55
1:A:217:ILE:HD13	1:A:265:PHE:CD1	2.43	0.54
4:B:36:GLN:NE2	4:B:85:TYR:OH	2.40	0.54
5:C:13:GLN:H	5:C:16:ARG:HE	1.55	0.54
5:C:34:MET:HB3	5:C:79:LEU:HD22	1.90	0.54
1:A:243:GLN:NE2	1:A:288:GLU:HG3	2.23	0.54
1:A:243:GLN:HE22	1:A:288:GLU:HG3	1.73	0.54
5:C:13:GLN:H	5:C:16:ARG:NE	2.06	0.53
8:A:635:HOH:O	5:C:105:SER:HB2	2.08	0.53
1:A:189:TYR:O	1:A:193:ARG:HG3	2.08	0.53
5:C:36:TRP:CZ3	5:C:96:CYS:HB3	2.44	0.53
1:A:147:ARG:HG2	1:A:247:THR:HG23	1.89	0.53
1:A:133:TYR:CD2	1:A:139:VAL:HG22	2.45	0.52
1:A:248:THR:HG22	1:A:249:SER:H	1.73	0.52
5:C:216:SER:OG	5:C:218:THR:OG1	2.17	0.52
5:C:36:TRP:NE1	5:C:81:LEU:HB2	2.25	0.52
4:B:81:ASP:O	4:B:104:LEU:HD23	2.10	0.51
1:A:45:VAL:HG22	1:A:50:CYS:HB2	1.92	0.51
1:A:192:LEU:HD13	1:A:305:PRO:HG2	1.91	0.51
4:B:38:LYS:HB2	4:B:41:GLN:NE2	2.26	0.50
5:C:30:SER:HB3	5:C:53:TYR:O	2.12	0.49
5:C:206:THR:HG23	5:C:223:LYS:HE3	1.94	0.49
2:L:82:GLU:HB2	2:L:172:ASN:HD21	1.77	0.49
1:A:141:ALA:O	1:A:143:PRO:HD3	2.12	0.49
3:H:45:LYS:HB3	3:H:45:LYS:NZ	2.27	0.49
5:C:100:GLY:HA2	5:C:114:ASP:OD1	2.13	0.48
4:B:53:ARG:NH2	4:B:61:PHE:O	2.37	0.48
1:A:84:ASN:OD1	1:A:87:SER:HB3	2.13	0.48
1:A:61:TRP:HA	1:A:62:LEU:HA	1.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:CYS:SG	1:A:208:SER:HB2	2.54	0.48
1:A:231:ILE:HG13	1:A:232:PRO:HD2	1.96	0.48
4:B:167:LYS:HD3	4:B:171:ASN:HA	1.95	0.47
4:B:125:GLU:HG2	4:B:130:LYS:O	2.15	0.47
1:A:7:LEU:O	1:A:8:PHE:HB2	2.15	0.47
4:B:167:LYS:HG2	4:B:173:TYR:CZ	2.49	0.47
3:H:100:GLU:OE1	3:H:111:ARG:NE	2.38	0.47
1:A:45:VAL:CG2	1:A:50:CYS:HB2	2.45	0.47
5:C:99:GLU:OE1	5:C:108:TYR:OH	2.25	0.46
1:A:34:ASN:HD21	1:A:144:TYR:H	1.63	0.46
1:A:120:TYR:CD2	1:A:121:LEU:HG	2.51	0.46
4:B:157:LYS:HB3	4:B:157:LYS:HE2	1.75	0.46
5:C:60:TYR:OH	5:C:70:ILE:HG22	2.15	0.46
4:B:38:LYS:HG2	4:B:83:ALA:HB2	1.98	0.46
1:A:34:ASN:ND2	1:A:144:TYR:H	2.14	0.46
1:A:395:LEU:HD23	1:A:395:LEU:HA	1.65	0.45
1:A:32:LEU:HD23	1:A:146:TRP:CH2	2.52	0.45
1:A:32:LEU:HA	1:A:146:TRP:CE2	2.51	0.45
1:A:154:GLU:HB2	8:A:651:HOH:O	2.17	0.45
5:C:34:MET:SD	5:C:98:ARG:HA	2.57	0.45
1:A:231:ILE:C	1:A:233:ILE:H	2.20	0.45
5:C:30:SER:O	5:C:53:TYR:HB2	2.18	0.44
4:B:136:LEU:HD13	5:C:194:VAL:CG2	2.46	0.44
5:C:67:ARG:NH2	5:C:90:ASP:OD2	2.51	0.44
1:A:58:PHE:CZ	5:C:106:PHE:HB3	2.53	0.44
1:A:29:PRO:HG3	1:A:34:ASN:HD22	1.82	0.44
1:A:217:ILE:HD12	1:A:323:ARG:HA	1.99	0.44
5:C:3:GLN:O	5:C:4:LEU:HD23	2.18	0.44
1:A:51:TYR:CZ	5:C:103:VAL:HG22	2.52	0.44
1:A:106:THR:O	1:A:110:GLU:HG3	2.18	0.44
1:A:269:PRO:HD3	1:A:327:TYR:O	2.18	0.44
1:A:248:THR:HG22	1:A:249:SER:N	2.33	0.43
3:H:206:THR:HG23	3:H:223:LYS:HE3	1.99	0.43
2:L:196:GLN:HG2	2:L:205:GLU:HG3	2.00	0.43
3:H:159:PHE:HA	3:H:160:PRO:HA	1.85	0.43
7:A:505:MAN:H2	7:A:507:MAN:H5	1.99	0.43
1:A:42:LYS:HD2	1:A:78:ASN:OD1	2.18	0.43
1:A:133:TYR:HD2	1:A:139:VAL:HG22	1.82	0.43
4:B:37:ARG:NH2	4:B:41:GLN:O	2.51	0.43
5:C:2:VAL:HA	5:C:26:GLY:HA3	2.00	0.43
5:C:58:LYS:HE3	5:C:58:LYS:HB2	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:O	1:A:167:MET:HG3	2.19	0.43
5:C:197:VAL:HG11	5:C:207:TYR:CE1	2.54	0.43
5:C:184:GLN:HB3	8:C:304:HOH:O	2.19	0.43
5:C:7:SER:CA	5:C:120:THR:HG21	2.48	0.42
2:L:7:ASP:HA	2:L:8:PRO:HD3	1.79	0.42
3:H:179:PHE:HE1	3:H:194:VAL:HG12	1.83	0.42
5:C:98:ARG:NH1	5:C:114:ASP:OD2	2.52	0.42
3:H:208:ILE:HG21	3:H:221:ASP:HB3	2.02	0.42
2:L:151:LYS:HB2	2:L:151:LYS:HE3	1.92	0.42
1:A:128:LEU:C	1:A:133:TYR:HB2	2.40	0.42
3:H:137:LEU:HD21	3:H:154:LEU:HB2	2.02	0.42
2:L:120:PHE:CD1	3:H:137:LEU:HB3	2.55	0.42
1:A:310:GLU:OE1	1:A:399:ARG:NH1	2.47	0.42
4:B:29:ASN:HD22	4:B:29:ASN:HA	1.66	0.42
1:A:68:LEU:HD12	5:C:107:TYR:HE2	1.85	0.42
1:A:296:GLN:HG2	1:A:296:GLN:O	2.19	0.42
4:B:38:LYS:HE3	4:B:41:GLN:HE22	1.85	0.42
4:B:58:PRO:HB2	4:B:61:PHE:CE1	2.55	0.42
5:C:67:ARG:NH1	5:C:87:ARG:HD2	2.35	0.42
5:C:53:TYR:HA	5:C:72:ARG:NH2	2.34	0.42
5:C:110:TYR:OH	5:C:113:MET:HG3	2.20	0.42
1:A:87:SER:OG	6:A:501:NAG:H83	2.19	0.41
1:A:147:ARG:HB3	1:A:247:THR:O	2.20	0.41
1:A:38:ALA:O	1:A:57:PHE:HA	2.20	0.41
3:H:4:LEU:HB3	3:H:97:CYS:SG	2.60	0.41
1:A:51:TYR:CD2	5:C:103:VAL:HG13	2.55	0.41
1:A:129:VAL:HG21	1:A:135:ARG:NH2	2.36	0.41
4:B:12:VAL:HG21	4:B:18:ALA:HB2	2.02	0.41
4:B:25:ASP:OD1	4:B:26:LYS:HG3	2.21	0.41
3:H:45:LYS:HB3	3:H:45:LYS:HZ2	1.86	0.40
4:B:139:ASP:HA	4:B:172:LYS:HB3	2.02	0.40
5:C:29:PHE:CD2	5:C:77:ASN:HA	2.56	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)
1:A:154:GLU:OE2	2:L:191:ARG:NH1[3_544]	2.11	0.09

## 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	371/422 (88%)	347 (94%)	18 (5%)	6 (2%)	12	11
2	L	208/214 (97%)	202 (97%)	6 (3%)	0	100	100
3	H	218/233 (94%)	205 (94%)	11 (5%)	2 (1%)	21	25
4	B	210/213 (99%)	193 (92%)	16 (8%)	1 (0%)	34	41
5	C	216/238 (91%)	199 (92%)	14 (6%)	3 (1%)	14	13
All	All	1223/1320 (93%)	1146 (94%)	65 (5%)	12 (1%)	19	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ILE
1	A	232	PRO
5	C	56	SER
1	A	136	ASP
4	B	66	SER
5	C	28	THR
1	A	396	GLY
3	H	169	SER
5	C	140	SER
1	A	41	ASP
1	A	395	LEU
3	H	200	SER

### 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	326/367 (89%)	321 (98%)	5 (2%)	72	84
2	L	175/179 (98%)	172 (98%)	3 (2%)	68	81
3	H	192/202 (95%)	187 (97%)	5 (3%)	54	70
4	B	180/181 (99%)	176 (98%)	4 (2%)	60	75
5	C	184/198 (93%)	173 (94%)	11 (6%)	24	33
All	All	1057/1127 (94%)	1029 (97%)	28 (3%)	54	70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	115	SER
1	A	136	ASP
1	A	176	PHE
1	A	366	PRO
2	L	29	SER
2	L	88	ASN
2	L	116	SER
3	H	16	GLN
3	H	52	TYR
3	H	105	SER
3	H	164	THR
3	H	217	ASN
4	B	22	CYS
4	B	33	SER
4	B	92	SER
4	B	157	LYS
5	C	3	GLN
5	C	16	ARG
5	C	31	SER
5	C	51	ILE
5	C	52	TRP
5	C	105	SER
5	C	128	SER
5	C	153	CYS
5	C	178	THR
5	C	210	ASN
5	C	219	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	127	ASN
1	A	228	ASN
1	A	279	GLN
1	A	391	ASN
2	L	41	GLN
2	L	78	GLN
2	L	88	ASN
2	L	172	ASN
3	H	3	GLN
3	H	79	GLN
3	H	177	HIS
4	B	29	ASN
4	B	36	GLN
4	B	41	GLN
4	B	88	GLN
4	B	109	GLN
5	C	184	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	NAG	A	501	1	14,14,15	1.80	2 (14%)	15,19,21	1.44	1 (6%)
6	NAG	A	502	1,6	14,14,15	0.33	0	15,19,21	0.42	0
6	NAG	A	503	7,6	14,14,15	0.89	1 (7%)	15,19,21	0.62	0
7	MAN	A	504	7,6	11,11,12	0.86	0	15,15,17	1.61	2 (13%)
7	MAN	A	505	7	11,11,12	0.95	0	15,15,17	0.95	1 (6%)
7	MAN	A	506	7	11,11,12	0.70	0	15,15,17	0.85	0
7	MAN	A	507	7	11,11,12	1.07	1 (9%)	15,15,17	1.46	1 (6%)
7	MAN	A	508	7	11,11,12	1.31	1 (9%)	15,15,17	1.10	1 (6%)
6	NAG	A	509	1	14,14,15	0.38	0	15,19,21	0.39	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
6	NAG	A	501	1	-	0/6/23/26	0/1/1/1
6	NAG	A	502	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	503	7,6	-	0/6/23/26	0/1/1/1
7	MAN	A	504	7,6	-	0/2/19/22	1/1/1/1
7	MAN	A	505	7	-	0/2/19/22	0/1/1/1
7	MAN	A	506	7	-	0/2/19/22	0/1/1/1
7	MAN	A	507	7	-	0/2/19/22	0/1/1/1
7	MAN	A	508	7	-	0/2/19/22	0/1/1/1
6	NAG	A	509	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	503	NAG	O5-C1	-3.09	1.38	1.43
7	A	507	MAN	C4-C3	2.09	1.57	1.52
7	A	508	MAN	C2-C3	3.12	1.56	1.52
6	A	501	NAG	O5-C1	3.58	1.49	1.43
6	A	501	NAG	C1-C2	5.47	1.60	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	505	MAN	O2-C2-C3	-2.30	105.55	110.19
7	A	508	MAN	C1-O5-C5	2.80	116.25	112.14
7	A	504	MAN	C1-C2-C3	3.20	113.43	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	504	MAN	C1-O5-C5	3.53	117.33	112.14
7	A	507	MAN	C1-O5-C5	4.51	118.77	112.14
6	A	501	NAG	C1-O5-C5	4.58	118.87	112.14

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	504	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	501	NAG	2	0
7	A	505	MAN	1	0
7	A	507	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 ⓘ

### 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	377/422 (89%)	-0.05	12 (3%) 51 54	25, 47, 76, 104	0
2	L	210/214 (98%)	-0.36	0 100 100	30, 42, 60, 73	0
3	H	222/233 (95%)	-0.18	4 (1%) 71 74	25, 42, 77, 90	0
4	B	212/213 (99%)	0.17	11 (5%) 31 34	32, 63, 96, 105	0
5	C	220/238 (92%)	0.34	11 (5%) 32 36	41, 68, 91, 98	0
All	All	1241/1320 (94%)	-0.02	38 (3%) 52 56	25, 50, 87, 105	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	GLY	6.6
1	A	229	GLN	4.0
1	A	231	ILE	3.8
1	A	228	ASN	3.5
1	A	21	HIS	3.4
4	B	55	SER	3.2
4	B	16	GLN	3.2
4	B	75	SER	3.0
4	B	1	SER	3.0
4	B	76	GLY	2.9
5	C	76	LYS	2.9
4	B	15	GLY	2.8
3	H	228	SER	2.8
1	A	227	ASP	2.7
5	C	26	GLY	2.7
1	A	86	SER	2.6
3	H	204	THR	2.5
5	C	5	VAL	2.5
5	C	75	SER	2.4
4	B	56	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
4	B	106	VAL	2.4
1	A	232	PRO	2.3
4	B	65	THR	2.3
5	C	118	GLN	2.3
1	A	226	GLY	2.2
5	C	66	GLY	2.2
5	C	113	MET	2.2
3	H	227	LYS	2.2
5	C	2	VAL	2.1
5	C	53	TYR	2.1
1	A	7	LEU	2.1
4	B	108	GLY	2.1
5	C	171	ALA	2.1
5	C	172	LEU	2.1
3	H	198	PRO	2.1
4	B	105	GLU	2.1
1	A	25	VAL	2.0
1	A	245	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	A	502	14/15	0.96	0.18	1.79	46,53,56,58	0
7	MAN	A	508	11/12	0.94	0.16	0.98	48,50,56,57	0
6	NAG	A	501	14/15	0.57	0.33	-	76,91,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	509	14/15	0.84	0.38	-	78,93,100,105	0
7	MAN	A	505	11/12	0.95	0.12	-	52,61,66,69	0
6	NAG	A	503	14/15	0.96	0.20	-	42,54,61,64	0
7	MAN	A	504	11/12	0.96	0.13	-	43,46,50,52	0
7	MAN	A	506	11/12	0.89	0.27	-	77,82,90,91	0
7	MAN	A	507	11/12	0.89	0.24	-	57,70,73,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.