



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 10:53 AM BST

PDB ID : 6URM  
Title : Crystal structure of vaccine-elicited receptor-binding site targeting antibody LPAF-a.01 in complex with Hemagglutinin H1 A/California/04/2009  
Authors : Zhou, T.; Cheung, S.F.; Kwong, P.D.  
Deposited on : 2019-10-23  
Resolution : 2.65 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.

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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 : 2.14.4.dev1  
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) : 2.14.4.dev1

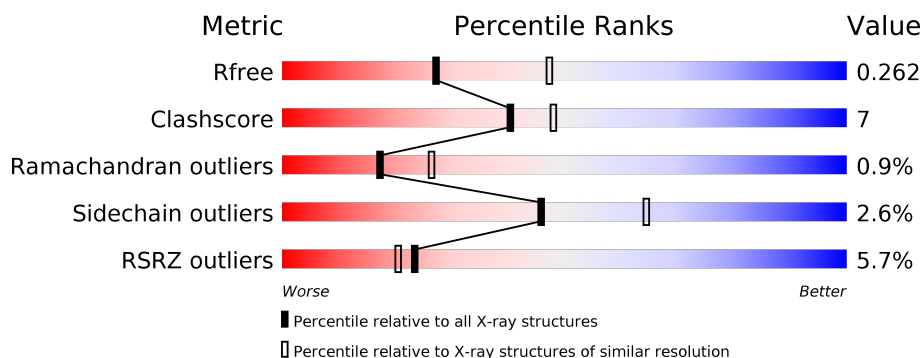
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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	C	505	<div> <div>8%</div> <div>34%</div> <div>8%</div> <div>57%</div> </div>
1	F	505	<div> <div>5%</div> <div>33%</div> <div>10%</div> <div>57%</div> </div>
2	D	227	<div> <div>%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
2	H	227	<div> <div>2%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
3	E	211	<div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div>
3	L	211	<div> <div>2%</div> <div>83%</div> <div>16%</div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
4	A	2	 100%
5	B	3	 33%  67%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10193 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	219	Total	C	N	O	S	0	0	0
			1733	1106	292	329	6			
1	C	217	Total	C	N	O	S	0	0	0
			1721	1098	290	327	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	506	SER	-	expression tag	UNP A0A3S7XTA4
F	507	GLY	-	expression tag	UNP A0A3S7XTA4
C	506	SER	-	expression tag	UNP A0A3S7XTA4
C	507	GLY	-	expression tag	UNP A0A3S7XTA4

- Molecule 2 is a protein called The heavy chain of antibody LPAF-a.01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1689	1069	281	331	8			
2	D	224	Total	C	N	O	S	0	0	0
			1689	1069	281	331	8			

- Molecule 3 is a protein called The light chain of antibody LPAF-a.01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1579	992	266	317	4			
3	E	209	Total	C	N	O	S	0	0	0
			1570	987	265	314	4			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



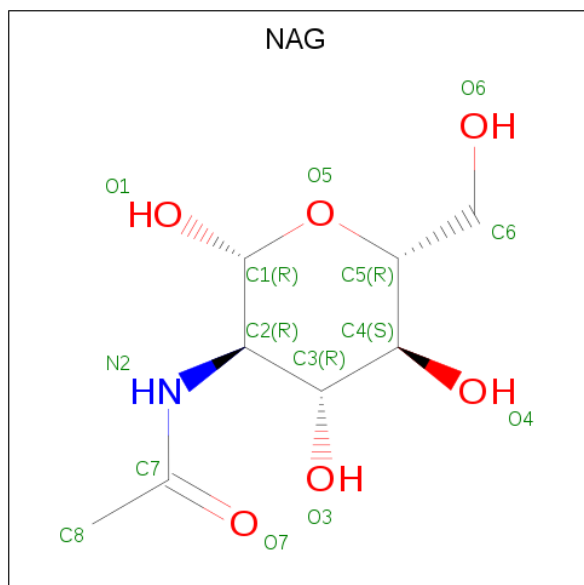
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



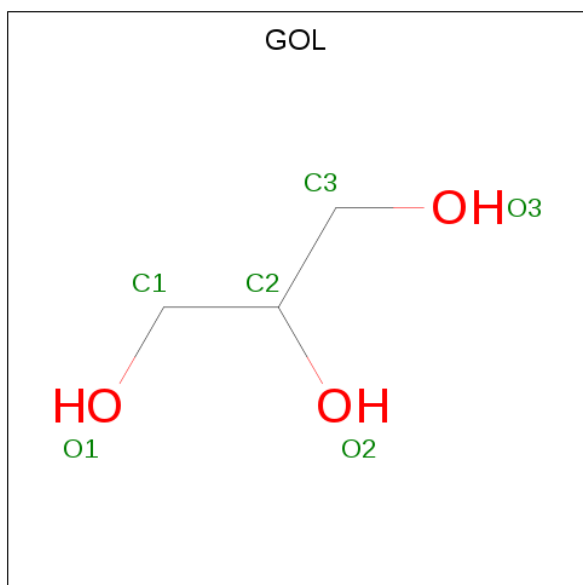
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

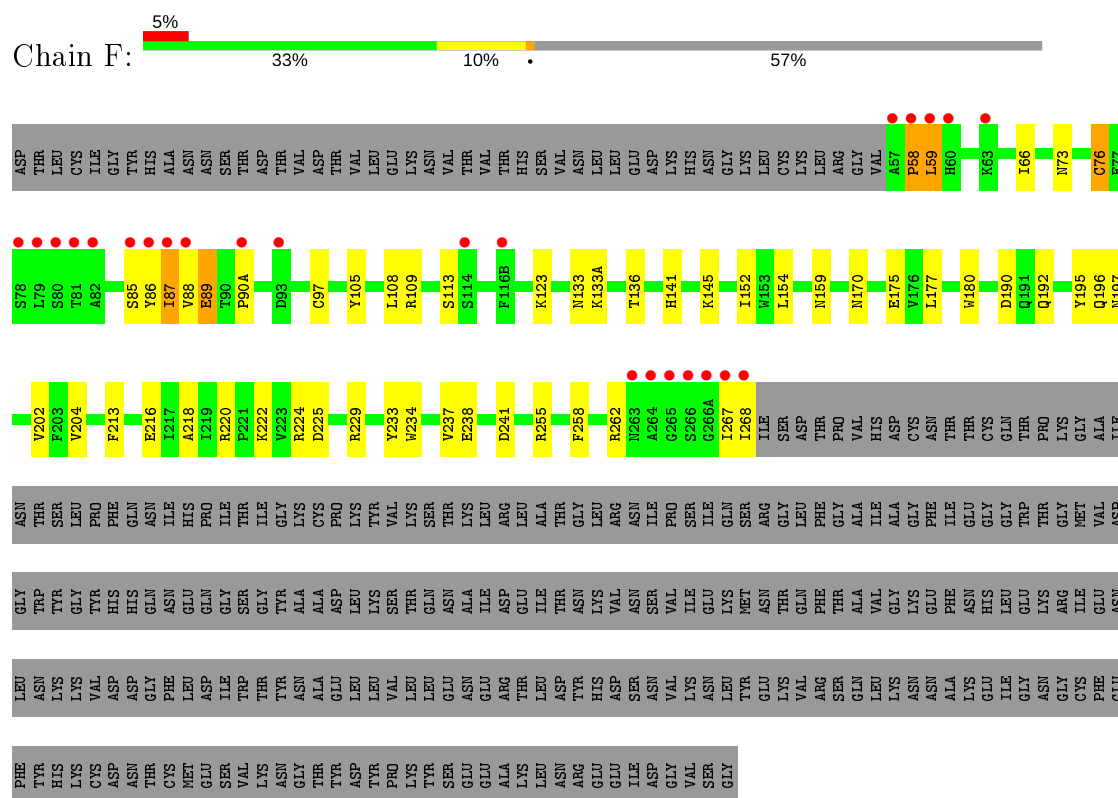
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	14	Total	O	0	0
			14	14		
9	H	15	Total	O	0	0
			15	15		
9	L	18	Total	O	0	0
			18	18		
9	C	8	Total	O	0	0
			8	8		
9	D	27	Total	O	0	0
			27	27		
9	E	17	Total	O	0	0
			17	17		

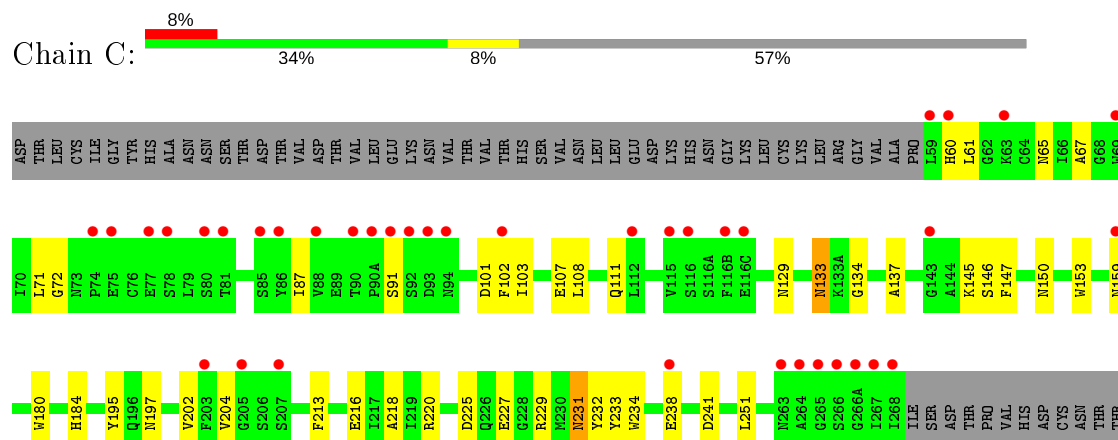
### 3 Residue-property plots

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: Hemagglutinin



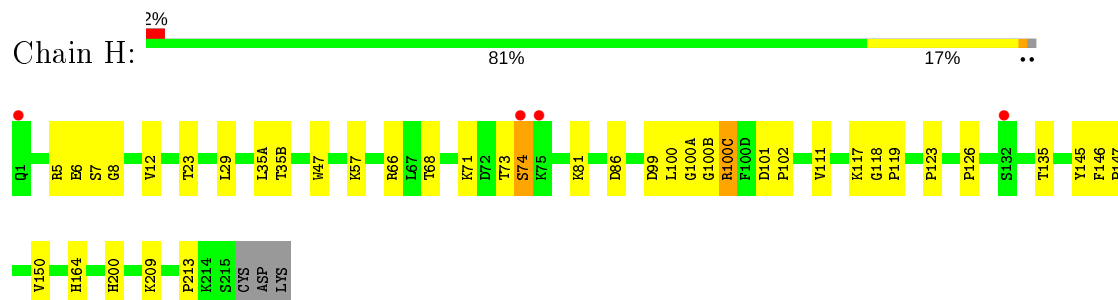
- Molecule 1: Hemagglutinin



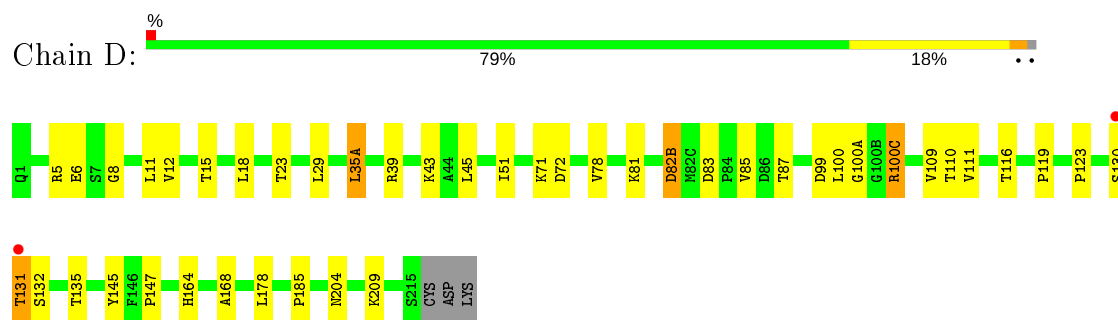


CYS	GLN	THR	PRO	GLY	ALA	ILE	ASN	THR	SER	LEU	PRO	PHE	GLN	ASN	ILE	HIS	GLN	ASN	GLY	THR	GLY	ILE	GLY	LYS	ALA	CYS	PRO	LEU	LYS	THR	GLN	SER	THR	ALA	LYS	ILE	ARG	ASN	VAL	ARG	ILE	PRO	SER	ILE	SER	ILE	GLN	THR	GLY	LEU	PHE	GLY	ALA	ILE	GLY	LYS	GLY	PHE	ILE	ASN
GLY	THR	TRP	GLY	ARG	VAL	ASP	GLY	TRP	TYR	LYS	TYR	HIS	VAL	ASP	ASP	GLN	THR	CYS	GLY	ASP	VAL	THR	LYS	GLY	ALA	ALA	ASP	LEU	LYS	THR	ASN	GLY	VAL	ASN	SER	VAL	ASN	SER	VAL	ASN	VAL	LYS	ASN	GLY	VAL	THR	GLY	ALA	GLN	THR	PHE	GLY	VAL	ILE	GLY	LYS	GLY	PHE	ILE	ASN
HIS	LEU	GLY	LYS	ARG	ILE	ASN	ASN	LEU	TYR	LYS	LYS	VAL	ASP	ASP	ASP	GLN	THR	CYS	GLY	ASP	VAL	THR	LYS	GLY	ALA	ALA	GLY	LEU	LYS	THR	ASN	GLY	VAL	ASN	SER	VAL	ASN	SER	VAL	ASN	VAL	LYS	ASN	GLY	VAL	THR	GLY	ALA	GLN	THR	PHE	GLY	VAL	ILE	GLY	LYS	GLY	PHE	ILE	ASN
GLY	ILE	GLY	ASN	GLY	PHE	GLY	PHE	TYR	HIS	LYS	LYS	CYS	ASP	ASP	ASN	THR	CYS	GLY	GLY	ASP	VAL	THR	LYS	GLY	ALA	ALA	GLY	LEU	LYS	THR	ASN	GLY	VAL	ASN	SER	VAL	ASN	SER	VAL	ASN	VAL	LYS	ASN	GLY	VAL	THR	GLY	ALA	GLN	THR	PHE	GLY	VAL	ILE	GLY	LYS	GLY	PHE	ILE	ASN

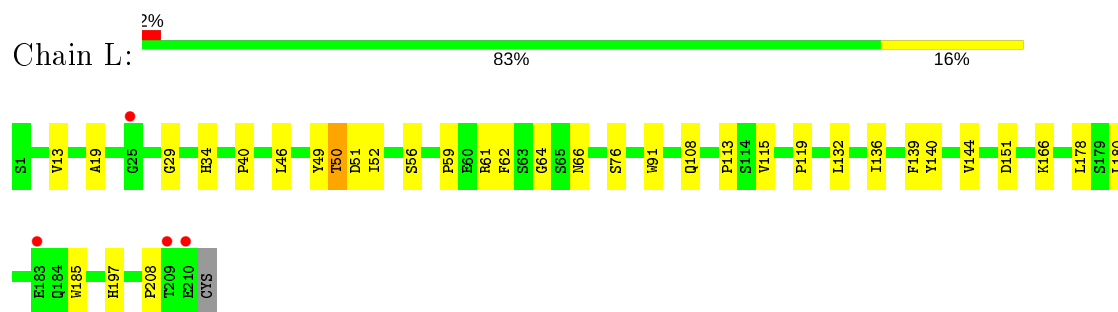
- Molecule 2: The heavy chain of antibody LPAF-a.01



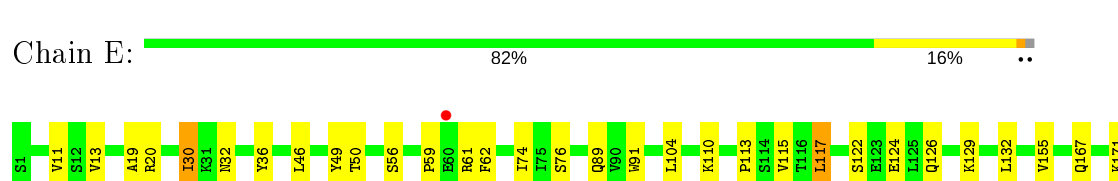
- Molecule 2: The heavy chain of antibody LPAF-a.01



- Molecule 3: The light chain of antibody LPAF-a.01



- Molecule 3: The light chain of antibody LPAF-a.01





- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  100%



- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  33% 67%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.41 Å   260.84 Å   66.45 Å 90.00°   96.93°   90.00°	Depositor
Resolution (Å)	40.06 – 2.65 40.06 – 2.63	Depositor EDS
% Data completeness (in resolution range)	88.6 (40.06-2.65) 88.6 (40.06-2.63)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.65 Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.215   ,   0.262 0.214   ,   0.262	Depositor DCC
$R_{free}$ test set	1996 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: GOL, SO4, 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	C	0.25	0/1770	0.43	0/2401
1	F	0.26	0/1783	0.43	0/2420
2	D	0.25	0/1729	0.48	0/2361
2	H	0.25	0/1729	0.48	0/2361
3	E	0.25	0/1607	0.45	0/2197
3	L	0.25	0/1616	0.45	0/2209
All	All	0.25	0/10234	0.45	0/13949

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

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	C	1721	0	1658	28	0
1	F	1733	0	1669	34	0
2	D	1689	0	1690	25	0
2	H	1689	0	1690	23	0
3	E	1570	0	1540	24	0
3	L	1579	0	1546	22	0
4	A	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	39	0	34	2	0
6	F	14	0	13	0	0
7	D	5	0	0	0	0
7	E	5	0	0	0	0
7	F	5	0	0	0	0
7	L	5	0	0	0	0
8	D	6	0	8	0	0
8	H	6	0	8	0	0
9	C	8	0	0	5	0
9	D	27	0	0	3	0
9	E	17	0	0	1	0
9	F	14	0	0	0	0
9	H	15	0	0	3	0
9	L	18	0	0	1	0
All	All	10193	0	9881	143	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 7.

All (143) 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:C:220:ARG:HG3	1:C:229:ARG:HG2	1.62	0.80
1:F:59:LEU:HD23	1:F:87:ILE:HG22	1.63	0.79
2:H:100(C):ARG:NH2	9:H:601:HOH:O	2.04	0.73
1:C:101:ASP:O	9:C:601:HOH:O	2.06	0.72
2:D:100(A):GLY:HA2	3:E:32:ASN:HD22	1.56	0.71
1:F:220:ARG:HG3	1:F:229:ARG:HG2	1.72	0.71
2:D:100(C):ARG:NH2	9:D:601:HOH:O	2.15	0.70
3:E:132:LEU:HD12	3:E:178:LEU:HD23	1.73	0.70
3:L:46:LEU:HD21	3:L:49:TYR:HB3	1.75	0.67
1:F:216:GLU:OE2	1:C:233:TYR:OH	2.10	0.64
1:F:87:ILE:HD13	1:F:113:SER:HA	1.80	0.64
2:D:87:THR:HG23	2:D:110:THR:HA	1.80	0.63
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.81	0.62
1:F:97:CYS:O	1:F:224:ARG:NH1	2.33	0.62
1:F:233:TYR:OH	1:C:216:GLU:OE2	2.14	0.60
2:D:130:SER:OG	3:E:115:VAL:O	2.15	0.59
3:L:180:LEU:O	9:L:401:HOH:O	2.16	0.59
2:D:100(A):GLY:O	3:E:91:TRP:HB3	2.02	0.59
2:D:81:LYS:NZ	9:D:603:HOH:O	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:VAL:HB	1:F:213:PHE:HB2	1.85	0.57
1:F:218:ALA:O	1:F:220:ARG:NH2	2.37	0.57
2:D:39:ARG:HG3	2:D:45:LEU:HD23	1.88	0.56
1:C:238:GLU:HG3	1:C:241:ASP:HB2	1.87	0.56
2:D:11:LEU:HD13	2:D:147:PRO:HG3	1.88	0.55
1:C:218:ALA:O	1:C:220:ARG:NH2	2.41	0.54
1:F:192:GLN:NE2	1:F:196:GLN:O	2.40	0.54
1:F:170:ASN:ND2	1:F:237:VAL:O	2.40	0.54
1:C:107:GLU:O	1:C:111:GLN:HG2	2.07	0.54
2:H:7:SER:O	9:H:602:HOH:O	2.18	0.52
3:E:117:LEU:HD21	3:E:206:VAL:HG22	1.91	0.52
1:C:137:ALA:HB1	3:E:30:ILE:HG22	1.91	0.52
3:L:13:VAL:HG11	3:L:19:ALA:HA	1.91	0.52
1:C:101:ASP:OD1	1:C:101:ASP:N	2.44	0.51
2:D:15:THR:HA	2:D:82(B):ASP:HB2	1.93	0.51
3:E:20:ARG:HG2	3:E:74:ILE:HG13	1.93	0.51
2:D:29:LEU:HD13	2:D:35(A):LEU:HD12	1.93	0.51
1:F:238:GLU:HG3	1:F:241:ASP:HB2	1.93	0.51
1:C:133:ASN:OD1	1:C:133:ASN:N	2.44	0.51
1:C:195:TYR:O	1:C:197:ASN:N	2.38	0.50
1:F:190:ASP:OD2	2:H:99:ASP:N	2.43	0.50
2:D:5:ARG:HE	2:D:23:THR:HB	1.75	0.50
1:C:71:LEU:O	9:C:602:HOH:O	2.20	0.50
1:C:72:GLY:HA3	9:C:602:HOH:O	2.12	0.50
2:D:18:LEU:HD22	2:D:109:VAL:HG11	1.93	0.50
2:H:29:LEU:HD22	2:H:35(A):LEU:HD12	1.94	0.50
1:F:87:ILE:HD11	1:F:267:ILE:HG13	1.93	0.50
2:D:51:ILE:HD11	2:D:71:LYS:HE2	1.94	0.49
3:L:115:VAL:HG22	3:L:136:ILE:HG23	1.93	0.49
1:F:152:ILE:HG13	1:F:255:ARG:HB2	1.94	0.49
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.43	0.49
3:E:204:LYS:NZ	9:E:407:HOH:O	2.44	0.49
2:D:131:THR:HG22	2:D:132:SER:H	1.78	0.48
3:L:132:LEU:HD12	3:L:178:LEU:HD23	1.94	0.48
2:D:119:PRO:HB3	2:D:145:TYR:HB3	1.94	0.48
1:F:195:TYR:O	1:F:197:ASN:N	2.42	0.48
2:H:100(A):GLY:N	9:H:601:HOH:O	2.45	0.48
3:L:113:PRO:HB3	3:L:139:PHE:HB3	1.96	0.48
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.49	0.48
3:E:113:PRO:HD3	3:E:197:HIS:CD2	2.48	0.48
1:F:58:PRO:HB3	1:F:85:SER:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:THR:HB	2:H:81:LYS:HB2	1.97	0.47
3:L:108:GLN:HB2	3:L:140:TYR:CE1	2.50	0.47
1:F:175:GLU:OE1	1:F:262:ARG:NH1	2.46	0.47
1:C:150:ASN:N	9:C:602:HOH:O	2.24	0.47
2:D:6:GLU:N	2:D:6:GLU:OE1	2.48	0.47
3:E:49:TYR:CD2	3:E:50:THR:HG22	2.50	0.47
1:F:222:LYS:HD2	1:F:225:ASP:HA	1.96	0.47
1:F:73:ASN:HB3	1:F:76:CYS:SG	2.55	0.47
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.96	0.47
2:H:6:GLU:OE1	2:H:6:GLU:N	2.48	0.47
3:L:119:PRO:HA	3:L:132:LEU:HD23	1.96	0.47
3:E:61:ARG:HB2	3:E:76:SER:O	2.15	0.47
5:B:2:NAG:H62	5:B:3:MAN:O2	2.15	0.46
1:C:227:GLU:H	2:D:99:ASP:CG	2.17	0.46
2:D:135:THR:HA	2:D:185:PRO:HA	1.96	0.46
1:C:102:PHE:CD2	1:C:232:TYR:HB2	2.50	0.46
1:C:108:LEU:HB2	1:C:234:TRP:CE2	2.51	0.46
2:H:5:ARG:HG3	2:H:23:THR:HB	1.96	0.46
3:E:46:LEU:HD21	3:E:49:TYR:HB3	1.97	0.46
3:L:132:LEU:HB2	3:L:178:LEU:HB3	1.97	0.46
1:F:136:THR:O	1:F:145:LYS:HB3	2.15	0.46
2:H:150:VAL:HG12	2:H:200:HIS:CD2	2.51	0.46
1:C:202:VAL:HB	1:C:213:PHE:HB2	1.98	0.45
3:L:52:ILE:HG22	3:L:64:GLY:O	2.17	0.45
2:H:209:LYS:HD2	2:H:209:LYS:HA	1.76	0.45
1:F:159:ASN:OD1	3:L:56:SER:HB3	2.17	0.45
1:F:108:LEU:HB2	1:F:234:TRP:CE2	2.52	0.45
2:H:100(C):ARG:HB3	3:L:34:HIS:CE1	2.52	0.45
3:L:40:PRO:HD2	3:L:166:LYS:HE2	1.99	0.45
1:F:177:LEU:HB3	1:F:258:PHE:HB2	1.98	0.45
2:D:35(A):LEU:HD13	2:D:78:VAL:HG21	1.97	0.45
2:H:35(B):THR:HG23	2:H:47:TRP:HE1	1.82	0.45
2:D:83:ASP:HB3	2:D:85:VAL:HG22	1.99	0.44
3:E:13:VAL:HG11	3:E:19:ALA:HA	1.98	0.44
3:L:51:ASP:OD1	3:L:66:ASN:ND2	2.45	0.44
1:F:123:LYS:NZ	1:F:133:ASN:OD1	2.37	0.44
2:H:117:LYS:HE2	2:H:118:GLY:O	2.17	0.44
1:C:145:LYS:NZ	3:E:32:ASN:OD1	2.26	0.44
1:C:159:ASN:OD1	3:E:56:SER:HB3	2.17	0.43
2:H:126:PRO:HD2	2:H:213:PRO:HA	1.99	0.43
1:C:65:ASN:HD21	1:C:67:ALA:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:LEU:HB3	2:D:100(C):ARG:NH2	2.33	0.43
2:D:123:PRO:HD3	2:D:209:LYS:HE3	1.99	0.43
3:E:122:SER:O	3:E:126:GLN:HG2	2.18	0.43
3:L:185:TRP:CE2	3:L:208:PRO:HB3	2.54	0.43
3:L:61:ARG:HB2	3:L:76:SER:O	2.18	0.43
2:H:100(B):GLY:HA3	3:L:91:TRP:CD1	2.54	0.43
2:H:73:THR:O	2:H:74:SER:HB3	2.18	0.43
3:L:144:VAL:HG12	3:L:197:HIS:HB2	2.01	0.43
1:F:145:LYS:NZ	3:L:29:GLY:O	2.48	0.43
3:E:11:VAL:O	3:E:104:LEU:HD12	2.19	0.43
1:C:231:ASN:N	1:C:231:ASN:OD1	2.51	0.43
3:E:167:GLN:HG2	3:E:171:LYS:O	2.18	0.43
2:H:123:PRO:HD3	2:H:209:LYS:HE2	2.01	0.43
1:F:133(A):LYS:HD2	3:L:52:ILE:HD12	2.01	0.43
3:E:36:TYR:HE2	3:E:89:GLN:HB3	1.83	0.42
2:H:29:LEU:HD23	2:H:71:LYS:HG3	2.01	0.42
9:D:622:HOH:O	5:B:2:NAG:H83	2.20	0.42
1:C:202:VAL:HG11	1:C:251:LEU:HD13	2.01	0.42
2:D:12:VAL:O	2:D:111:VAL:HA	2.18	0.42
3:E:124:GLU:HG2	3:E:129:LYS:HB2	2.02	0.42
1:F:105:TYR:CE2	1:F:109:ARG:HD2	2.54	0.42
1:C:146:SER:OG	1:C:147:PHE:N	2.51	0.41
2:D:168:ALA:HA	2:D:178:LEU:HB3	2.01	0.41
2:H:146:PHE:HA	2:H:147:PRO:HA	1.87	0.41
1:F:88:VAL:HG12	1:F:268:ILE:HB	2.02	0.41
3:E:49:TYR:HD2	3:E:50:THR:HG22	1.85	0.41
1:F:58:PRO:HB2	1:F:86:TYR:O	2.20	0.41
3:E:115:VAL:O	3:E:204:LYS:HD2	2.19	0.41
3:E:59:PRO:HG2	3:E:62:PHE:CD1	2.55	0.41
1:C:184:HIS:HB3	1:C:220:ARG:HH12	1.84	0.41
2:D:29:LEU:HD23	2:D:71:LYS:HD3	2.01	0.41
1:F:180:TRP:CE2	1:F:204:VAL:HG21	2.55	0.41
1:C:103:ILE:HD12	9:C:601:HOH:O	2.19	0.41
1:F:89:GLU:OE2	1:F:109:ARG:NH1	2.54	0.41
2:H:12:VAL:O	2:H:111:VAL:HA	2.21	0.41
3:L:59:PRO:HG2	3:L:62:PHE:CD1	2.56	0.41
3:E:13:VAL:HG21	3:E:19:ALA:HB2	2.03	0.40
2:H:101:ASP:HA	2:H:102:PRO:HA	1.87	0.40
1:F:175:GLU:OE2	1:F:262:ARG:HD3	2.21	0.40
3:L:13:VAL:HG21	3:L:19:ALA:HB2	2.03	0.40
1:F:66:ILE:HD12	1:F:109:ARG:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:LEU:HA	1:F:154:LEU:HD23	1.83	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	C	215/505 (43%)	204 (95%)	10 (5%)	1 (0%)	29	43
1	F	217/505 (43%)	204 (94%)	11 (5%)	2 (1%)	17	26
2	D	222/227 (98%)	204 (92%)	15 (7%)	3 (1%)	11	16
2	H	222/227 (98%)	211 (95%)	8 (4%)	3 (1%)	11	16
3	E	207/211 (98%)	197 (95%)	10 (5%)	0	100	100
3	L	208/211 (99%)	199 (96%)	7 (3%)	2 (1%)	15	23
All	All	1291/1886 (68%)	1219 (94%)	61 (5%)	11 (1%)	17	26

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	43	LYS
2	D	82(B)	ASP
1	F	58	PRO
2	H	8	GLY
2	H	135	THR
3	L	151	ASP
2	H	74	SER
3	L	50	THR
2	D	8	GLY
1	C	91	SER
1	F	90(A)	PRO

### 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	C	188/440 (43%)	181 (96%)	7 (4%)	34	50
1	F	189/440 (43%)	184 (97%)	5 (3%)	46	64
2	D	196/199 (98%)	189 (96%)	7 (4%)	35	51
2	H	196/199 (98%)	192 (98%)	4 (2%)	55	73
3	E	176/178 (99%)	171 (97%)	5 (3%)	43	61
3	L	177/178 (99%)	176 (99%)	1 (1%)	86	92
All	All	1122/1634 (69%)	1093 (97%)	29 (3%)	46	64

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	59	LEU
1	F	76	CYS
1	F	87	ILE
1	F	89	GLU
1	F	141	HIS
2	H	57	LYS
2	H	100	LEU
2	H	100(C)	ARG
2	H	164	HIS
3	L	50	THR
1	C	60	HIS
1	C	61	LEU
1	C	87	ILE
1	C	129	ASN
1	C	133	ASN
1	C	225	ASP
1	C	231	ASN
2	D	35(A)	LEU
2	D	72	ASP
2	D	100(C)	ARG
2	D	116	THR
2	D	131	THR

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Mol	Chain	Res	Type
2	D	164	HIS
2	D	204	ASN
3	E	30	ILE
3	E	110	LYS
3	E	117	LEU
3	E	155	VAL
3	E	209	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	192	GLN
3	L	32	ASN
1	C	192	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](#)

5 monosaccharides 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	1	2,4	14,14,15	0.27	0	17,19,21	0.51	0
4	NAG	A	2	4	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	B	1	2,5	14,14,15	0.20	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	2	5	14,14,15	1.31	2 (14%)	17,19,21	2.59	4 (23%)
5	MAN	B	3	5	11,11,12	1.66	4 (36%)	15,15,17	1.78	3 (20%)

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	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
5	NAG	B	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2	5	-	2/6/23/26	0/1/1/1
5	MAN	B	3	5	-	1/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2	NAG	C1-C2	3.65	1.57	1.52
5	B	2	NAG	O5-C1	3.13	1.48	1.43
5	B	3	MAN	C4-C5	3.10	1.59	1.53
5	B	3	MAN	O2-C2	2.26	1.48	1.43
5	B	3	MAN	C4-C3	2.22	1.58	1.52
5	B	3	MAN	C1-C2	2.09	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2	NAG	C1-O5-C5	6.87	121.50	112.19
5	B	2	NAG	O4-C4-C5	5.94	124.06	109.30
5	B	3	MAN	O5-C5-C6	-4.51	100.14	107.20
5	B	2	NAG	C3-C4-C5	-3.95	103.19	110.24
5	B	3	MAN	O2-C2-C1	3.21	115.72	109.15
5	B	3	MAN	C1-O5-C5	2.55	115.65	112.19
5	B	2	NAG	O5-C5-C4	-2.06	105.81	110.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2	NAG	C8-C7-N2-C2
5	B	2	NAG	O7-C7-N2-C2
4	A	2	NAG	C4-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6
5	B	3	MAN	O5-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3	MAN	1	0
5	B	2	NAG	2	0

## 5.6 Ligand geometry [i](#)

7 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	$\# Z  > 2$
8	GOL	D	504	-	5,5,5	0.91	0	5,5,5	1.01	0
8	GOL	H	503	-	5,5,5	0.92	0	5,5,5	1.03	0
6	NAG	F	601	1	14,14,15	0.36	0	17,19,21	0.46	0
7	SO4	F	602	-	4,4,4	0.14	0	6,6,6	0.06	0
7	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.08	0
7	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.08	0
7	SO4	E	301	-	4,4,4	0.14	0	6,6,6	0.07	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
8	GOL	D	504	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	H	503	-	-	2/4/4/4	-
6	NAG	F	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	503	GOL	O1-C1-C2-C3
8	D	504	GOL	O2-C2-C3-O3
8	D	504	GOL	C1-C2-C3-O3
8	H	503	GOL	O1-C1-C2-O2
8	D	504	GOL	O1-C1-C2-C3

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	C	217/505 (42%)	0.90	38 (17%) <b>1</b> <b>1</b>	52, 82, 159, 194	6 (2%)
1	F	219/505 (43%)	0.67	25 (11%) <b>5</b> <b>3</b>	41, 71, 134, 180	6 (2%)
2	D	224/227 (98%)	0.03	2 (0%) <b>84</b> <b>83</b>	31, 54, 100, 166	0
2	H	224/227 (98%)	0.02	4 (1%) <b>68</b> <b>65</b>	29, 55, 98, 143	0
3	E	209/211 (99%)	-0.02	1 (0%) <b>91</b> <b>91</b>	36, 54, 77, 117	0
3	L	210/211 (99%)	-0.01	4 (1%) <b>66</b> <b>63</b>	33, 53, 84, 153	0
All	All	1303/1886 (69%)	0.26	74 (5%) <b>23</b> <b>20</b>	29, 61, 117, 194	12 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	266	SER	9.3
1	F	57	ALA	9.1
1	F	268	ILE	9.0
1	C	266(A)	GLY	8.3
1	F	266	SER	8.1
1	C	90(A)	PRO	8.1
1	C	265	GLY	7.3
1	F	267	ILE	6.7
1	C	267	ILE	6.3
1	C	93	ASP	5.9
1	C	268	ILE	5.6
1	C	60	HIS	5.1
1	F	264	ALA	4.9
1	C	90	THR	4.7
1	C	263	ASN	4.7
1	F	81	THR	4.6
1	C	78	SER	4.6
1	F	58	PRO	4.5
1	F	87	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	90(A)	PRO	4.3
2	D	130	SER	4.3
1	C	80	SER	4.2
2	H	132	SER	4.2
1	F	79	LEU	4.1
1	F	265	GLY	4.1
1	C	86	TYR	4.0
1	F	59	LEU	4.0
1	C	63	LYS	3.8
2	D	131	THR	3.8
1	C	59	LEU	3.8
2	H	75	LYS	3.6
2	H	74	SER	3.6
1	F	114	SER	3.5
1	C	116	SER	3.5
1	C	143	GLY	3.5
1	C	77	GLU	3.4
1	C	264	ALA	3.4
1	F	80	SER	3.4
3	L	210	GLU	3.4
1	C	94	ASN	3.1
1	F	63	LYS	3.1
1	C	159	ASN	3.1
1	C	203	PHE	3.1
1	C	112	LEU	3.1
1	F	85	SER	3.0
1	C	81	THR	3.0
1	F	263	ASN	2.9
1	C	85	SER	2.8
1	C	88	VAL	2.8
1	C	205	GLY	2.8
1	C	91	SER	2.7
3	L	25	GLY	2.7
1	F	82	ALA	2.7
1	F	88	VAL	2.5
1	C	207	SER	2.5
1	F	78	SER	2.5
1	C	74	PRO	2.5
1	C	115	VAL	2.5
1	C	92	SER	2.5
3	L	209	THR	2.4
1	C	238	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	1	GLN	2.3
1	C	116(C)	GLU	2.3
1	F	116(B)	PHE	2.3
1	F	86	TYR	2.2
1	C	69	TRP	2.2
1	F	266(A)	GLY	2.2
1	C	116(B)	PHE	2.2
3	L	183	GLU	2.2
1	C	75	GLU	2.1
3	E	60	GLU	2.1
1	C	102	PHE	2.1
1	F	60	HIS	2.0
1	F	93	ASP	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](#)

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	MAN	B	3	11/12	0.63	0.25	89,92,98,99	0
5	NAG	B	2	14/15	0.78	0.27	79,84,95,97	0
4	NAG	A	1	14/15	0.85	0.19	63,70,78,78	0
4	NAG	A	2	14/15	0.87	0.27	83,88,91,94	0
5	NAG	B	1	14/15	0.95	0.15	41,48,60,69	0

## 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( $\text{\AA}^2$ )	Q<0.9
8	GOL	H	503	6/6	0.82	0.23	55,60,61,63	0
7	SO4	D	505	5/5	0.85	0.28	122,124,125,128	0
6	NAG	F	601	14/15	0.88	0.25	57,68,76,78	0
8	GOL	D	504	6/6	0.88	0.20	65,70,71,72	0
7	SO4	L	301	5/5	0.89	0.23	105,106,106,108	0
7	SO4	F	602	5/5	0.94	0.14	90,92,92,93	0
7	SO4	E	301	5/5	0.95	0.19	92,92,93,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.