



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 07:52 PM EDT

PDB ID : 8EEO  
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing human antibodies WRAIR-2063 and WRAIR-2151  
Authors : Jensen, J.L.; Sankhala, R.S.; Joyce, M.G.  
Deposited on : 2022-10-03  
Resolution : 2.77 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 : 2.36  
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) : 2.36

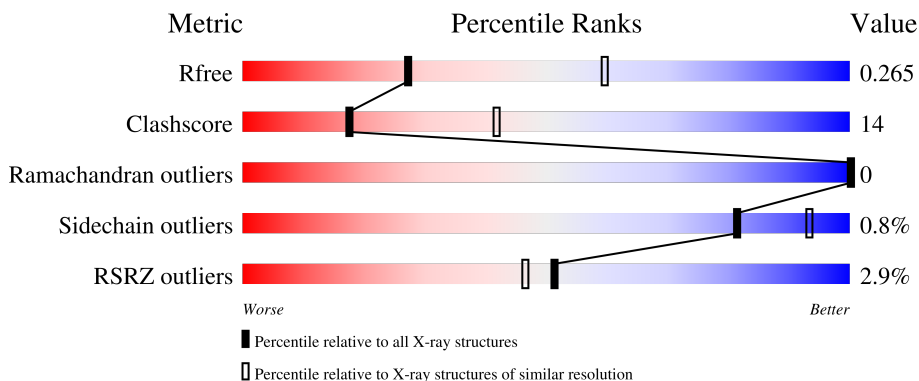
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	A	223	 3% 69% 29%
1	F	223	 4% 66% 31%
2	B	216	 % 77% 21%
2	K	216	 5% 70% 28%
3	C	205	 3% 74% 21%

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Mol	Chain	Length	Quality of chain
3	D	205	
4	E	227	
4	H	227	
5	J	219	
5	L	219	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	B	301	-	-	-	X
6	GOL	D	602	-	-	-	X
6	GOL	K	301	-	-	-	X

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 16527 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 WRAIR-2151 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	Total 1639	C 1046	N 267	O 322	S 4	0	0	0
1	F	217	Total 1633	C 1043	N 266	O 320	S 4	0	0	0

- Molecule 2 is a protein called WRAIR-2151 antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	Total 1609	C 1001	N 268	O 335	S 5	0	0	0
2	K	214	Total 1618	C 1006	N 269	O 338	S 5	0	0	0

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	196	Total 1546	C 990	N 258	O 290	S 8	0	0	0
3	D	197	Total 1555	C 997	N 259	O 291	S 8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	528	GLY	-	expression tag	UNP P0DTC2
C	529	SER	-	expression tag	UNP P0DTC2
C	530	HIS	-	expression tag	UNP P0DTC2
C	531	HIS	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	528	GLY	-	expression tag	UNP P0DTC2
D	529	SER	-	expression tag	UNP P0DTC2
D	530	HIS	-	expression tag	UNP P0DTC2
D	531	HIS	-	expression tag	UNP P0DTC2
D	532	HIS	-	expression tag	UNP P0DTC2
D	533	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2
D	535	HIS	-	expression tag	UNP P0DTC2

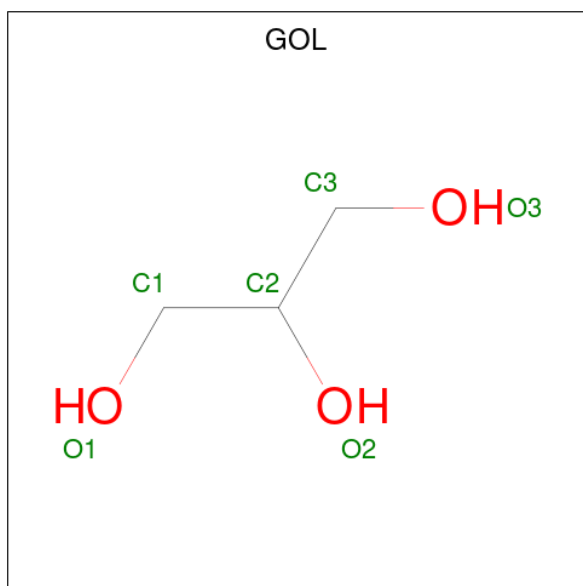
- Molecule 4 is a protein called WRAIR-2063 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	226	Total	C	N	O	S	0	0	0
			1704	1078	287	332	7			
4	H	226	Total	C	N	O	S	0	0	0
			1704	1078	287	332	7			

- Molecule 5 is a protein called WRAIR-2063 antibody Fab light chain.

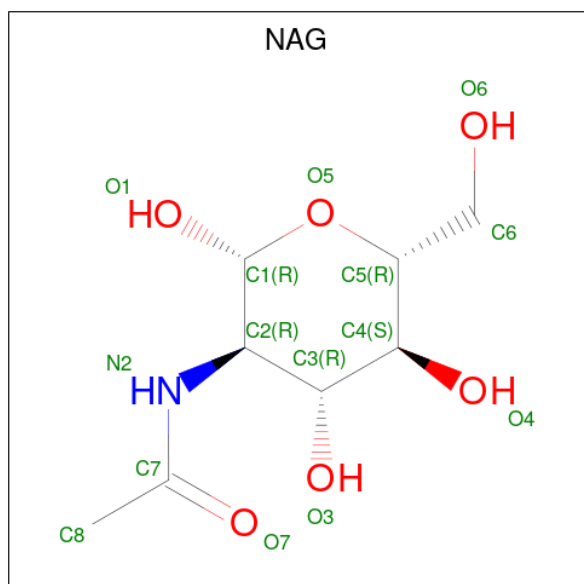
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	J	219	Total	C	N	O	S	0	0	0
			1692	1055	291	339	7			
5	L	218	Total	C	N	O	S	0	0	0
			1686	1052	290	338	6			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	K	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total	O	0	0
			7	7		

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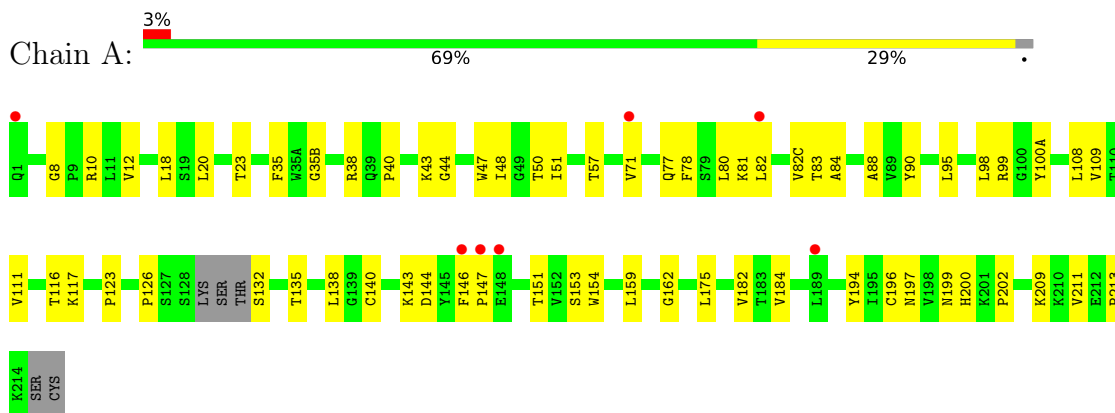
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
8	B	8	Total O 8 8	0	0
8	C	5	Total O 5 5	0	0
8	D	6	Total O 6 6	0	0
8	E	10	Total O 10 10	0	0
8	F	6	Total O 6 6	0	0
8	H	9	Total O 9 9	0	0
8	J	11	Total O 11 11	0	0
8	K	8	Total O 8 8	0	0
8	L	7	Total O 7 7	0	0

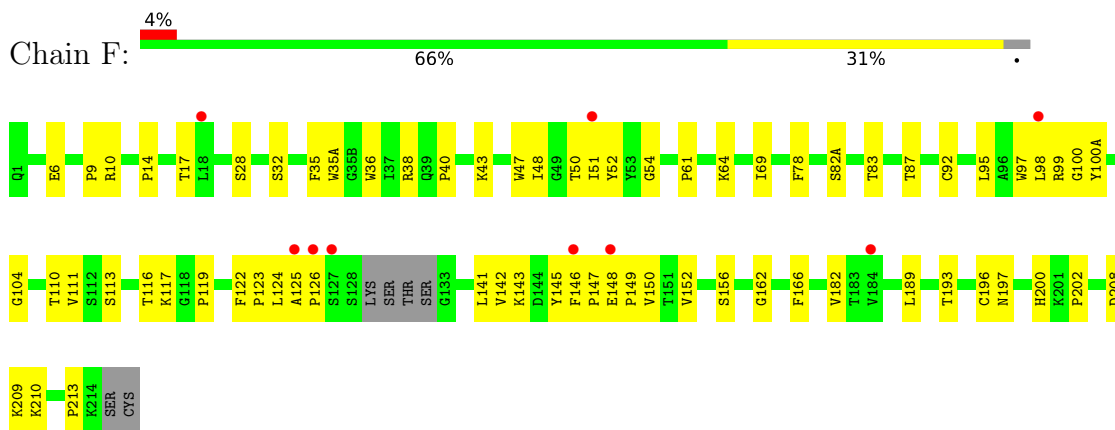
### 3 Residue-property plots [i](#)

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.

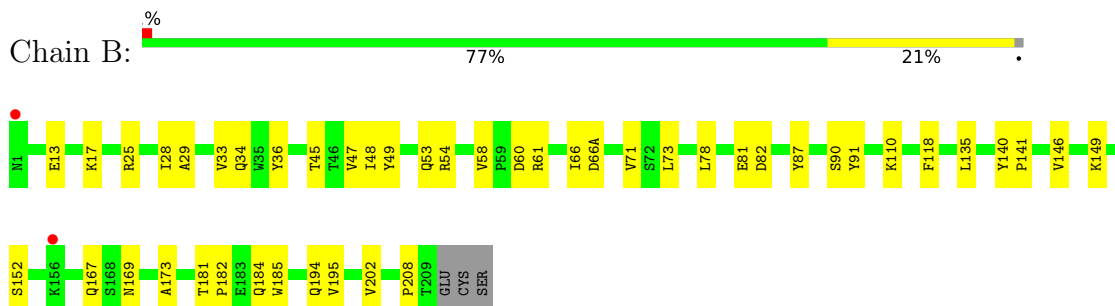
- Molecule 1: WRAIR-2151 antibody Fab heavy chain



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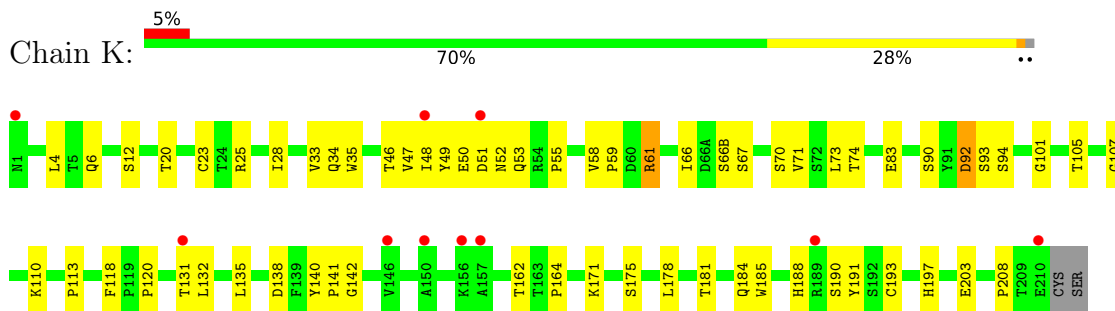


- Molecule 2: WRAIR-2151 antibody Fab light chain

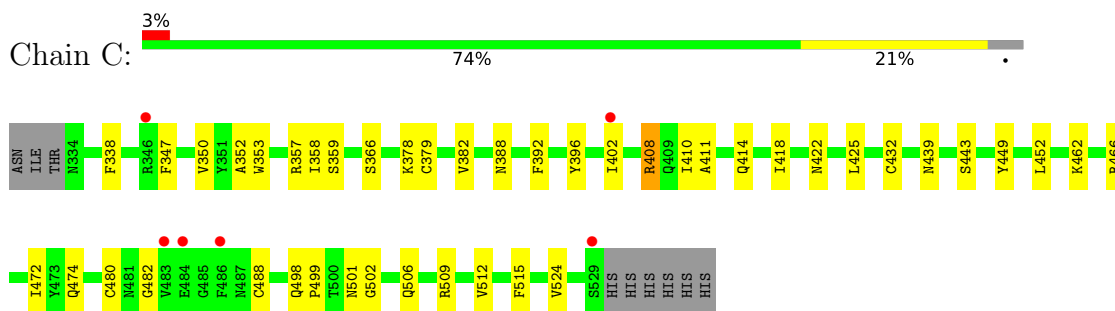




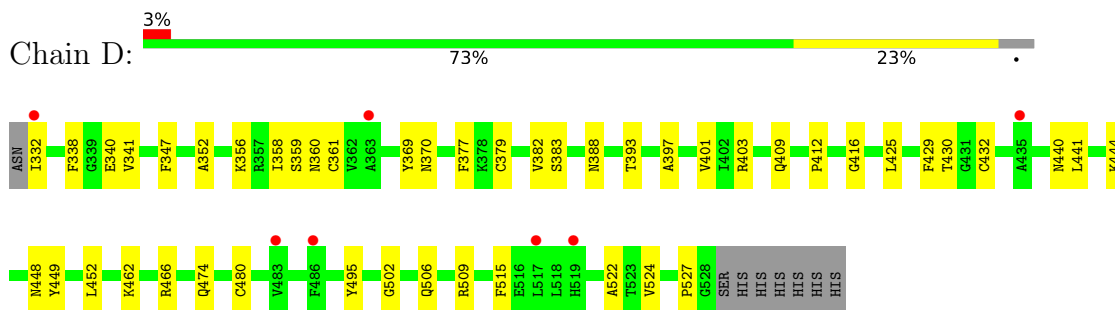
- Molecule 2: WRAIR-2151 antibody Fab light chain



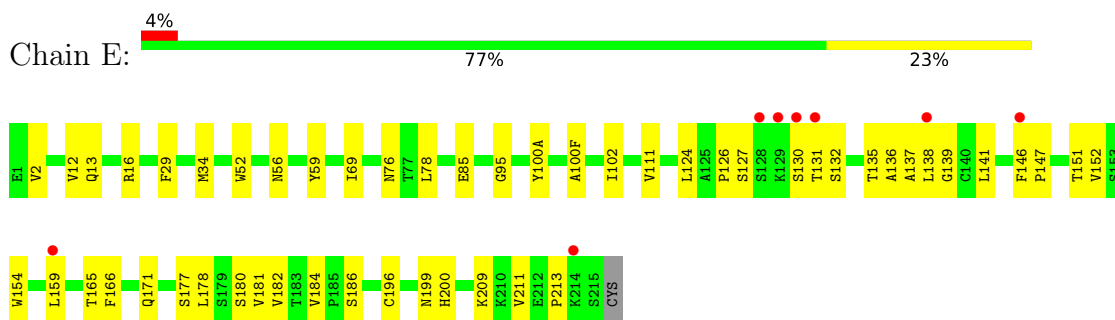
- Molecule 3: Spike protein S1



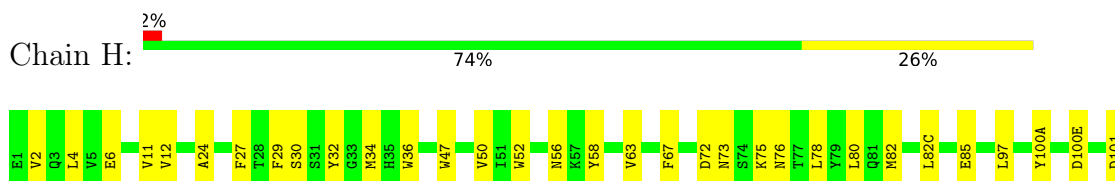
- Molecule 3: Spike protein S1



- Molecule 4: WRAIR-2063 antibody Fab heavy chain

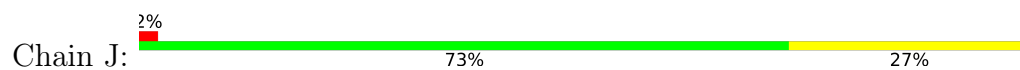


- Molecule 4: WRAIR-2063 antibody Fab heavy chain





- Molecule 5: WRAIR-2063 antibody Fab light chain



- Molecule 5: WRAIR-2063 antibody Fab light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.07Å 97.41Å 141.13Å 90.00° 99.76° 90.00°	Depositor
Resolution (Å)	19.95 – 2.77 139.09 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.95-2.77) 88.5 (139.09-2.76)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.54 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.194 , 0.255 0.218 , 0.265	Depositor DCC
$R_{free}$ test set	1986 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.8	Xtrriage
Anisotropy	0.309	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.43	0/1683	0.63	0/2301
1	F	0.43	0/1677	0.69	0/2293
2	B	0.46	0/1649	0.62	0/2253
2	K	0.44	0/1658	0.63	0/2265
3	C	0.51	0/1590	0.64	0/2164
3	D	0.47	0/1599	0.66	0/2177
4	E	0.49	0/1748	0.69	0/2380
4	H	0.48	0/1748	0.70	0/2380
5	J	0.50	0/1729	0.70	0/2344
5	L	0.50	0/1723	0.70	0/2336
All	All	0.47	0/16804	0.67	0/22893

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1639	0	1606	51	0
1	F	1633	0	1601	73	0
2	B	1609	0	1540	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1618	0	1546	51	0
3	C	1546	0	1462	34	0
3	D	1555	0	1473	38	0
4	E	1704	0	1656	38	0
4	H	1704	0	1656	44	0
5	J	1692	0	1644	52	0
5	L	1686	0	1639	54	0
6	B	12	0	16	0	0
6	D	6	0	8	3	0
6	F	6	0	8	0	0
6	K	6	0	8	1	0
6	L	6	0	8	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
8	A	7	0	0	0	0
8	B	8	0	0	0	0
8	C	5	0	0	0	0
8	D	6	0	0	0	0
8	E	10	0	0	0	0
8	F	6	0	0	0	0
8	H	9	0	0	0	0
8	J	11	0	0	0	0
8	K	8	0	0	0	0
8	L	7	0	0	0	0
All	All	16527	0	15897	442	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 14.

All (442) 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)
3:C:480:CYS:SG	3:C:488:CYS:SG	1.44	1.38
3:D:332:ILE:HD12	3:D:361:CYS:N	1.62	1.12
1:A:51:ILE:HG13	1:A:57:THR:HG22	1.31	1.07
1:F:51:ILE:HG21	1:F:69:ILE:CG2	1.86	1.05
1:F:126:PRO:HG3	1:F:213:PRO:HA	1.39	1.03
1:F:51:ILE:HG21	1:F:69:ILE:HG22	1.44	0.96
1:A:71:VAL:HG12	1:A:78:PHE:HB3	1.47	0.96
1:A:98:LEU:HD23	1:A:99:ARG:HG3	1.49	0.95
1:A:71:VAL:HG12	1:A:78:PHE:CB	1.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:LEU:HD12	1:F:98:LEU:O	1.70	0.91
5:J:9:LEU:HG	5:J:10:SER:H	1.41	0.85
3:D:332:ILE:HD12	3:D:361:CYS:CA	2.06	0.84
3:D:462:LYS:HB2	5:J:94:TRP:CD1	2.12	0.84
4:E:127:SER:HB2	4:E:130:SER:HB2	1.62	0.81
1:F:51:ILE:CG2	1:F:69:ILE:HG21	2.11	0.81
5:J:36:PHE:HZ	5:J:89:MET:HE1	1.45	0.81
3:D:332:ILE:CD1	3:D:361:CYS:N	2.42	0.80
1:F:51:ILE:CG2	1:F:69:ILE:CG2	2.61	0.79
1:F:51:ILE:HG21	1:F:69:ILE:HG21	1.66	0.78
1:F:47:TRP:HE1	1:F:50:THR:HG23	1.49	0.77
1:A:51:ILE:HG13	1:A:57:THR:CG2	2.14	0.76
3:D:338:PHE:HE1	3:D:358:ILE:HD13	1.53	0.74
4:H:152:VAL:HG22	4:H:198:VAL:HG22	1.68	0.73
1:A:47:TRP:HE1	1:A:50:THR:HG23	1.52	0.73
4:H:171:GLN:NE2	4:H:177:SER:HB2	2.03	0.72
2:K:47:VAL:O	2:K:48:ILE:HD13	1.90	0.71
4:H:147:PRO:HD2	4:H:200:HIS:CE1	2.26	0.71
4:H:147:PRO:HD2	4:H:200:HIS:HE1	1.54	0.71
3:C:410:ILE:O	3:C:425:LEU:HD12	1.91	0.70
5:J:8:PRO:HG2	5:J:21:ILE:HA	1.73	0.70
2:B:48:ILE:HD12	2:B:73:LEU:HD13	1.73	0.70
1:F:156:SER:H	1:F:197:ASN:ND2	1.90	0.70
1:A:100(A):TYR:HB3	2:B:34:GLN:HG2	1.73	0.70
1:A:51:ILE:CG1	1:A:57:THR:HG22	2.17	0.70
5:J:9:LEU:HG	5:J:10:SER:N	2.05	0.70
5:J:9:LEU:O	5:J:102:THR:HG23	1.92	0.69
4:H:34:MET:HB3	4:H:78:LEU:HD22	1.73	0.69
4:E:165:THR:HG22	4:E:178:LEU:HD21	1.73	0.69
3:C:462:LYS:HB2	5:L:94:TRP:CD1	2.28	0.69
2:K:101:GLY:HA3	6:K:301:GOL:H2	1.75	0.69
4:E:136:ALA:HB2	4:E:186:SER:HA	1.74	0.68
5:L:108:ARG:HG3	5:L:171:SER:HB2	1.74	0.68
3:C:480:CYS:CB	3:C:488:CYS:HG	2.00	0.68
2:B:13:GLU:HG3	2:B:17:LYS:HB2	1.76	0.68
4:H:114:ALA:HB3	4:H:146:PHE:CD1	2.28	0.68
1:A:71:VAL:HG12	1:A:78:PHE:HB2	1.76	0.68
5:J:8:PRO:HB2	5:J:102:THR:HG21	1.75	0.68
2:K:34:GLN:HG3	2:K:49:TYR:HA	1.76	0.68
1:F:100(A):TYR:HB3	2:K:34:GLN:HG2	1.76	0.67
3:D:440:ASN:OD1	3:D:441:LEU:HG	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:138:LEU:HG	4:E:211:VAL:HG11	1.76	0.67
1:A:18:LEU:HD11	1:A:109:VAL:HG21	1.74	0.67
1:F:97:TRP:CH2	1:F:99:ARG:HA	2.29	0.67
2:B:48:ILE:HD12	2:B:73:LEU:CD1	2.25	0.67
1:F:35:PHE:CD1	1:F:97:TRP:HB2	2.29	0.66
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.77	0.66
5:J:36:PHE:CZ	5:J:89:MET:HE1	2.30	0.66
5:J:141:PRO:HD2	5:J:198:HIS:CE1	2.30	0.65
5:J:8:PRO:HB2	5:J:102:THR:CG2	2.27	0.64
5:L:35:TRP:HB2	5:L:48:ILE:HB	1.79	0.63
4:E:2:VAL:HG11	4:E:102:ILE:HD13	1.79	0.63
3:D:370:ASN:OD1	1:F:97:TRP:HB3	1.98	0.63
2:B:28:ILE:HG12	2:B:71:VAL:HG13	1.82	0.62
4:H:130:SER:HA	5:L:116:PHE:HD1	1.66	0.61
2:B:34:GLN:HG3	2:B:49:TYR:HA	1.81	0.61
4:H:52:TRP:CD1	4:H:56:ASN:HB2	2.35	0.61
1:F:17:THR:HG22	1:F:82(A):SER:HA	1.81	0.61
1:A:38:ARG:HB3	1:A:48:ILE:HD11	1.83	0.61
4:E:138:LEU:CD2	4:E:154:TRP:CH2	2.85	0.60
2:B:118:PHE:HE2	2:B:135:LEU:HD12	1.65	0.60
1:F:51:ILE:HG23	1:F:69:ILE:HG21	1.83	0.60
5:J:50:LYS:HB2	5:J:53:LYS:HG3	1.83	0.60
2:B:47:VAL:HA	2:B:58:VAL:HG21	1.84	0.60
3:D:338:PHE:CE1	3:D:358:ILE:HD13	2.36	0.60
2:K:140:TYR:HB3	2:K:141:PRO:HD3	1.84	0.60
1:F:38:ARG:HB3	1:F:48:ILE:HD11	1.83	0.60
1:F:35:PHE:HB2	1:F:95:LEU:HB3	1.83	0.60
1:A:138:LEU:CD1	1:A:211:VAL:CG1	2.81	0.59
1:A:138:LEU:HD11	1:A:211:VAL:CG1	2.33	0.59
1:A:138:LEU:HD12	1:A:211:VAL:HG11	1.84	0.59
3:D:332:ILE:HD12	3:D:360:ASN:C	2.22	0.59
3:D:370:ASN:HA	1:F:97:TRP:HD1	1.67	0.59
5:L:108:ARG:HB3	5:L:140:TYR:CG	2.38	0.59
1:F:98:LEU:HD12	1:F:98:LEU:C	2.22	0.59
5:L:120:PRO:HD3	5:L:132:VAL:HG22	1.84	0.59
3:D:370:ASN:HA	1:F:97:TRP:CD1	2.38	0.58
4:H:32:TYR:CE2	4:H:97:LEU:HB2	2.37	0.58
5:L:7:SER:HB3	5:L:22:SER:H	1.68	0.58
1:A:10:ARG:HH12	1:A:108:LEU:HB3	1.66	0.58
5:L:89:MET:SD	5:L:98:PHE:CE2	2.96	0.58
3:C:338:PHE:HE1	3:C:358:ILE:HD13	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:PRO:HG3	1:F:213:PRO:CA	2.26	0.58
5:L:151:ASP:HA	5:L:191:VAL:CG1	2.34	0.58
1:F:145:TYR:CE2	1:F:150:VAL:CG2	2.87	0.58
3:D:382:VAL:HG12	3:D:383:SER:O	2.03	0.58
2:K:52:ASN:C	2:K:52:ASN:OD1	2.42	0.58
3:D:430:THR:HB	6:D:602:GOL:H12	1.84	0.58
2:K:49:TYR:O	2:K:53:GLN:HB2	2.04	0.58
5:J:187:GLU:HG2	5:J:211:ARG:HH22	1.69	0.57
3:D:474:GLN:HG2	3:D:480:CYS:SG	2.44	0.57
1:F:145:TYR:CE2	1:F:150:VAL:HG21	2.39	0.57
5:J:33:LEU:HB3	5:J:51:VAL:HG22	1.86	0.57
2:K:59:PRO:HB2	2:K:61:ARG:HG3	1.86	0.57
4:H:50:VAL:HG12	4:H:58:TYR:HB2	1.85	0.57
2:K:110:LYS:HA	2:K:140:TYR:HB3	1.87	0.57
1:A:40:PRO:HB2	1:A:43:LYS:HD2	1.86	0.57
1:A:84:ALA:HA	1:A:111:VAL:HG23	1.85	0.57
5:J:36:PHE:CZ	5:J:89:MET:CE	2.87	0.57
1:A:126:PRO:HG3	1:A:138:LEU:HD13	1.87	0.56
1:F:40:PRO:HB2	1:F:43:LYS:HD2	1.87	0.56
5:J:36:PHE:HZ	5:J:89:MET:CE	2.16	0.56
2:B:61:ARG:NH1	2:B:82:ASP:OD2	2.32	0.56
4:E:136:ALA:HB3	4:E:184:VAL:HG23	1.88	0.56
5:L:141:PRO:HD2	5:L:198:HIS:CE1	2.40	0.56
4:H:147:PRO:HB2	4:H:202:PRO:HG2	1.88	0.56
5:L:108:ARG:HD3	5:L:140:TYR:HB2	1.88	0.55
2:K:66(B):SER:O	2:K:67:SER:HB2	2.07	0.55
4:E:181:VAL:HG21	5:J:135:LEU:HD22	1.89	0.55
3:D:430:THR:H	6:D:602:GOL:H31	1.72	0.55
4:E:131:THR:HG21	5:J:118:PHE:CE2	2.42	0.55
4:H:52:TRP:CG	4:H:56:ASN:HB2	2.42	0.55
5:J:34:ASN:OD1	5:J:46:ARG:HD2	2.07	0.55
2:B:181:THR:O	2:B:184:GLN:HG2	2.07	0.54
1:A:138:LEU:CD1	1:A:211:VAL:HG11	2.37	0.54
2:K:184:GLN:O	2:K:191:TYR:OH	2.26	0.54
2:K:185:TRP:CZ2	2:K:208:PRO:HA	2.42	0.54
1:F:152:VAL:HA	1:F:197:ASN:O	2.08	0.54
5:J:141:PRO:HD2	5:J:198:HIS:HE1	1.70	0.54
3:D:403:ARG:HD3	3:D:495:TYR:HE1	1.72	0.54
1:F:156:SER:H	1:F:197:ASN:HD21	1.52	0.54
2:K:33:VAL:HG11	2:K:71:VAL:HG21	1.89	0.54
2:B:167:GLN:OE1	2:B:173:ALA:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:TRP:HE1	1:F:50:THR:CG2	2.20	0.54
4:H:117:LYS:HD3	4:H:144:ASP:O	2.07	0.54
2:K:120:PRO:HB3	2:K:131:THR:H	1.73	0.54
4:H:72:ASP:OD2	4:H:75:LYS:HB2	2.08	0.54
1:F:98:LEU:O	1:F:98:LEU:CD1	2.49	0.53
2:K:49:TYR:HD1	2:K:55:PRO:HD3	1.74	0.53
2:B:149:LYS:HD3	2:B:152:SER:HA	1.91	0.53
2:B:33:VAL:HG11	2:B:71:VAL:HG21	1.89	0.53
5:J:51:VAL:O	5:J:64:GLY:HA3	2.07	0.53
3:C:366:SER:HB3	3:C:388:ASN:HD21	1.72	0.53
4:E:166:PHE:O	4:E:178:LEU:HG	2.09	0.53
5:J:7:SER:HB3	5:J:22:SER:HB3	1.91	0.53
5:J:35:TRP:CZ3	5:J:88:CYS:HB3	2.43	0.53
2:B:140:TYR:HB3	2:B:141:PRO:HD3	1.91	0.53
2:B:185:TRP:CZ2	2:B:208:PRO:HA	2.44	0.53
4:E:171:GLN:NE2	4:E:177:SER:HB2	2.24	0.52
1:A:35:PHE:HB2	1:A:95:LEU:HB3	1.90	0.52
1:A:44:GLY:HA2	2:B:87:TYR:OH	2.09	0.52
2:K:141:PRO:HD2	2:K:197:HIS:NE2	2.24	0.52
3:C:472:ILE:HG13	3:C:482:GLY:O	2.08	0.52
4:E:138:LEU:CD2	4:E:154:TRP:CZ3	2.92	0.52
1:F:166:PHE:CE2	2:K:135:LEU:HD22	2.44	0.52
1:A:126:PRO:HD2	1:A:213:PRO:HA	1.90	0.52
1:A:117:LYS:H	1:A:147:PRO:HD3	1.74	0.52
1:F:162:GLY:O	1:F:182:VAL:HA	2.09	0.52
2:K:47:VAL:HA	2:K:58:VAL:HG21	1.92	0.52
2:K:66:ILE:HG23	2:K:71:VAL:HG12	1.91	0.52
5:L:2:VAL:HG21	5:L:93:HIS:CG	2.44	0.52
4:E:29:PHE:CD2	4:E:76:ASN:HA	2.45	0.52
4:E:131:THR:HG22	5:J:116:PHE:HB3	1.92	0.52
2:B:13:GLU:CG	2:B:17:LYS:HB2	2.39	0.52
5:L:189:HIS:O	5:L:211:ARG:HD3	2.10	0.52
4:E:124:LEU:HD12	4:E:139:GLY:HA3	1.91	0.52
1:F:147:PRO:HB2	1:F:200:HIS:NE2	2.25	0.51
4:H:154:TRP:CZ3	4:H:196:CYS:HB3	2.45	0.51
2:B:33:VAL:HG22	2:B:90:SER:HB2	1.91	0.51
3:C:439:ASN:HD21	3:C:499:PRO:HA	1.73	0.51
4:H:85:GLU:H	4:H:85:GLU:CD	2.14	0.51
3:C:338:PHE:CE1	3:C:358:ILE:HD13	2.45	0.51
4:H:100(E):ASP:OD1	4:H:100(E):ASP:O	2.29	0.51
4:E:52:TRP:CG	4:E:56:ASN:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:52:ASN:OD1	2:K:53:GLN:HG2	2.11	0.51
3:D:340:GLU:OE1	3:D:356:LYS:HE2	2.11	0.51
4:E:95:GLY:HA2	4:E:100(F):ALA:HB1	1.92	0.51
5:J:145:LYS:HB3	5:J:197:THR:HB	1.92	0.51
3:C:347:PHE:CD2	3:C:509:ARG:HD3	2.46	0.51
3:C:439:ASN:O	3:C:443:SER:HB2	2.11	0.51
4:H:126:PRO:HG3	4:H:138:LEU:HD12	1.93	0.51
1:A:151:THR:OG1	1:A:199:ASN:HB3	2.10	0.51
1:F:193:THR:CG2	1:F:210:LYS:HE2	2.40	0.51
4:H:159:LEU:HD21	4:H:182:VAL:HG21	1.93	0.51
2:K:35:TRP:CE2	2:K:73:LEU:HB2	2.46	0.51
3:C:462:LYS:HG3	5:L:94:TRP:CG	2.45	0.51
1:F:200:HIS:CD2	1:F:202:PRO:HD2	2.46	0.51
4:H:36:TRP:NE1	4:H:80:LEU:HB2	2.26	0.51
1:F:83:THR:O	1:F:111:VAL:HG21	2.12	0.50
3:C:402:ILE:HD13	3:C:410:ILE:HD11	1.94	0.50
4:H:6:GLU:OE2	4:H:104:GLY:HA3	2.11	0.50
1:A:116:THR:HA	1:A:146:PHE:HD2	1.77	0.50
4:E:159:LEU:HD21	4:E:182:VAL:HG21	1.93	0.50
1:A:80:LEU:HD12	1:A:81:LYS:N	2.26	0.50
3:D:341:VAL:HG11	3:D:397:ALA:HB1	1.94	0.50
1:F:52:TYR:HD2	1:F:54:GLY:H	1.57	0.50
5:J:23:CYS:HB2	5:J:35:TRP:CH2	2.46	0.50
4:H:2:VAL:HG11	4:H:102:ILE:HD13	1.94	0.50
5:J:148:TRP:HB2	5:J:155:GLN:HB2	1.94	0.50
1:A:83:THR:O	1:A:111:VAL:HG21	2.12	0.50
1:F:47:TRP:NE1	1:F:50:THR:HG23	2.23	0.50
1:F:197:ASN:OD1	1:F:208:ASP:OD1	2.30	0.50
4:E:146:PHE:HB3	4:E:147:PRO:HD3	1.94	0.49
4:E:131:THR:HB	4:E:137:ALA:HB3	1.93	0.49
2:K:83:GLU:HG3	2:K:105:THR:HA	1.94	0.49
4:E:147:PRO:HD2	4:E:200:HIS:CE1	2.47	0.49
2:K:162:THR:HB	2:K:175:SER:H	1.77	0.49
2:B:167:GLN:HE21	2:B:169:ASN:HB2	1.77	0.49
1:F:117:LYS:H	1:F:147:PRO:HD3	1.77	0.49
3:C:352:ALA:HB1	3:C:466:ARG:HH21	1.78	0.49
1:F:141:LEU:HG	1:F:143:LYS:HG3	1.94	0.49
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.48	0.49
2:K:188:HIS:O	2:K:208:PRO:HG3	2.13	0.49
2:B:66:ILE:O	2:B:66(A):ASP:OD1	2.30	0.49
2:B:195:VAL:HB	2:B:202:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:4:LEU:HD12	4:H:102:ILE:HG22	1.94	0.48
4:H:12:VAL:O	4:H:111:VAL:HA	2.13	0.48
4:H:134:GLY:O	4:H:135:THR:HG23	2.13	0.48
5:J:9:LEU:CG	5:J:10:SER:H	2.18	0.48
5:L:9:LEU:O	5:L:103:LYS:N	2.46	0.48
1:A:162:GLY:O	1:A:182:VAL:HA	2.13	0.48
2:B:146:VAL:HA	2:B:194:GLN:O	2.13	0.48
5:J:2:VAL:HG21	5:J:93:HIS:CG	2.48	0.48
5:J:94:TRP:HA	5:J:94:TRP:CE3	2.48	0.48
5:J:187:GLU:HA	5:J:211:ARG:HH22	1.78	0.48
4:E:52:TRP:N	4:E:52:TRP:CD1	2.82	0.48
5:J:108:ARG:NH2	5:J:111:ALA:HB2	2.28	0.48
5:J:187:GLU:HA	5:J:211:ARG:NH2	2.29	0.48
1:A:23:THR:HG22	1:A:77:GLN:OE1	2.12	0.48
3:D:332:ILE:HD13	3:D:360:ASN:HA	1.95	0.48
5:J:124:GLN:HG2	5:J:129:THR:O	2.14	0.48
4:E:34:MET:HB3	4:E:78:LEU:HD22	1.95	0.48
1:A:98:LEU:HD21	2:B:91:TYR:CE2	2.49	0.48
1:F:35:PHE:CE1	1:F:97:TRP:HB2	2.49	0.48
3:C:359:SER:HA	3:C:524:VAL:HG22	1.96	0.47
5:J:48:ILE:HG21	5:J:51:VAL:O	2.14	0.47
1:F:51:ILE:HD13	1:F:69:ILE:CG2	2.43	0.47
2:K:25:ARG:HB2	2:K:28:ILE:HD13	1.96	0.47
1:A:154:TRP:CH2	1:A:196:CYS:HB3	2.49	0.47
3:C:462:LYS:HG3	5:L:94:TRP:CD1	2.49	0.47
1:F:87:THR:HG23	1:F:110:THR:HA	1.96	0.47
4:H:50:VAL:CG1	4:H:58:TYR:HB2	2.44	0.47
3:D:382:VAL:HG12	3:D:383:SER:N	2.30	0.47
1:F:100:GLY:O	2:K:34:GLN:NE2	2.48	0.47
5:J:89:MET:SD	5:J:98:PHE:CE2	3.08	0.47
3:D:403:ARG:HD3	3:D:495:TYR:CE1	2.50	0.47
4:E:151:THR:OG1	4:E:199:ASN:HB3	2.15	0.47
1:F:61:PRO:HA	1:F:64:LYS:HG3	1.96	0.47
5:L:151:ASP:OD1	5:L:191:VAL:HG12	2.15	0.47
1:A:8:GLY:HA3	1:A:20:LEU:HD23	1.97	0.47
1:A:80:LEU:HD12	1:A:81:LYS:H	1.79	0.46
2:K:49:TYR:O	2:K:50:GLU:HB2	2.16	0.46
5:L:193:ALA:HB2	5:L:208:SER:HB3	1.96	0.46
4:E:132:SER:O	4:E:135:THR:O	2.33	0.46
1:F:28:SER:O	1:F:32:SER:HB3	2.14	0.46
1:F:145:TYR:CE2	1:F:150:VAL:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:THR:HG23	1:F:210:LYS:HE2	1.96	0.46
5:L:184:ALA:O	5:L:188:LYS:HG3	2.15	0.46
3:D:412:PRO:HG3	3:D:429:PHE:HB3	1.97	0.46
1:F:116:THR:HG23	1:F:147:PRO:HG2	1.97	0.46
5:J:147:GLN:O	5:J:194:CYS:HA	2.16	0.46
2:K:73:LEU:HD12	2:K:74:THR:N	2.30	0.46
5:L:108:ARG:HB3	5:L:140:TYR:CD1	2.51	0.46
5:L:136:LEU:HB3	5:L:139:PHE:CE1	2.50	0.46
3:C:350:VAL:O	3:C:353:TRP:HD1	1.99	0.46
5:J:8:PRO:CG	5:J:21:ILE:HA	2.45	0.46
5:L:163:VAL:HG22	5:L:164:THR:N	2.31	0.46
5:J:108:ARG:HD2	5:J:170:ASP:O	2.15	0.46
1:F:97:TRP:CE3	1:F:97:TRP:HA	2.50	0.46
1:A:12:VAL:O	1:A:111:VAL:HA	2.16	0.46
3:D:401:VAL:HG22	3:D:509:ARG:HG2	1.98	0.46
3:D:388:ASN:HD22	3:D:527:PRO:HD2	1.81	0.45
1:F:156:SER:N	1:F:197:ASN:HD21	2.13	0.45
3:C:408:ARG:HH11	3:C:408:ARG:HB2	1.80	0.45
1:A:143:LYS:HB3	1:A:143:LYS:HE3	1.76	0.45
2:B:29:ALA:O	3:C:378:LYS:HE3	2.15	0.45
4:H:130:SER:HA	5:L:116:PHE:CD1	2.49	0.45
2:K:35:TRP:CD2	2:K:73:LEU:HB2	2.50	0.45
5:L:94:TRP:CE3	5:L:94:TRP:HA	2.50	0.45
5:L:136:LEU:HD21	5:L:196:VAL:HG13	1.98	0.45
1:A:132:SER:HB2	1:A:135:THR:OG1	2.17	0.45
3:D:393:THR:HA	3:D:522:ALA:HA	1.97	0.45
4:E:138:LEU:HD23	4:E:154:TRP:CH2	2.51	0.45
3:D:379:CYS:HA	3:D:432:CYS:HA	1.99	0.45
1:F:9:PRO:O	1:F:10:ARG:HB2	2.17	0.45
1:F:147:PRO:HD2	1:F:200:HIS:CE1	2.50	0.45
2:K:132:LEU:HD13	2:K:178:LEU:HD23	1.98	0.45
1:A:144:ASP:HB3	1:A:175:LEU:HD13	1.99	0.45
3:C:350:VAL:HG22	3:C:422:ASN:HB3	1.99	0.45
5:J:27(D):TYR:CG	5:J:27(E):SER:N	2.84	0.45
5:L:108:ARG:CD	5:L:140:TYR:HB2	2.47	0.45
5:J:146:VAL:HG12	5:J:196:VAL:HG22	1.98	0.45
3:C:379:CYS:HB3	3:C:382:VAL:HG23	1.98	0.45
4:E:209:LYS:HA	4:E:209:LYS:HD3	1.79	0.45
2:K:47:VAL:O	2:K:55:PRO:HD2	2.17	0.45
2:K:193:CYS:O	2:K:203:GLU:HA	2.16	0.45
3:C:418:ILE:HA	3:C:422:ASN:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:502:GLY:O	3:C:506:GLN:HG3	2.17	0.45
2:K:25:ARG:HH22	2:K:92:ASP:CG	2.21	0.45
3:C:357:ARG:HG3	3:C:396:TYR:CE2	2.52	0.44
3:C:474:GLN:HG2	3:C:480:CYS:SG	2.57	0.44
1:F:14:PRO:HD2	1:F:113:SER:OG	2.17	0.44
1:F:97:TRP:CZ3	1:F:99:ARG:HA	2.52	0.44
1:F:123:PRO:HG3	1:F:209:LYS:NZ	2.32	0.44
5:J:192:TYR:HB2	5:J:209:PHE:CZ	2.53	0.44
5:L:186:TYR:O	5:L:192:TYR:OH	2.36	0.44
1:A:123:PRO:HD3	1:A:209:LYS:HZ3	1.82	0.44
3:D:425:LEU:HD23	3:D:425:LEU:HA	1.85	0.44
4:H:52:TRP:CH2	4:H:100(A):TYR:CD1	3.05	0.44
3:D:444:LYS:HG2	3:D:448:ASN:HB2	1.99	0.44
3:D:515:PHE:O	6:D:602:GOL:H11	2.18	0.44
1:F:36:TRP:CZ3	1:F:92:CYS:HB3	2.53	0.44
5:J:142:ARG:HB2	5:J:173:TYR:CE2	2.53	0.44
5:L:124:GLN:O	5:L:127:SER:HB3	2.18	0.44
1:A:35(B):GLY:HA2	1:A:50:THR:HA	2.00	0.44
3:D:352:ALA:C	3:D:466:ARG:HE	2.21	0.44
4:H:143:LYS:HG2	4:H:144:ASP:N	2.32	0.44
5:J:34:ASN:HB2	5:J:89:MET:HE2	1.99	0.44
2:K:46:THR:HG22	2:K:55:PRO:HG3	1.99	0.44
5:L:54:ARG:NE	5:L:60:ASP:HA	2.32	0.44
2:K:20:THR:HG22	2:K:74:THR:OG1	2.18	0.44
3:C:411:ALA:O	3:C:414:GLN:HB2	2.17	0.43
1:F:100(A):TYR:CB	2:K:34:GLN:HG2	2.46	0.43
1:A:138:LEU:CD1	1:A:211:VAL:HG12	2.48	0.43
3:C:472:ILE:HG22	3:C:488:CYS:HB3	1.99	0.43
3:D:409:GLN:NE2	3:D:416:GLY:HA3	2.33	0.43
4:E:85:GLU:H	4:E:85:GLU:CD	2.21	0.43
1:F:35:PHE:CE1	1:F:52:TYR:CD1	3.06	0.43
5:L:3:VAL:HB	5:L:26:SER:HB3	2.00	0.43
5:L:27(D):TYR:CG	5:L:27(E):SER:N	2.86	0.43
1:A:18:LEU:HB3	1:A:82:LEU:HB3	2.00	0.43
2:B:54:ARG:NE	2:B:60:ASP:HA	2.34	0.43
1:F:35(A):TRP:HB3	1:F:78:PHE:CZ	2.53	0.43
5:J:37:GLN:HB2	5:J:47:LEU:HD11	2.00	0.43
2:K:23:CYS:O	2:K:70:SER:HA	2.19	0.43
5:L:48:ILE:HD13	5:L:54:ARG:HA	2.00	0.43
4:H:143:LYS:HG3	4:H:177:SER:OG	2.18	0.43
5:J:8:PRO:HG2	5:J:21:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:13:GLN:HB2	4:E:16:ARG:HD3	2.00	0.43
4:H:29:PHE:CD2	4:H:76:ASN:HA	2.54	0.43
5:L:108:ARG:CB	5:L:140:TYR:CD1	3.02	0.43
4:E:52:TRP:CD1	4:E:56:ASN:HB2	2.54	0.43
4:E:124:LEU:HD21	4:E:141:LEU:HB2	2.00	0.43
3:D:359:SER:HA	3:D:524:VAL:CG2	2.49	0.43
1:F:147:PRO:HB2	1:F:202:PRO:HG2	1.99	0.43
4:H:47:TRP:HB2	5:L:98:PHE:HE1	1.84	0.43
2:K:113:PRO:HD3	2:K:197:HIS:ND1	2.34	0.43
5:L:33:LEU:HA	5:L:89:MET:O	2.19	0.43
5:L:185:ASP:HA	5:L:188:LYS:HD2	2.01	0.43
3:C:379:CYS:HA	3:C:432:CYS:HA	1.99	0.43
4:E:52:TRP:HZ3	4:E:100(A):TYR:CD2	2.37	0.43
4:E:165:THR:CG2	4:E:178:LEU:HD21	2.44	0.43
3:C:425:LEU:HD21	3:C:512:VAL:HG11	2.01	0.42
1:F:124:LEU:HD21	1:F:141:LEU:HB2	2.01	0.42
1:F:125:ALA:HB3	2:K:118:PHE:HD1	1.84	0.42
4:H:24:ALA:HB1	4:H:27:PHE:CE1	2.54	0.42
1:A:88:ALA:HB3	1:A:90:TYR:CE1	2.54	0.42
1:F:189:LEU:HD23	1:F:189:LEU:HA	1.87	0.42
5:J:125:LEU:HD23	5:J:125:LEU:HA	1.86	0.42
2:K:4:LEU:HB3	2:K:23:CYS:SG	2.59	0.42
2:K:181:THR:OG1	2:K:184:GLN:HG2	2.20	0.42
3:D:502:GLY:O	3:D:506:GLN:HG3	2.20	0.42
2:K:190:SER:HA	2:K:208:PRO:HD3	2.01	0.42
5:L:108:ARG:NE	5:L:140:TYR:HB2	2.34	0.42
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.79	0.42
1:F:51:ILE:HD13	1:F:69:ILE:HG22	2.01	0.42
4:H:101:ASP:O	4:H:102:ILE:HG13	2.19	0.42
1:A:82(C):VAL:HG22	1:A:111:VAL:HG11	2.02	0.42
2:B:110:LYS:HA	2:B:140:TYR:HB3	2.01	0.42
5:J:6:GLN:HA	5:J:22:SER:O	2.19	0.42
5:L:139:PHE:HZ	5:L:175:LEU:HB2	1.83	0.42
3:D:347:PHE:CE2	3:D:509:ARG:HB3	2.55	0.42
2:K:73:LEU:HD12	2:K:74:THR:H	1.85	0.42
1:A:153:SER:OG	1:A:197:ASN:HB2	2.20	0.42
1:A:159:LEU:HD21	1:A:182:VAL:HG21	2.01	0.42
2:B:36:TYR:HA	2:B:45:THR:O	2.20	0.42
1:F:35:PHE:CE1	1:F:52:TYR:HD1	2.38	0.42
4:H:82:MET:HB3	4:H:82(C):LEU:HD21	2.02	0.42
5:L:47:LEU:HA	5:L:58:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:PRO:HB2	1:F:142:VAL:HG13	2.01	0.42
4:H:63:VAL:HB	4:H:67:PHE:CG	2.55	0.42
5:J:125:LEU:O	5:J:183:LYS:HD2	2.19	0.42
2:K:93:SER:OG	2:K:94:SER:N	2.53	0.42
5:L:6:GLN:HE21	5:L:6:GLN:HB3	1.66	0.42
1:F:146:PHE:HB3	1:F:147:PRO:HD3	2.01	0.41
5:J:6:GLN:HE21	5:J:6:GLN:HB3	1.68	0.41
5:L:37:GLN:CB	5:L:47:LEU:HD11	2.46	0.41
1:A:184:VAL:HG11	1:A:194:TYR:CE1	2.55	0.41
4:E:152:VAL:HG11	4:E:180:SER:CB	2.50	0.41
2:K:138:ASP:HA	2:K:171:LYS:HD3	2.00	0.41
5:L:50:LYS:O	5:L:52:SER:N	2.46	0.41
5:L:124:GLN:HG2	5:L:129:THR:O	2.20	0.41
2:B:81:GLU:H	2:B:81:GLU:HG2	1.72	0.41
5:J:9:LEU:O	5:J:102:THR:CG2	2.65	0.41
5:L:130:ALA:O	5:L:180:THR:HA	2.20	0.41
1:A:10:ARG:NH2	1:A:108:LEU:H	2.19	0.41
3:C:498:GLN:HB2	3:C:501:ASN:ND2	2.35	0.41
1:F:122:PHE:CD2	1:F:143:LYS:HD3	2.56	0.41
2:K:25:ARG:HB2	2:K:28:ILE:CD1	2.50	0.41
3:C:449:TYR:CD2	3:D:452:LEU:HD11	2.55	0.41
4:E:126:PRO:HG2	4:E:213:PRO:HB3	2.03	0.41
4:H:134:GLY:O	4:H:135:THR:CG2	2.69	0.41
5:L:13:VAL:HG21	5:L:78:VAL:HG11	2.01	0.41
3:C:392:PHE:CD1	3:C:515:PHE:HB3	2.55	0.41
3:C:462:LYS:HB2	5:L:94:TRP:NE1	2.35	0.41
4:H:30:SER:HA	4:H:73:ASN:ND2	2.36	0.41
4:H:138:LEU:HG	4:H:211:VAL:HG11	2.02	0.41
4:H:166:PHE:HE2	5:L:174:SER:O	2.04	0.41
5:L:34:ASN:HB2	5:L:89:MET:HE2	2.03	0.41
5:L:35:TRP:CE2	5:L:73:LEU:HB2	2.56	0.41
5:L:111:ALA:O	5:L:139:PHE:HA	2.20	0.41
1:A:35:PHE:CZ	1:A:98:LEU:HB2	2.55	0.41
4:E:154:TRP:CH2	4:E:196:CYS:HB3	2.55	0.41
1:F:6:GLU:OE2	1:F:104:GLY:HA3	2.21	0.41
4:H:27:PHE:CE2	4:H:29:PHE:HA	2.55	0.41
5:J:94:TRP:N	5:J:95:PRO:CD	2.84	0.41
2:K:28:ILE:HG12	2:K:71:VAL:HG13	2.03	0.41
3:D:369:TYR:HB3	3:D:377:PHE:CZ	2.56	0.41
4:E:12:VAL:O	4:E:111:VAL:HA	2.20	0.41
5:J:95:PRO:HB2	5:J:97:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ARG:HE	2:B:60:ASP:HA	1.86	0.40
2:B:181:THR:HG23	2:B:182:PRO:HD2	2.03	0.40
1:F:156:SER:N	1:F:197:ASN:ND2	2.64	0.40
4:H:2:VAL:HG13	4:H:27:PHE:CD1	2.56	0.40
2:K:185:TRP:CH2	2:K:208:PRO:HA	2.56	0.40
1:A:140:CYS:SG	1:A:154:TRP:CH2	3.15	0.40
4:E:59:TYR:CZ	4:E:69:ILE:HG22	2.57	0.40
2:K:107:GLY:N	2:K:140:TYR:OH	2.49	0.40
3:C:452:LEU:HD11	3:D:449:TYR:CD1	2.56	0.40
1:F:98:LEU:HD11	1:F:100:GLY:CA	2.51	0.40
1:F:148:GLU:N	1:F:149:PRO:HD2	2.36	0.40
4:H:11:VAL:HG11	4:H:146:PHE:CE2	2.57	0.40
2:K:142:GLY:O	2:K:164:PRO:HG2	2.21	0.40
2:B:48:ILE:HA	2:B:53:GLN:O	2.22	0.40
3:D:382:VAL:CG1	3:D:383:SER:N	2.85	0.40
1:F:145:TYR:CD2	1:F:150:VAL:HG21	2.56	0.40
4:H:154:TRP:CH2	4:H:196:CYS:HB3	2.55	0.40
5:L:140:TYR:HB3	5:L:141:PRO:HD3	2.02	0.40
1:A:147:PRO:HB2	1:A:200:HIS:NE2	2.36	0.40
2:B:184:GLN:HE21	2:B:184:GLN:HB3	1.52	0.40
2:K:12:SER:HA	2:K:105:THR:O	2.22	0.40
5:L:9:LEU:HA	5:L:102:THR:HA	2.03	0.40
5:L:90:GLN:NE2	5:L:96:LEU:HA	2.37	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	A	214/223 (96%)	200 (94%)	14 (6%)	0	100 100
1	F	213/223 (96%)	202 (95%)	11 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	211/216 (98%)	204 (97%)	7 (3%)	0	100	100
2	K	212/216 (98%)	202 (95%)	10 (5%)	0	100	100
3	C	194/205 (95%)	185 (95%)	9 (5%)	0	100	100
3	D	195/205 (95%)	186 (95%)	9 (5%)	0	100	100
4	E	224/227 (99%)	214 (96%)	10 (4%)	0	100	100
4	H	224/227 (99%)	219 (98%)	5 (2%)	0	100	100
5	J	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
5	L	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
All	All	2120/2180 (97%)	2034 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	186/191 (97%)	186 (100%)	0	100	100
1	F	185/191 (97%)	184 (100%)	1 (0%)	88	95
2	B	186/189 (98%)	185 (100%)	1 (0%)	88	95
2	K	187/189 (99%)	182 (97%)	5 (3%)	44	75
3	C	168/177 (95%)	167 (99%)	1 (1%)	86	95
3	D	169/177 (96%)	169 (100%)	0	100	100
4	E	189/190 (100%)	189 (100%)	0	100	100
4	H	189/190 (100%)	189 (100%)	0	100	100
5	J	194/194 (100%)	190 (98%)	4 (2%)	53	81
5	L	193/194 (100%)	190 (98%)	3 (2%)	62	86
All	All	1846/1882 (98%)	1831 (99%)	15 (1%)	81	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	25	ARG
3	C	408	ARG
1	F	196	CYS
5	J	55	ASP
5	J	61	ARG
5	J	162	SER
5	J	211	ARG
2	K	6	GLN
2	K	51	ASP
2	K	61	ARG
2	K	90	SER
2	K	92	ASP
5	L	6	GLN
5	L	7	SER
5	L	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	169	ASN
1	F	197	ASN
1	F	199	ASN
2	K	53	GLN
5	L	6	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 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	D	602	-	5,5,5	0.09	0	5,5,5	0.31	0
6	GOL	B	301	-	5,5,5	0.09	0	5,5,5	0.32	0
6	GOL	L	301	-	5,5,5	0.88	0	5,5,5	1.21	0
6	GOL	F	301	-	5,5,5	0.89	0	5,5,5	1.00	0
6	GOL	B	302	-	5,5,5	1.07	0	5,5,5	0.84	0
6	GOL	K	301	-	5,5,5	0.09	0	5,5,5	0.35	0
7	NAG	D	601	3	14,14,15	0.29	0	17,19,21	0.58	0
7	NAG	C	601	3	14,14,15	1.32	2 (14%)	17,19,21	0.95	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	D	602	-	-	2/4/4/4	-
6	GOL	B	301	-	-	2/4/4/4	-
6	GOL	L	301	-	-	2/4/4/4	-
6	GOL	F	301	-	-	2/4/4/4	-
6	GOL	B	302	-	-	2/4/4/4	-
6	GOL	K	301	-	-	2/4/4/4	-
7	NAG	D	601	3	-	2/6/23/26	0/1/1/1
7	NAG	C	601	3	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	601	NAG	O5-C1	3.46	1.49	1.43
7	C	601	NAG	C1-C2	3.28	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	C	601	NAG	C1-O5-C5	3.25	116.60	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	302	GOL	O1-C1-C2-O2
6	B	302	GOL	O1-C1-C2-C3
6	D	602	GOL	C1-C2-C3-O3
6	K	301	GOL	C1-C2-C3-O3
7	C	601	NAG	O5-C5-C6-O6
7	C	601	NAG	C4-C5-C6-O6
7	C	601	NAG	C8-C7-N2-C2
7	C	601	NAG	O7-C7-N2-C2
7	D	601	NAG	C8-C7-N2-C2
7	D	601	NAG	O7-C7-N2-C2
6	F	301	GOL	O2-C2-C3-O3
6	K	301	GOL	O2-C2-C3-O3
6	F	301	GOL	C1-C2-C3-O3
6	L	301	GOL	O1-C1-C2-C3
6	D	602	GOL	O2-C2-C3-O3
6	L	301	GOL	O1-C1-C2-O2
6	B	301	GOL	C1-C2-C3-O3
6	B	301	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	602	GOL	3	0
6	K	301	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	218/223 (97%)	0.47	7 (3%) 47 42	66, 93, 128, 169	0
1	F	217/223 (97%)	0.52	9 (4%) 37 32	77, 99, 131, 210	0
2	B	213/216 (98%)	0.21	2 (0%) 84 82	61, 84, 126, 155	0
2	K	214/216 (99%)	0.40	10 (4%) 31 25	72, 96, 140, 178	0
3	C	196/205 (95%)	0.49	6 (3%) 49 44	66, 87, 149, 180	0
3	D	197/205 (96%)	0.42	7 (3%) 42 37	69, 87, 144, 176	0
4	E	226/227 (99%)	0.33	8 (3%) 44 38	64, 85, 116, 210	0
4	H	226/227 (99%)	0.22	4 (1%) 68 65	63, 82, 114, 153	0
5	J	219/219 (100%)	0.33	4 (1%) 68 65	63, 83, 118, 173	0
5	L	218/219 (99%)	0.37	5 (2%) 60 55	70, 83, 104, 131	0
All	All	2144/2180 (98%)	0.38	62 (2%) 51 46	61, 88, 129, 210	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	GLU	6.9
1	F	127	SER	6.9
3	D	332	ILE	5.8
5	J	94	TRP	5.1
5	L	9	LEU	4.6
3	C	483	VAL	4.6
3	C	486	PHE	4.6
1	A	146	PHE	4.5
5	L	140	TYR	4.4
1	F	146	PHE	4.2
5	L	94	TRP	4.1
1	F	125	ALA	3.9
1	F	148	GLU	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	K	156	LYS	3.7
4	E	146	PHE	3.3
3	D	363	ALA	3.3
3	C	484	GLU	3.3
5	L	142	ARG	3.2
1	A	147	PRO	3.2
2	K	1	ASN	3.2
1	A	1	GLN	3.2
4	E	129	LYS	3.1
4	H	146	PHE	3.0
3	D	483	VAL	3.0
2	B	1	ASN	2.9
4	H	214	LYS	2.9
2	B	156	LYS	2.9
1	F	51	ILE	2.8
5	J	9	LEU	2.7
3	D	519	HIS	2.7
3	D	486	PHE	2.7
4	E	159	LEU	2.7
1	F	18	LEU	2.7
5	L	7	SER	2.6
3	D	435	ALA	2.6
4	E	131	THR	2.6
1	F	126	PRO	2.5
5	J	7	SER	2.5
3	C	346	ARG	2.4
1	A	71	VAL	2.4
4	H	147	PRO	2.4
4	E	138	LEU	2.4
4	E	128	SER	2.4
3	C	529	SER	2.4
2	K	189	ARG	2.4
2	K	51	ASP	2.4
1	F	98	LEU	2.3
1	A	82	LEU	2.3
4	E	214	LYS	2.3
2	K	157	ALA	2.2
2	K	48	ILE	2.2
3	C	402	ILE	2.2
2	K	150	ALA	2.2
2	K	210	GLU	2.2
3	D	517	LEU	2.1

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	F	184	VAL	2.1
2	K	131	THR	2.1
1	A	189	LEU	2.0
5	J	96	LEU	2.0
4	H	195	ILE	2.0
4	E	130	SER	2.0
2	K	146	VAL	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
6	GOL	B	301	6/6	0.55	0.57	80,85,86,90	0
6	GOL	K	301	6/6	0.55	0.61	86,89,91,93	0
6	GOL	D	602	6/6	0.58	0.57	84,88,91,95	0
7	NAG	D	601	14/15	0.67	0.32	116,130,134,134	0
7	NAG	C	601	14/15	0.69	0.34	101,113,116,118	0
6	GOL	B	302	6/6	0.87	0.28	99,104,106,108	0
6	GOL	L	301	6/6	0.88	0.44	79,83,85,86	0
6	GOL	F	301	6/6	0.89	0.20	81,84,86,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.