



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:24 PM GMT

PDB ID : 3X2D  
Title : Crystal structure of Marburg virus GP in complex with the human survivor antibody MR78  
Authors : Hashiguchi, T.; Fusco, M.L.; Bornholdt, Z.A.; Lee, J.E.; Flyak, A.I.; Matsuoka, R.; Kohda, D.; Yanagi, Y.; Hammel, M.; Crowe, J.E.; Saphire, E.O.  
Deposited on : 2014-12-20  
Resolution : 3.60 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

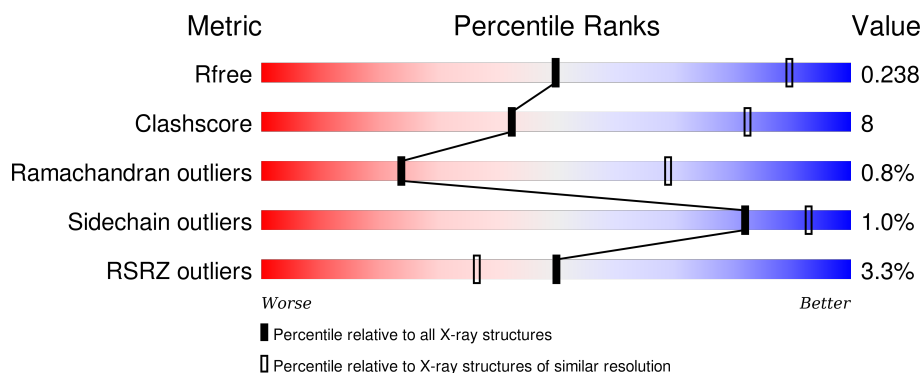
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	250	<div> <div></div> <div>45%17%38%</div> </div>
1	E	250	<div> <div>%</div> <div>51%11%38%</div> </div>
1	I	250	<div> <div></div> <div>46%14%39%</div> </div>
1	M	250	<div> <div>3%</div> <div>49%12%39%</div> </div>
2	B	237	<div> <div></div> <div>27%7%65%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	237	
2	J	237	
2	N	237	
3	C	211	
3	G	211	
3	K	211	
3	O	211	
4	D	226	
4	H	226	
4	L	226	
4	P	226	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20841 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 Envelope glycoprotein GP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1183	748	209	220	6			
1	E	154	Total	C	N	O	S	0	0	0
			1172	742	207	217	6			
1	I	152	Total	C	N	O	S	0	0	0
			1158	733	204	215	6			
1	M	152	Total	C	N	O	S	0	0	0
			1162	736	205	215	6			

- Molecule 2 is a protein called Virion spike glycoprotein GP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	S	0	0	0
			651	420	118	111	2			
2	F	83	Total	C	N	O	S	0	0	0
			651	420	118	111	2			
2	J	83	Total	C	N	O	S	0	0	0
			651	420	118	111	2			
2	N	83	Total	C	N	O	S	0	0	0
			651	420	118	111	2			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	438	LEU	PHE	ENGINEERED MUTATION	UNP Q1PDC7
B	439	ALA	TRP	ENGINEERED MUTATION	UNP Q1PDC7
B	445	GLY	PHE	ENGINEERED MUTATION	UNP Q1PDC7
B	447	ASN	PHE	ENGINEERED MUTATION	UNP Q1PDC7
B	638	ASP	-	EXPRESSION TAG	UNP Q1PDC7
B	639	ASP	-	EXPRESSION TAG	UNP Q1PDC7
B	640	ASP	-	EXPRESSION TAG	UNP Q1PDC7
B	641	ASP	-	EXPRESSION TAG	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	642	LYS	-	EXPRESSION TAG	UNP Q1PDC7
B	643	ALA	-	EXPRESSION TAG	UNP Q1PDC7
B	644	GLY	-	EXPRESSION TAG	UNP Q1PDC7
B	645	TRP	-	EXPRESSION TAG	UNP Q1PDC7
B	646	SER	-	EXPRESSION TAG	UNP Q1PDC7
B	647	HIS	-	EXPRESSION TAG	UNP Q1PDC7
B	648	PRO	-	EXPRESSION TAG	UNP Q1PDC7
B	649	GLN	-	EXPRESSION TAG	UNP Q1PDC7
B	650	PHE	-	EXPRESSION TAG	UNP Q1PDC7
B	651	GLU	-	EXPRESSION TAG	UNP Q1PDC7
B	652	LYS	-	EXPRESSION TAG	UNP Q1PDC7
B	653	GLY	-	EXPRESSION TAG	UNP Q1PDC7
B	654	GLY	-	EXPRESSION TAG	UNP Q1PDC7
B	655	GLY	-	EXPRESSION TAG	UNP Q1PDC7
B	656	SER	-	EXPRESSION TAG	UNP Q1PDC7
B	657	GLY	-	EXPRESSION TAG	UNP Q1PDC7
B	658	GLY	-	EXPRESSION TAG	UNP Q1PDC7
B	659	GLY	-	EXPRESSION TAG	UNP Q1PDC7
B	660	SER	-	EXPRESSION TAG	UNP Q1PDC7
B	661	GLY	-	EXPRESSION TAG	UNP Q1PDC7
B	662	GLY	-	EXPRESSION TAG	UNP Q1PDC7
B	663	GLY	-	EXPRESSION TAG	UNP Q1PDC7
B	664	SER	-	EXPRESSION TAG	UNP Q1PDC7
B	665	TRP	-	EXPRESSION TAG	UNP Q1PDC7
B	666	SER	-	EXPRESSION TAG	UNP Q1PDC7
B	667	HIS	-	EXPRESSION TAG	UNP Q1PDC7
B	668	PRO	-	EXPRESSION TAG	UNP Q1PDC7
B	669	GLN	-	EXPRESSION TAG	UNP Q1PDC7
B	670	PHE	-	EXPRESSION TAG	UNP Q1PDC7
B	671	GLU	-	EXPRESSION TAG	UNP Q1PDC7
B	672	LYS	-	EXPRESSION TAG	UNP Q1PDC7
F	438	LEU	PHE	ENGINEERED MUTATION	UNP Q1PDC7
F	439	ALA	TRP	ENGINEERED MUTATION	UNP Q1PDC7
F	445	GLY	PHE	ENGINEERED MUTATION	UNP Q1PDC7
F	447	ASN	PHE	ENGINEERED MUTATION	UNP Q1PDC7
F	638	ASP	-	EXPRESSION TAG	UNP Q1PDC7
F	639	ASP	-	EXPRESSION TAG	UNP Q1PDC7
F	640	ASP	-	EXPRESSION TAG	UNP Q1PDC7
F	641	ASP	-	EXPRESSION TAG	UNP Q1PDC7
F	642	LYS	-	EXPRESSION TAG	UNP Q1PDC7
F	643	ALA	-	EXPRESSION TAG	UNP Q1PDC7
F	644	GLY	-	EXPRESSION TAG	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	645	TRP	-	EXPRESSION TAG	UNP Q1PDC7
F	646	SER	-	EXPRESSION TAG	UNP Q1PDC7
F	647	HIS	-	EXPRESSION TAG	UNP Q1PDC7
F	648	PRO	-	EXPRESSION TAG	UNP Q1PDC7
F	649	GLN	-	EXPRESSION TAG	UNP Q1PDC7
F	650	PHE	-	EXPRESSION TAG	UNP Q1PDC7
F	651	GLU	-	EXPRESSION TAG	UNP Q1PDC7
F	652	LYS	-	EXPRESSION TAG	UNP Q1PDC7
F	653	GLY	-	EXPRESSION TAG	UNP Q1PDC7
F	654	GLY	-	EXPRESSION TAG	UNP Q1PDC7
F	655	GLY	-	EXPRESSION TAG	UNP Q1PDC7
F	656	SER	-	EXPRESSION TAG	UNP Q1PDC7
F	657	GLY	-	EXPRESSION TAG	UNP Q1PDC7
F	658	GLY	-	EXPRESSION TAG	UNP Q1PDC7
F	659	GLY	-	EXPRESSION TAG	UNP Q1PDC7
F	660	SER	-	EXPRESSION TAG	UNP Q1PDC7
F	661	GLY	-	EXPRESSION TAG	UNP Q1PDC7
F	662	GLY	-	EXPRESSION TAG	UNP Q1PDC7
F	663	GLY	-	EXPRESSION TAG	UNP Q1PDC7
F	664	SER	-	EXPRESSION TAG	UNP Q1PDC7
F	665	TRP	-	EXPRESSION TAG	UNP Q1PDC7
F	666	SER	-	EXPRESSION TAG	UNP Q1PDC7
F	667	HIS	-	EXPRESSION TAG	UNP Q1PDC7
F	668	PRO	-	EXPRESSION TAG	UNP Q1PDC7
F	669	GLN	-	EXPRESSION TAG	UNP Q1PDC7
F	670	PHE	-	EXPRESSION TAG	UNP Q1PDC7
F	671	GLU	-	EXPRESSION TAG	UNP Q1PDC7
F	672	LYS	-	EXPRESSION TAG	UNP Q1PDC7
J	438	LEU	PHE	ENGINEERED MUTATION	UNP Q1PDC7
J	439	ALA	TRP	ENGINEERED MUTATION	UNP Q1PDC7
J	445	GLY	PHE	ENGINEERED MUTATION	UNP Q1PDC7
J	447	ASN	PHE	ENGINEERED MUTATION	UNP Q1PDC7
J	638	ASP	-	EXPRESSION TAG	UNP Q1PDC7
J	639	ASP	-	EXPRESSION TAG	UNP Q1PDC7
J	640	ASP	-	EXPRESSION TAG	UNP Q1PDC7
J	641	ASP	-	EXPRESSION TAG	UNP Q1PDC7
J	642	LYS	-	EXPRESSION TAG	UNP Q1PDC7
J	643	ALA	-	EXPRESSION TAG	UNP Q1PDC7
J	644	GLY	-	EXPRESSION TAG	UNP Q1PDC7
J	645	TRP	-	EXPRESSION TAG	UNP Q1PDC7
J	646	SER	-	EXPRESSION TAG	UNP Q1PDC7
J	647	HIS	-	EXPRESSION TAG	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	648	PRO	-	EXPRESSION TAG	UNP Q1PDC7
J	649	GLN	-	EXPRESSION TAG	UNP Q1PDC7
J	650	PHE	-	EXPRESSION TAG	UNP Q1PDC7
J	651	GLU	-	EXPRESSION TAG	UNP Q1PDC7
J	652	LYS	-	EXPRESSION TAG	UNP Q1PDC7
J	653	GLY	-	EXPRESSION TAG	UNP Q1PDC7
J	654	GLY	-	EXPRESSION TAG	UNP Q1PDC7
J	655	GLY	-	EXPRESSION TAG	UNP Q1PDC7
J	656	SER	-	EXPRESSION TAG	UNP Q1PDC7
J	657	GLY	-	EXPRESSION TAG	UNP Q1PDC7
J	658	GLY	-	EXPRESSION TAG	UNP Q1PDC7
J	659	GLY	-	EXPRESSION TAG	UNP Q1PDC7
J	660	SER	-	EXPRESSION TAG	UNP Q1PDC7
J	661	GLY	-	EXPRESSION TAG	UNP Q1PDC7
J	662	GLY	-	EXPRESSION TAG	UNP Q1PDC7
J	663	GLY	-	EXPRESSION TAG	UNP Q1PDC7
J	664	SER	-	EXPRESSION TAG	UNP Q1PDC7
J	665	TRP	-	EXPRESSION TAG	UNP Q1PDC7
J	666	SER	-	EXPRESSION TAG	UNP Q1PDC7
J	667	HIS	-	EXPRESSION TAG	UNP Q1PDC7
J	668	PRO	-	EXPRESSION TAG	UNP Q1PDC7
J	669	GLN	-	EXPRESSION TAG	UNP Q1PDC7
J	670	PHE	-	EXPRESSION TAG	UNP Q1PDC7
J	671	GLU	-	EXPRESSION TAG	UNP Q1PDC7
J	672	LYS	-	EXPRESSION TAG	UNP Q1PDC7
N	438	LEU	PHE	ENGINEERED MUTATION	UNP Q1PDC7
N	439	ALA	TRP	ENGINEERED MUTATION	UNP Q1PDC7
N	445	GLY	PHE	ENGINEERED MUTATION	UNP Q1PDC7
N	447	ASN	PHE	ENGINEERED MUTATION	UNP Q1PDC7
N	638	ASP	-	EXPRESSION TAG	UNP Q1PDC7
N	639	ASP	-	EXPRESSION TAG	UNP Q1PDC7
N	640	ASP	-	EXPRESSION TAG	UNP Q1PDC7
N	641	ASP	-	EXPRESSION TAG	UNP Q1PDC7
N	642	LYS	-	EXPRESSION TAG	UNP Q1PDC7
N	643	ALA	-	EXPRESSION TAG	UNP Q1PDC7
N	644	GLY	-	EXPRESSION TAG	UNP Q1PDC7
N	645	TRP	-	EXPRESSION TAG	UNP Q1PDC7
N	646	SER	-	EXPRESSION TAG	UNP Q1PDC7
N	647	HIS	-	EXPRESSION TAG	UNP Q1PDC7
N	648	PRO	-	EXPRESSION TAG	UNP Q1PDC7
N	649	GLN	-	EXPRESSION TAG	UNP Q1PDC7
N	650	PHE	-	EXPRESSION TAG	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
N	651	GLU	-	EXPRESSION TAG	UNP Q1PDC7
N	652	LYS	-	EXPRESSION TAG	UNP Q1PDC7
N	653	GLY	-	EXPRESSION TAG	UNP Q1PDC7
N	654	GLY	-	EXPRESSION TAG	UNP Q1PDC7
N	655	GLY	-	EXPRESSION TAG	UNP Q1PDC7
N	656	SER	-	EXPRESSION TAG	UNP Q1PDC7
N	657	GLY	-	EXPRESSION TAG	UNP Q1PDC7
N	658	GLY	-	EXPRESSION TAG	UNP Q1PDC7
N	659	GLY	-	EXPRESSION TAG	UNP Q1PDC7
N	660	SER	-	EXPRESSION TAG	UNP Q1PDC7
N	661	GLY	-	EXPRESSION TAG	UNP Q1PDC7
N	662	GLY	-	EXPRESSION TAG	UNP Q1PDC7
N	663	GLY	-	EXPRESSION TAG	UNP Q1PDC7
N	664	SER	-	EXPRESSION TAG	UNP Q1PDC7
N	665	TRP	-	EXPRESSION TAG	UNP Q1PDC7
N	666	SER	-	EXPRESSION TAG	UNP Q1PDC7
N	667	HIS	-	EXPRESSION TAG	UNP Q1PDC7
N	668	PRO	-	EXPRESSION TAG	UNP Q1PDC7
N	669	GLN	-	EXPRESSION TAG	UNP Q1PDC7
N	670	PHE	-	EXPRESSION TAG	UNP Q1PDC7
N	671	GLU	-	EXPRESSION TAG	UNP Q1PDC7
N	672	LYS	-	EXPRESSION TAG	UNP Q1PDC7

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1640	1028	274	333	5			
3	G	211	Total	C	N	O	S	0	0	0
			1640	1028	274	333	5			
3	K	211	Total	C	N	O	S	0	0	0
			1640	1028	274	333	5			
3	O	211	Total	C	N	O	S	0	0	0
			1640	1028	274	333	5			

- Molecule 4 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	226	Total	C	N	O	S	0	0	0
			1683	1071	268	339	5			
4	H	226	Total	C	N	O	S	0	0	0
			1683	1071	268	339	5			

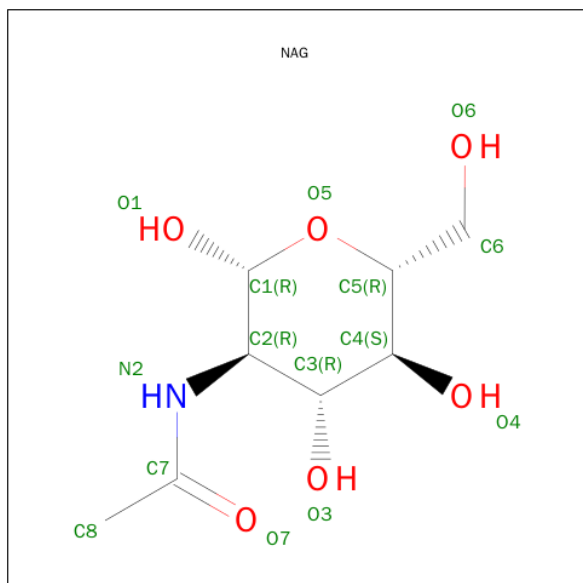
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	226	Total	C	N	O	S	0	0	0
			1683	1071	268	339	5			
4	P	226	Total	C	N	O	S	0	0	0
			1683	1071	268	339	5			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	4	Total	C	N	O	0	0
			50	28	2	20		
6	F	4	Total	C	N	O	0	0
			50	28	2	20		

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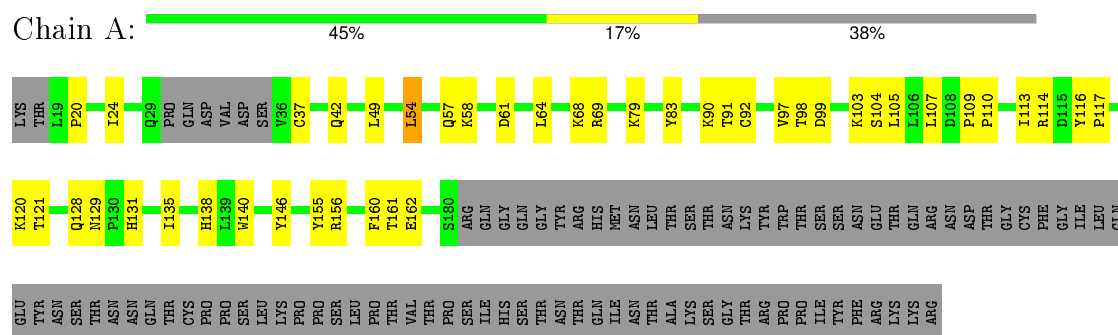
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	J	4	Total	C	N	O	0	0
			50	28	2	20		
6	N	4	Total	C	N	O	0	0
			50	28	2	20		

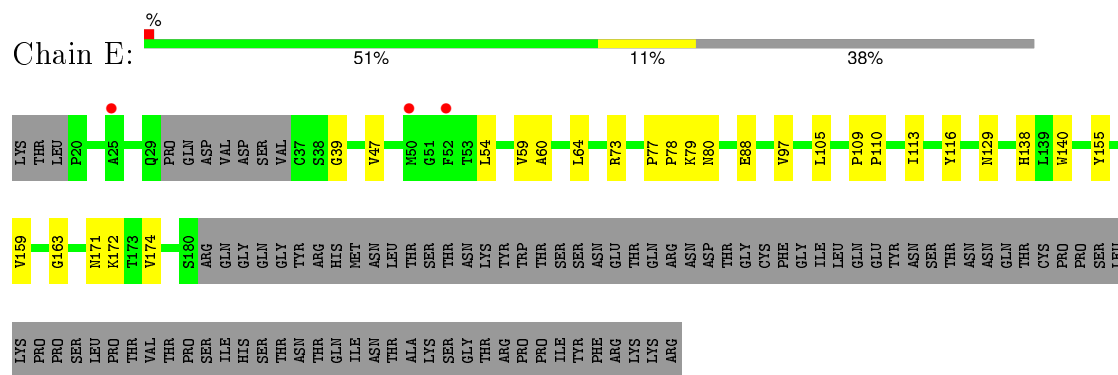
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

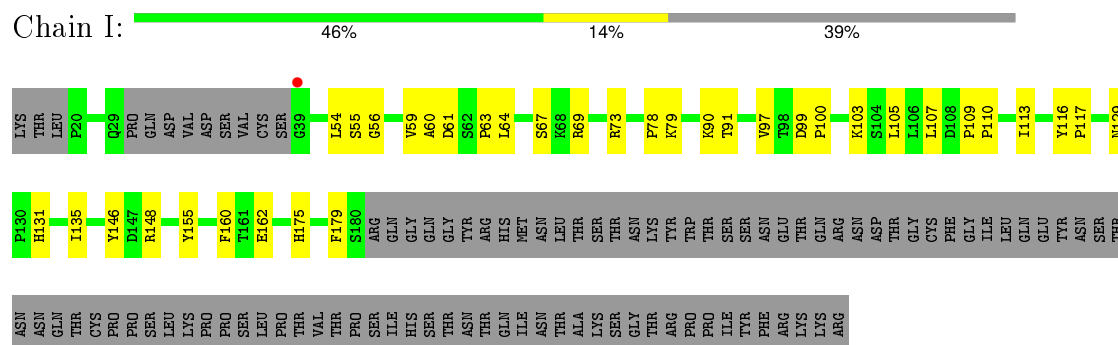
#### • Molecule 1: Envelope glycoprotein GP1



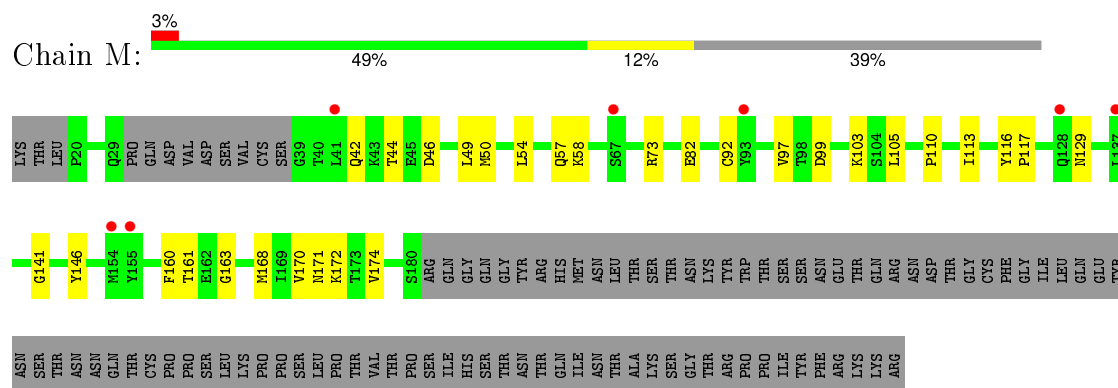
#### • Molecule 1: Envelope glycoprotein GP1



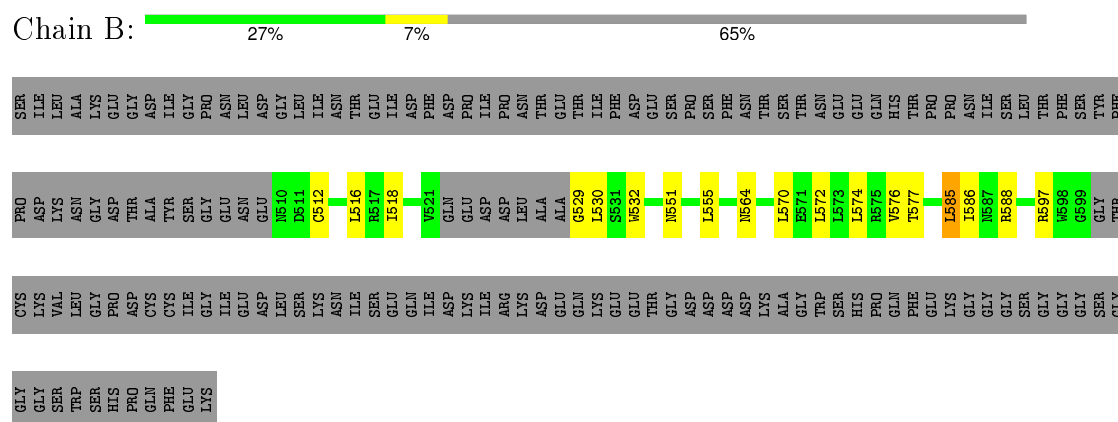
#### • Molecule 1: Envelope glycoprotein GP1



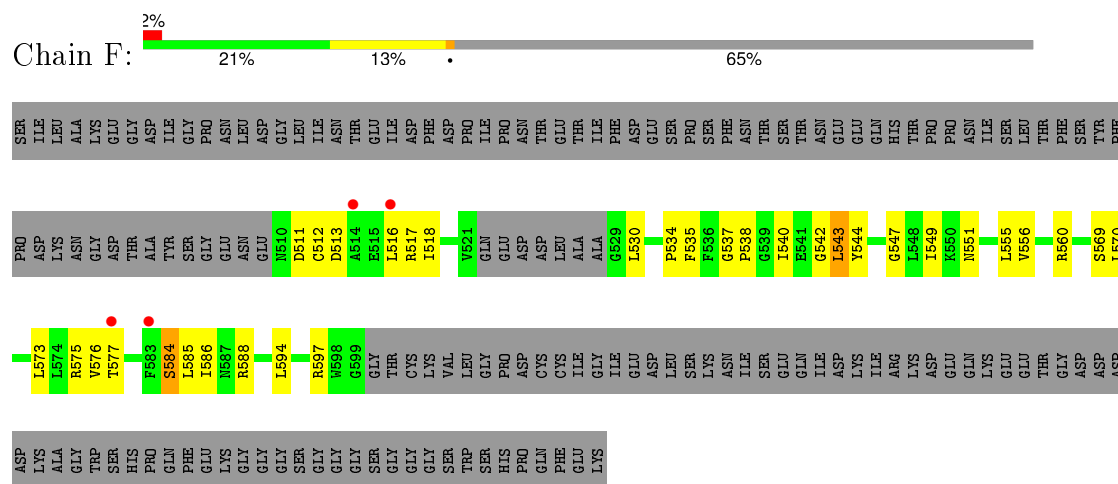
- Molecule 1: Envelope glycoprotein GP1



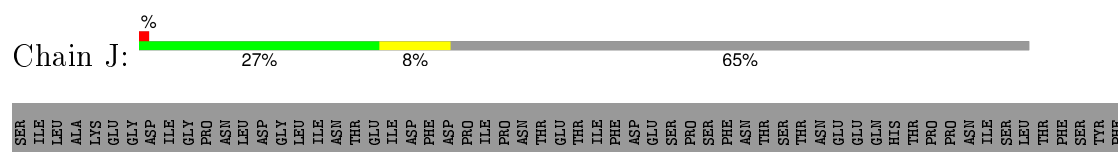
- Molecule 2: Virion spike glycoprotein GP2



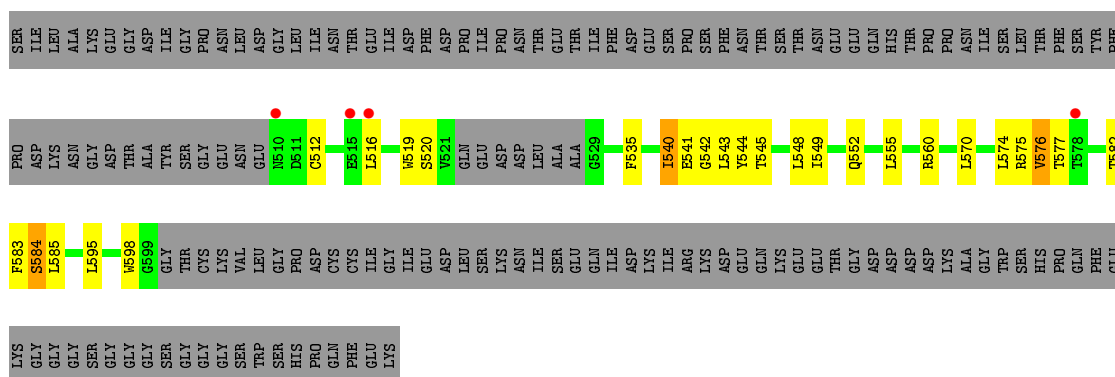
- Molecule 2: Virion spike glycoprotein GP2



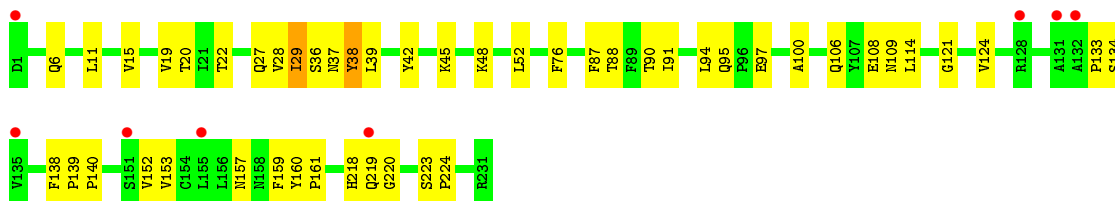
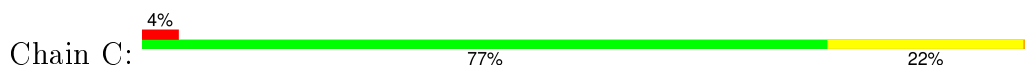
- Molecule 2: Virion spike glycoprotein GP2



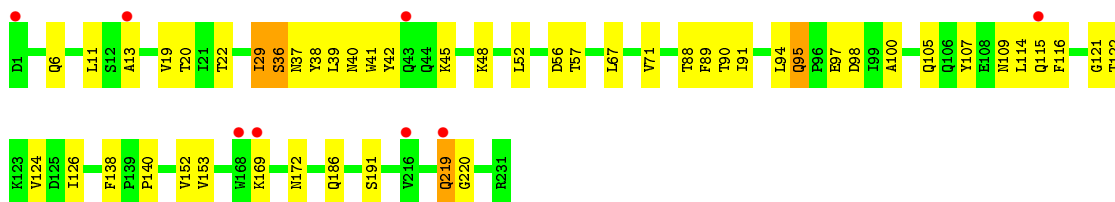
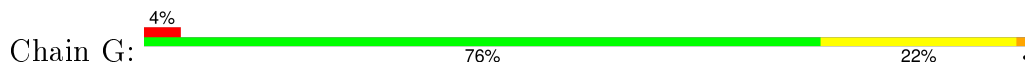
- Molecule 2: Virion spike glycoprotein GP2



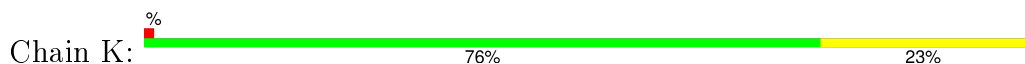
- Molecule 3: Fab light chain

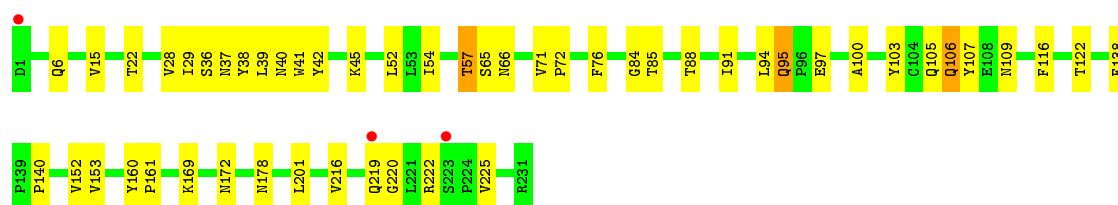


- Molecule 3: Fab light chain

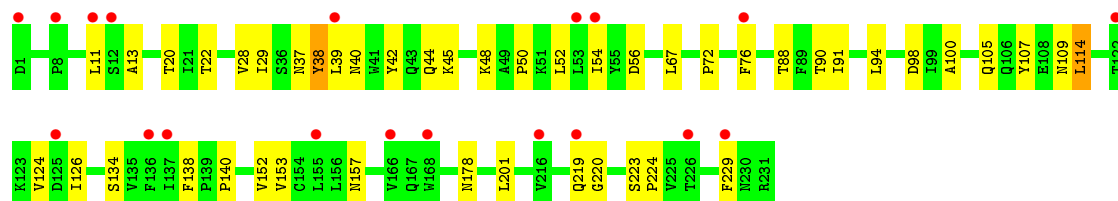
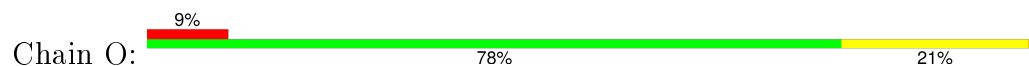


- Molecule 3: Fab light chain

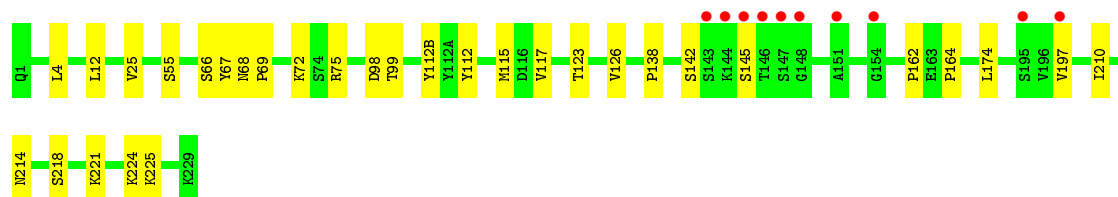
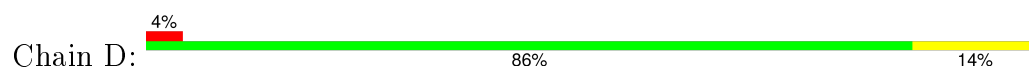




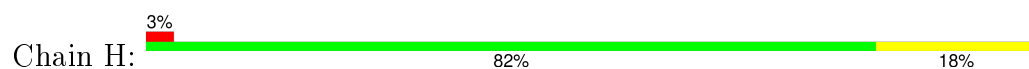
- Molecule 3: Fab light chain



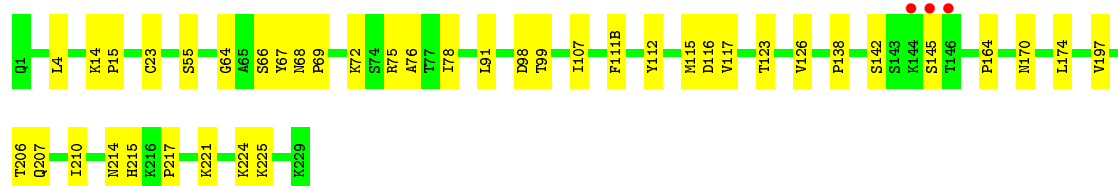
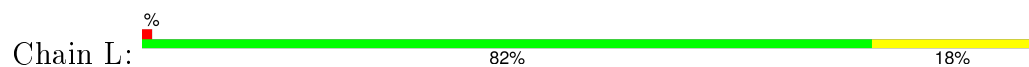
- Molecule 4: Fab heavy chain



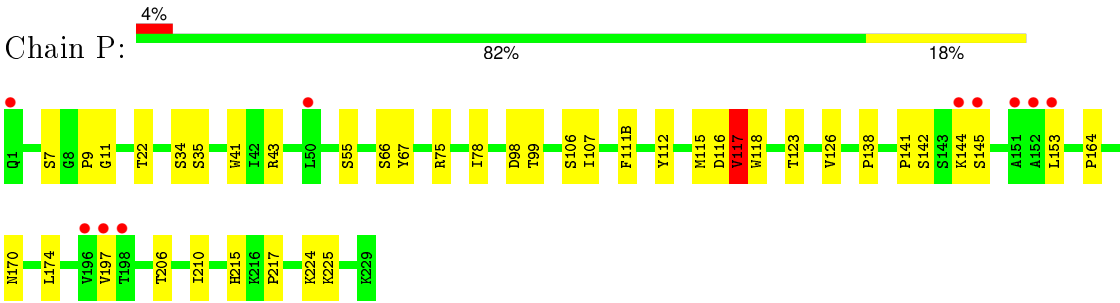
- Molecule 4: Fab heavy chain



- Molecule 4: Fab heavy chain



- Molecule 4: Fab heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.65Å 204.65Å 192.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.74 – 3.60 130.53 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (84.74-3.60) 94.2 (130.53-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.247 , 0.279 0.215 , 0.238	Depositor DCC
$R_{free}$ test set	2541 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 75.4	EDS
Estimated twinning fraction	0.186 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 52793 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	20841	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/1210	0.76	1/1641 (0.1%)
1	E	0.25	0/1199	0.43	0/1626
1	I	0.23	0/1185	0.42	0/1608
1	M	0.22	0/1189	0.43	0/1612
2	B	0.33	0/663	0.61	0/899
2	F	0.32	0/663	0.67	0/899
2	J	0.32	0/663	0.59	0/899
2	N	0.32	0/663	0.67	1/899 (0.1%)
3	C	0.25	0/1675	0.48	0/2274
3	G	0.25	0/1675	0.51	0/2274
3	K	0.25	0/1675	0.51	0/2274
3	O	0.23	0/1675	0.49	1/2274 (0.0%)
4	D	0.24	0/1729	0.44	0/2360
4	H	0.25	0/1729	0.47	0/2360
4	L	0.24	0/1729	0.44	0/2360
4	P	0.23	0/1729	0.44	0/2360
All	All	0.27	0/21051	0.51	3/28619 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	LEU	CB-CG-CD2	10.11	128.19	111.00
2	N	584	SER	N-CA-C	-6.33	93.92	111.00
3	O	114	LEU	CA-CB-CG	6.03	129.17	115.30

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	A	1183	0	1129	28	0
1	E	1172	0	1124	17	0
1	I	1158	0	1109	23	0
1	M	1162	0	1120	21	0
2	B	651	0	652	12	0
2	F	651	0	652	24	0
2	J	651	0	652	13	0
2	N	651	0	652	21	0
3	C	1640	0	1597	31	0
3	G	1640	0	1597	37	0
3	K	1640	0	1597	37	0
3	O	1640	0	1597	30	0
4	D	1683	0	1638	18	0
4	H	1683	0	1638	27	0
4	L	1683	0	1638	24	0
4	P	1683	0	1638	23	0
5	A	28	0	26	0	0
5	E	14	0	13	0	0
5	I	14	0	13	0	0
5	M	14	0	13	0	0
6	B	50	0	43	0	0
6	F	50	0	43	0	0
6	J	50	0	43	0	0
6	N	50	0	43	0	0
All	All	20841	0	20267	342	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 8.

All (342) 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:K:140:PRO:HD3	3:K:152:VAL:HG22	1.63	0.79
1:A:110:PRO:HG2	1:A:113:ILE:HD13	1.65	0.79
2:B:576:VAL:HG13	2:B:577:THR:HG23	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:PRO:HD3	3:C:152:VAL:HG22	1.67	0.77
4:H:99:THR:HG22	4:H:126:VAL:H	1.51	0.76
3:O:38:TYR:HB2	3:O:56:ASP:HA	1.68	0.76
1:E:39:GLY:O	2:F:597:ARG:NH1	2.19	0.76
3:G:219:GLN:HG3	3:G:220:GLY:HA3	1.67	0.76
4:L:99:THR:HG22	4:L:126:VAL:H	1.50	0.76
1:A:129:ASN:HB2	4:D:112(B):TYR:HA	1.66	0.75
2:F:512:CYS:SG	2:F:513:ASP:N	2.59	0.75
4:D:99:THR:HG22	4:D:126:VAL:H	1.52	0.74
3:O:140:PRO:HD3	3:O:152:VAL:HG22	1.67	0.73
4:P:99:THR:HG22	4:P:126:VAL:H	1.54	0.72
3:G:38:TYR:HB2	3:G:56:ASP:HA	1.69	0.72
3:G:140:PRO:HD3	3:G:152:VAL:HG22	1.71	0.72
4:P:141:PRO:HG3	4:P:153:LEU:HB3	1.71	0.71
3:C:27:GLN:HB2	3:C:108:GLU:HG3	1.74	0.70
1:E:64:LEU:HD11	3:G:38:TYR:HB3	1.73	0.70
2:J:512:CYS:SG	2:J:513:ASP:N	2.64	0.69
1:A:37:CYS:O	2:B:597:ARG:NH1	2.25	0.69
4:L:75:ARG:NH2	4:L:98:ASP:OD2	2.27	0.68
4:D:142:SER:H	4:D:145:SER:HB3	1.58	0.68
3:K:178:ASN:HD22	3:K:201:LEU:HD21	1.59	0.68
4:H:12:LEU:HD23	4:H:162:PRO:HD3	1.76	0.68
4:L:142:SER:H	4:L:145:SER:HB3	1.57	0.67
2:J:545:THR:OG1	2:J:546:ALA:N	2.27	0.67
3:K:95:GLN:NE2	3:K:97:GLU:OE1	2.27	0.67
3:O:91:ILE:HD13	3:O:94:LEU:HD12	1.77	0.67
2:F:511:ASP:HA	2:F:512:CYS:HB3	1.77	0.67
4:H:208:THR:HG23	4:H:225:LYS:HE2	1.76	0.67
2:J:588:ARG:HG3	1:M:44:THR:HG21	1.77	0.67
4:H:174:LEU:HD21	4:H:197:VAL:HG21	1.76	0.66
1:M:82:GLU:HB2	2:N:582:THR:HB	1.77	0.66
3:K:22:THR:HG22	3:K:88:THR:HG22	1.77	0.66
1:I:73:ARG:NH1	2:N:535:PHE:O	2.28	0.66
3:K:40:ASN:ND2	3:K:105:GLN:OE1	2.28	0.66
1:A:58:LYS:NZ	2:B:512:CYS:O	2.28	0.65
3:K:29:ILE:HG12	3:K:36:SER:H	1.61	0.65
3:O:29:ILE:HD11	3:O:38:TYR:HA	1.79	0.65
3:K:52:LEU:HD21	4:L:116:ASP:HB3	1.78	0.64
3:G:29:ILE:HG12	3:G:36:SER:H	1.63	0.64
2:F:535:PHE:O	1:M:73:ARG:NH1	2.31	0.64
3:O:42:TYR:HA	3:O:52:LEU:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:540:ILE:O	2:N:542:GLY:N	2.31	0.63
3:C:29:ILE:O	3:C:37:ASN:N	2.31	0.63
3:K:6:GLN:HE21	3:K:122:THR:HG23	1.63	0.63
4:L:107:ILE:HG12	4:L:115:MET:HG2	1.79	0.62
1:M:58:LYS:NZ	2:N:512:CYS:O	2.30	0.62
3:K:37:ASN:HD21	3:K:107:TYR:HD1	1.45	0.62
4:D:75:ARG:NH2	4:D:98:ASP:OD2	2.33	0.62
4:D:174:LEU:HD21	4:D:197:VAL:HG21	1.81	0.61
1:I:129:ASN:ND2	4:L:111(B):PHE:O	2.30	0.61
2:N:516:LEU:HB3	2:N:549:ILE:HB	1.82	0.61
4:H:109:GLY:HA2	4:H:113:PHE:HA	1.82	0.61
1:A:54:LEU:HD12	1:A:162:GLU:HB3	1.81	0.61
3:C:45:LYS:HG2	3:C:100:ALA:HB2	1.81	0.61
4:P:174:LEU:HD21	4:P:197:VAL:HG21	1.83	0.61
3:G:95:GLN:NE2	3:G:97:GLU:OE1	2.32	0.61
3:K:28:VAL:HG13	3:K:29:ILE:HB	1.83	0.61
4:D:123:THR:HB	4:D:164:PRO:HD3	1.82	0.60
4:D:214:ASN:HD22	4:D:221:LYS:HG2	1.66	0.60
1:E:129:ASN:HB2	4:H:112(B):TYR:HA	1.84	0.60
3:G:138:PHE:HB2	3:G:153:VAL:HG22	1.84	0.59
4:H:75:ARG:NH2	4:H:98:ASP:OD2	2.36	0.59
2:B:529:GLY:O	2:B:532:TRP:NE1	2.36	0.59
4:H:117:VAL:HG22	4:H:118:TRP:H	1.67	0.59
3:C:22:THR:HG22	3:C:88:THR:HG22	1.84	0.59
4:L:214:ASN:HD22	4:L:221:LYS:HG2	1.68	0.58
3:G:20:THR:HG22	3:G:90:THR:HG23	1.85	0.57
3:K:138:PHE:HB2	3:K:153:VAL:HG22	1.85	0.57
3:O:229:PHE:HB2	4:P:144:LYS:HD2	1.87	0.57
4:L:215:HIS:CD2	4:L:217:PRO:HD2	2.40	0.57
4:L:123:THR:HB	4:L:164:PRO:HD3	1.87	0.57
4:H:215:HIS:CD2	4:H:217:PRO:HD2	2.40	0.56
4:P:75:ARG:NH2	4:P:98:ASP:OD2	2.36	0.56
2:B:530:LEU:H	2:B:530:LEU:HD23	1.70	0.56
4:H:123:THR:HB	4:H:164:PRO:HD3	1.85	0.56
1:I:107:LEU:HD12	1:I:135:ILE:HG21	1.86	0.56
3:G:91:ILE:HD13	3:G:94:LEU:HD12	1.87	0.56
3:C:138:PHE:HB2	3:C:153:VAL:HG22	1.87	0.56
1:M:170:VAL:HG13	1:M:174:VAL:HG22	1.86	0.56
1:E:110:PRO:HD2	1:E:113:ILE:HD13	1.87	0.56
3:G:6:GLN:NE2	3:G:121:GLY:O	2.38	0.56
1:A:49:LEU:HD12	1:A:83:TYR:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:SER:O	4:D:66:SER:OG	2.23	0.56
4:P:210:ILE:HG22	4:P:225:LYS:HG2	1.88	0.55
3:O:109:ASN:O	3:O:114:LEU:HG	2.06	0.55
3:O:45:LYS:HG3	3:O:48:LYS:HE2	1.88	0.55
1:A:90:LYS:O	1:A:120:LYS:HB3	2.06	0.55
4:L:174:LEU:HD21	4:L:197:VAL:HG21	1.88	0.55
2:J:577:THR:HG21	2:J:583:PHE:HE1	1.71	0.55
1:M:171:ASN:OD1	1:M:172:LYS:N	2.40	0.55
3:K:36:SER:OG	3:K:107:TYR:O	2.22	0.55
1:A:57:GLN:NE2	2:B:564:ASN:OD1	2.38	0.54
2:B:551:ASN:OD1	2:B:555:LEU:N	2.41	0.54
4:P:123:THR:HB	4:P:164:PRO:HD3	1.89	0.54
4:D:210:ILE:HG22	4:D:225:LYS:HG2	1.89	0.54
3:G:22:THR:HG22	3:G:88:THR:HG22	1.90	0.54
4:D:12:LEU:HB2	4:D:162:PRO:HG3	1.89	0.54
3:K:40:ASN:HB2	3:K:105:GLN:HB3	1.90	0.53
2:N:516:LEU:HD23	2:N:549:ILE:HD12	1.89	0.53
3:G:45:LYS:HG3	3:G:48:LYS:HE2	1.89	0.53
3:K:40:ASN:HD22	3:K:105:GLN:HB3	1.71	0.53
2:B:576:VAL:HG22	2:B:577:THR:H	1.73	0.53
2:N:570:LEU:HD11	2:N:585:LEU:HD21	1.90	0.53
1:A:69:ARG:NH1	1:A:162:GLU:OE1	2.41	0.53
4:P:55:SER:O	4:P:66:SER:OG	2.26	0.53
3:O:138:PHE:HB2	3:O:153:VAL:HG22	1.90	0.53
4:H:12:LEU:HB3	4:H:162:PRO:HG3	1.92	0.52
4:P:215:HIS:CD2	4:P:217:PRO:HD2	2.45	0.52
3:G:37:ASN:HB2	3:G:107:TYR:HB3	1.90	0.52
1:E:88:GLU:OE2	2:F:517:ARG:NH2	2.42	0.52
3:C:106:GLN:HE21	3:C:108:GLU:HB2	1.74	0.52
1:A:107:LEU:HD12	1:A:135:ILE:HG21	1.90	0.52
3:O:178:ASN:HD22	3:O:201:LEU:HD21	1.74	0.52
3:O:54:ILE:HG13	3:O:67:LEU:HG	1.90	0.52
1:M:129:ASN:ND2	4:P:111(B):PHE:O	2.41	0.52
3:O:219:GLN:HB2	3:O:220:GLY:HA3	1.92	0.52
3:K:28:VAL:HG21	3:K:85:THR:HA	1.91	0.52
4:P:106:SER:OG	4:P:116:ASP:O	2.28	0.52
4:H:68:ASN:OD1	4:H:70:SER:OG	2.23	0.52
1:A:131:HIS:ND1	1:A:131:HIS:O	2.42	0.52
3:C:42:TYR:CE2	4:D:115:MET:HB2	2.44	0.52
1:I:64:LEU:O	1:I:67:SER:OG	2.22	0.52
2:N:576:VAL:HG23	2:N:577:THR:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:105:GLN:HE21	3:K:116:PHE:HB3	1.74	0.51
2:F:588:ARG:HH22	2:J:586:ILE:HD12	1.75	0.51
1:I:54:LEU:HD22	1:I:59:VAL:HG21	1.92	0.51
3:K:37:ASN:HD22	4:L:112:TYR:HA	1.75	0.51
2:N:520:SER:O	2:N:544:TYR:HA	2.10	0.51
3:C:20:THR:HG22	3:C:90:THR:HG23	1.92	0.51
4:D:138:PRO:HD3	4:D:224:LYS:HE2	1.91	0.51
1:E:109:PRO:HB3	1:E:155:TYR:HB3	1.93	0.51
3:G:219:GLN:CG	3:G:220:GLY:HA3	2.38	0.51
3:C:42:TYR:HA	3:C:52:LEU:HA	1.91	0.51
2:F:530:LEU:H	2:F:530:LEU:HD23	1.76	0.51
3:C:38:TYR:CE1	4:D:112:TYR:HB3	2.45	0.51
2:N:542:GLY:C	2:N:544:TYR:H	2.15	0.51
3:C:11:LEU:HB3	3:C:124:VAL:HG12	1.93	0.50
3:G:29:ILE:O	3:G:36:SER:OG	2.23	0.50
3:G:11:LEU:HB3	3:G:124:VAL:HG12	1.93	0.50
3:C:95:GLN:NE2	3:C:97:GLU:OE1	2.43	0.50
1:I:109:PRO:HB3	1:I:155:TYR:HB3	1.91	0.50
3:O:22:THR:HG22	3:O:88:THR:HG22	1.94	0.50
3:K:28:VAL:HG21	3:K:84:GLY:O	2.11	0.50
4:P:43:ARG:NH2	4:P:98:ASP:HA	2.27	0.50
3:O:45:LYS:HB2	3:O:48:LYS:HG2	1.93	0.50
3:G:115:GLN:N	3:G:115:GLN:OE1	2.45	0.50
1:I:61:ASP:HB3	1:I:91:THR:HG21	1.94	0.50
3:O:20:THR:HG22	3:O:90:THR:HG23	1.92	0.50
4:L:138:PRO:HD3	4:L:224:LYS:HE2	1.92	0.50
1:M:99:ASP:OD2	1:M:103:LYS:N	2.44	0.50
3:C:19:VAL:HG13	3:C:91:ILE:HG23	1.93	0.49
3:G:42:TYR:CD2	3:G:52:LEU:HB3	2.48	0.49
3:C:219:GLN:HB2	3:C:220:GLY:HA3	1.94	0.49
2:F:534:PRO:HD2	1:M:141:GLY:HA2	1.94	0.49
4:P:138:PRO:HD3	4:P:224:LYS:HE2	1.93	0.49
2:F:584:SER:OG	2:F:585:LEU:N	2.45	0.49
4:D:218:SER:O	4:H:85:ASN:HB2	2.12	0.49
2:J:530:LEU:HD23	2:J:530:LEU:H	1.78	0.49
4:L:55:SER:O	4:L:66:SER:OG	2.29	0.48
1:E:54:LEU:HD13	1:E:163:GLY:HA2	1.94	0.48
1:A:61:ASP:HB3	1:A:91:THR:HG21	1.95	0.48
1:M:97:VAL:HG12	1:M:105:LEU:HD12	1.95	0.48
3:G:186:GLN:HE21	3:G:191:SER:HB3	1.79	0.48
1:I:175:HIS:CE1	1:I:179:PHE:HE2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:ASN:HD21	4:D:112:TYR:HA	1.77	0.48
1:I:55:SER:HB3	1:I:90:LYS:HB3	1.95	0.48
1:E:116:TYR:H	1:E:159:VAL:HG23	1.79	0.48
3:O:45:LYS:HG2	3:O:100:ALA:HB2	1.96	0.47
1:I:59:VAL:HG12	1:I:60:ALA:H	1.79	0.47
4:L:210:ILE:HG22	4:L:225:LYS:HG2	1.96	0.47
1:I:78:PRO:O	1:I:79:LYS:HG3	2.14	0.47
3:O:11:LEU:HB3	3:O:124:VAL:HG12	1.95	0.47
3:G:52:LEU:HD21	4:H:116:ASP:HB2	1.96	0.47
1:M:57:GLN:HG2	2:N:560:ARG:HD3	1.95	0.47
3:K:219:GLN:HB3	3:K:220:GLY:HA3	1.97	0.47
2:F:542:GLY:HA2	2:F:543:LEU:CB	2.44	0.47
3:G:39:LEU:HD22	4:H:114:TYR:HA	1.97	0.47
1:A:97:VAL:HG12	1:A:105:LEU:HD12	1.96	0.47
1:A:99:ASP:OD1	1:A:103:LYS:N	2.48	0.47
3:O:38:TYR:CE1	4:P:112:TYR:HB3	2.50	0.47
3:G:41:TRP:CE2	3:G:89:PHE:HB2	2.50	0.47
2:F:516:LEU:HD23	2:F:556:VAL:HG13	1.96	0.47
1:E:171:ASN:OD1	1:E:172:LYS:N	2.45	0.47
1:I:110:PRO:HD2	1:I:113:ILE:HD13	1.96	0.47
3:G:19:VAL:HG13	3:G:91:ILE:HG23	1.97	0.46
3:K:72:PRO:HG2	3:K:76:PHE:CD2	2.50	0.46
4:H:4:LEU:HD22	4:H:25:VAL:HG12	1.96	0.46
2:J:551:ASN:OD1	2:J:555:LEU:N	2.48	0.46
3:C:6:GLN:NE2	3:C:121:GLY:O	2.48	0.46
1:E:59:VAL:HG22	1:E:60:ALA:H	1.79	0.46
1:A:92:CYS:SG	1:A:161:THR:OG1	2.74	0.46
1:I:63:PRO:HG2	3:K:29:ILE:HG22	1.98	0.46
3:G:45:LYS:HB2	3:G:48:LYS:HG2	1.97	0.46
4:P:41:TRP:HD1	4:P:78:ILE:HD13	1.80	0.46
1:M:171:ASN:CG	1:M:172:LYS:H	2.17	0.46
2:B:516:LEU:HG	2:B:518:ILE:HD11	1.96	0.46
1:I:97:VAL:HG12	1:I:105:LEU:HD12	1.98	0.46
1:I:56:GLY:O	2:J:513:ASP:HB2	2.16	0.46
3:G:45:LYS:HE3	3:G:100:ALA:HB2	1.97	0.46
3:G:115:GLN:HB2	4:H:52:TRP:CE3	2.51	0.46
2:F:516:LEU:HG	2:F:549:ILE:HB	1.97	0.46
1:E:171:ASN:HB3	1:E:174:VAL:HG12	1.97	0.46
1:E:97:VAL:HG12	1:E:105:LEU:HD23	1.97	0.46
2:F:594:LEU:HD21	2:N:595:LEU:HD23	1.98	0.46
4:P:117:VAL:O	4:P:118:TRP:CD1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:GLN:HG3	3:C:28:VAL:H	1.81	0.45
1:I:146:TYR:CE2	1:I:160:PHE:HB3	2.51	0.45
1:A:98:THR:HG22	1:A:104:SER:HA	1.97	0.45
2:N:520:SER:OG	2:N:545:THR:OG1	2.32	0.45
3:G:45:LYS:HG2	3:G:100:ALA:HB2	1.99	0.45
1:A:99:ASP:OD2	1:A:103:LYS:HB3	2.16	0.45
3:O:40:ASN:HB2	3:O:105:GLN:HB3	1.98	0.45
3:O:94:LEU:HG	3:O:98:ASP:HB2	1.98	0.45
1:A:138:HIS:CE1	1:A:140:TRP:HB2	2.52	0.45
3:K:45:LYS:HG2	3:K:100:ALA:HB2	1.98	0.45
1:E:138:HIS:CE1	1:E:140:TRP:HB2	2.52	0.45
1:A:109:PRO:HB3	1:A:155:TYR:HB3	1.99	0.45
2:N:570:LEU:O	2:N:574:LEU:HB2	2.16	0.45
4:H:55:SER:O	4:H:66:SER:OG	2.34	0.45
3:K:38:TYR:HB3	3:K:39:LEU:H	1.43	0.45
3:K:216:VAL:HB	3:K:225:VAL:HB	1.98	0.45
4:L:170:ASN:HD22	4:L:174:LEU:HB2	1.82	0.45
1:I:69:ARG:HD2	1:I:162:GLU:OE2	2.16	0.45
3:G:42:TYR:HA	3:G:52:LEU:HA	1.99	0.45
2:J:598:TRP:HB3	2:N:598:TRP:CZ2	2.51	0.45
1:I:100:PRO:HB2	4:L:64:GLY:HA2	1.99	0.45
2:J:575:ARG:HE	2:N:543:LEU:HD21	1.82	0.45
3:G:42:TYR:CE2	3:G:52:LEU:HB3	2.52	0.45
2:F:588:ARG:NH2	2:J:586:ILE:HD12	2.32	0.45
3:C:76:PHE:CE1	3:C:91:ILE:HD12	2.52	0.45
2:F:576:VAL:HG23	2:F:577:THR:HG23	1.99	0.45
1:A:104:SER:HB3	1:A:156:ARG:HE	1.82	0.45
4:P:9:PRO:HA	4:P:11:GLY:HA3	1.63	0.45
3:O:72:PRO:HG2	3:O:76:PHE:CD2	2.52	0.44
3:K:41:TRP:HA	3:K:103:TYR:O	2.16	0.44
2:F:569:SER:O	2:F:573:LEU:HD13	2.16	0.44
1:A:116:TYR:HA	1:A:117:PRO:HD3	1.70	0.44
1:A:146:TYR:CE2	1:A:160:PHE:HB3	2.51	0.44
4:L:4:LEU:HB3	4:L:23:CYS:SG	2.56	0.44
4:L:116:ASP:HA	4:L:117:VAL:HA	1.62	0.44
2:F:575:ARG:O	1:I:148:ARG:NH1	2.50	0.44
2:B:585:LEU:O	2:B:588:ARG:N	2.49	0.44
4:H:142:SER:H	4:H:145:SER:HB3	1.82	0.44
1:E:77:PRO:HA	1:E:78:PRO:HD3	1.88	0.44
1:A:64:LEU:O	1:A:68:LYS:HG3	2.18	0.44
3:K:6:GLN:NE2	3:K:122:THR:HG23	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:44:GLN:HB2	3:O:50:PRO:HB3	1.98	0.44
4:P:34:SER:HA	4:P:35:SER:HA	1.86	0.44
3:G:39:LEU:HD23	4:H:112:TYR:O	2.18	0.44
3:G:40:ASN:OD1	3:G:57:THR:N	2.51	0.44
2:B:572:LEU:HA	2:B:572:LEU:HD12	1.83	0.44
3:K:169:LYS:HE2	3:K:172:ASN:HA	1.99	0.44
4:H:43:ARG:NH2	4:H:98:ASP:HA	2.33	0.44
2:J:574:LEU:HA	2:J:574:LEU:HD23	1.84	0.44
1:M:49:LEU:HD13	2:N:585:LEU:HD23	2.00	0.43
3:C:15:VAL:HA	3:C:94:LEU:HD11	1.99	0.43
3:G:169:LYS:HE2	3:G:172:ASN:HA	1.99	0.43
3:K:76:PHE:CE1	3:K:91:ILE:HD12	2.53	0.43
3:C:108:GLU:OE2	3:C:109:ASN:ND2	2.52	0.43
1:A:49:LEU:HD11	2:B:585:LEU:HD22	2.00	0.43
1:E:73:ARG:NH1	2:J:535:PHE:O	2.51	0.43
1:I:99:ASP:OD2	1:I:103:LYS:N	2.51	0.43
4:P:107:ILE:HG12	4:P:115:MET:HG2	2.00	0.43
3:C:109:ASN:O	3:C:114:LEU:HB2	2.19	0.43
1:E:80:ASN:ND2	1:E:113:ILE:HD11	2.34	0.43
3:O:37:ASN:HB2	3:O:107:TYR:HB3	2.01	0.43
3:O:39:LEU:HD22	3:O:105:GLN:O	2.19	0.43
1:A:42:GLN:N	1:A:42:GLN:OE1	2.52	0.43
3:O:13:ALA:O	3:O:126:ILE:HA	2.19	0.43
2:F:551:ASN:OD1	2:F:555:LEU:N	2.52	0.43
2:F:513:ASP:OD2	2:F:560:ARG:NH2	2.52	0.43
3:C:29:ILE:HD13	3:C:87:PHE:CZ	2.54	0.43
3:O:67:LEU:HD21	3:O:76:PHE:O	2.19	0.43
3:G:39:LEU:HD11	3:G:105:GLN:CD	2.39	0.43
3:G:13:ALA:O	3:G:126:ILE:HA	2.18	0.43
2:N:552:GLN:O	2:N:555:LEU:HB2	2.19	0.42
3:K:39:LEU:HD12	3:K:40:ASN:H	1.84	0.42
3:G:94:LEU:HG	3:G:98:ASP:HB2	2.00	0.42
3:G:67:LEU:HB2	3:G:71:VAL:HG21	1.99	0.42
3:K:42:TYR:CE2	3:K:52:LEU:HB3	2.55	0.42
1:M:42:GLN:HB2	1:M:46:ASP:OD1	2.19	0.42
3:C:160:TYR:CG	3:C:161:PRO:HA	2.54	0.42
4:L:76:ALA:HB2	4:L:91:LEU:HD13	1.99	0.42
2:F:538:PRO:HG2	2:N:575:ARG:HH12	1.83	0.42
1:M:50:MET:HG3	1:M:168:MET:SD	2.60	0.42
3:O:39:LEU:HD13	3:O:40:ASN:N	2.34	0.42
3:C:133:PRO:HB3	3:C:159:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:SER:HB2	3:C:224:PRO:C	2.40	0.42
4:P:142:SER:H	4:P:145:SER:HB3	1.84	0.42
1:E:47:VAL:HG13	2:F:586:ILE:HG23	2.02	0.42
1:I:131:HIS:O	1:I:131:HIS:ND1	2.52	0.42
1:M:116:TYR:HA	1:M:117:PRO:HD3	1.84	0.42
4:D:68:ASN:HA	4:D:69:PRO:HD3	1.94	0.42
3:O:134:SER:OG	3:O:157:ASN:HB3	2.19	0.42
3:C:39:LEU:HD13	3:C:87:PHE:CD1	2.55	0.42
3:C:134:SER:HB2	3:C:157:ASN:HB3	2.01	0.42
3:G:116:PHE:HB2	4:H:52:TRP:CG	2.55	0.42
1:M:110:PRO:HD2	1:M:113:ILE:HD13	2.02	0.42
4:H:37:TYR:CZ	4:H:108:TYR:HD1	2.38	0.42
2:N:574:LEU:HD12	2:N:574:LEU:HA	1.79	0.41
4:H:34:SER:HA	4:H:35:SER:HA	1.88	0.41
3:O:107:TYR:CZ	3:O:114:LEU:HA	2.55	0.41
1:A:98:THR:O	1:A:128:GLN:HA	2.20	0.41
3:O:223:SER:HB2	3:O:224:PRO:C	2.40	0.41
4:L:67:TYR:HE2	4:L:78:ILE:HG13	1.85	0.41
4:P:7:SER:HB3	4:P:22:THR:OG1	2.20	0.41
4:P:170:ASN:HD22	4:P:174:LEU:HB2	1.84	0.41
3:C:138:PHE:HA	3:C:139:PRO:HD2	1.88	0.41
1:I:99:ASP:OD1	1:I:103:LYS:HB3	2.20	0.41
2:F:542:GLY:CA	2:F:544:TYR:H	2.34	0.41
1:A:114:ARG:O	1:A:146:TYR:HB3	2.20	0.41
3:K:28:VAL:HA	3:K:29:ILE:HA	1.75	0.41
3:K:105:GLN:HG2	3:K:106:GLN:N	2.36	0.41
1:A:120:LYS:HG2	1:A:121:THR:HG23	2.02	0.41
2:N:584:SER:OG	2:N:585:LEU:N	2.53	0.41
1:M:42:GLN:OE1	1:M:42:GLN:N	2.54	0.41
4:D:67:TYR:HB2	4:D:72:LYS:HG3	2.03	0.41
3:K:160:TYR:CG	3:K:161:PRO:HA	2.56	0.41
4:H:41:TRP:HD1	4:H:78:ILE:HD13	1.86	0.41
1:M:146:TYR:CE2	1:M:160:PHE:HB3	2.56	0.41
4:L:68:ASN:HA	4:L:69:PRO:HD3	1.93	0.41
1:M:92:CYS:SG	1:M:161:THR:OG1	2.79	0.41
4:P:67:TYR:HE2	4:P:78:ILE:HG13	1.86	0.40
2:F:518:ILE:HG13	2:F:547:GLY:HA3	2.03	0.40
4:H:116:ASP:HA	4:H:117:VAL:HA	1.67	0.40
2:F:537:GLY:HA3	2:F:538:PRO:HD2	1.86	0.40
4:L:67:TYR:HB2	4:L:72:LYS:HG3	2.02	0.40
3:K:54:ILE:HG23	3:K:66:ASN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:206:THR:OG1	4:L:207:GLN:N	2.54	0.40
3:K:15:VAL:HA	3:K:94:LEU:HD11	2.04	0.40
4:L:14:LYS:HA	4:L:15:PRO:HD3	1.97	0.40
3:C:133:PRO:HD3	3:C:218:HIS:CD2	2.56	0.40
3:K:71:VAL:HA	3:K:72:PRO:HD2	1.93	0.40
1:I:116:TYR:HA	1:I:117:PRO:HD3	1.82	0.40
3:C:45:LYS:HB2	3:C:48:LYS:HG2	2.03	0.40
4:D:4:LEU:HD22	4:D:25:VAL:HG12	2.03	0.40
3:K:57:THR:O	3:K:65:SER:OG	2.26	0.40
4:H:22:THR:HG22	4:H:88:SER:HB3	2.03	0.40
1:M:54:LEU:HD13	1:M:163:GLY:HA2	2.04	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	152/250 (61%)	142 (93%)	8 (5%)	2 (1%)	15	60
1	E	150/250 (60%)	143 (95%)	7 (5%)	0	100	100
1	I	148/250 (59%)	142 (96%)	6 (4%)	0	100	100
1	M	148/250 (59%)	140 (95%)	8 (5%)	0	100	100
2	B	79/237 (33%)	70 (89%)	7 (9%)	2 (2%)	7	48
2	F	79/237 (33%)	66 (84%)	12 (15%)	1 (1%)	15	60
2	J	79/237 (33%)	66 (84%)	12 (15%)	1 (1%)	15	60
2	N	79/237 (33%)	64 (81%)	11 (14%)	4 (5%)	2	28
3	C	209/211 (99%)	195 (93%)	12 (6%)	2 (1%)	19	66
3	G	209/211 (99%)	191 (91%)	14 (7%)	4 (2%)	10	53
3	K	209/211 (99%)	189 (90%)	18 (9%)	2 (1%)	19	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	209/211 (99%)	196 (94%)	13 (6%)	0	100	100
4	D	224/226 (99%)	208 (93%)	15 (7%)	1 (0%)	39	80
4	H	224/226 (99%)	210 (94%)	13 (6%)	1 (0%)	39	80
4	L	224/226 (99%)	209 (93%)	15 (7%)	0	100	100
4	P	224/226 (99%)	210 (94%)	13 (6%)	1 (0%)	39	80
All	All	2646/3696 (72%)	2441 (92%)	184 (7%)	21 (1%)	24	69

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
3	C	36	SER
3	G	29	ILE
2	N	541	GLU
3	C	29	ILE
3	G	36	SER
2	J	540	ILE
2	N	540	ILE
4	P	117	VAL
1	A	24	ILE
2	B	586	ILE
2	F	584	SER
3	G	109	ASN
3	G	114	LEU
3	K	57	THR
3	K	109	ASN
2	N	583	PHE
2	B	585	LEU
4	H	114	TYR
4	D	117	VAL
2	N	576	VAL

### 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	122/222 (55%)	121 (99%)	1 (1%)	86	95
1	E	121/222 (54%)	120 (99%)	1 (1%)	86	95
1	I	120/222 (54%)	120 (100%)	0	100	100
1	M	121/222 (54%)	121 (100%)	0	100	100
2	B	67/202 (33%)	65 (97%)	2 (3%)	48	82
2	F	67/202 (33%)	64 (96%)	3 (4%)	34	74
2	J	67/202 (33%)	65 (97%)	2 (3%)	48	82
2	N	67/202 (33%)	65 (97%)	2 (3%)	48	82
3	C	189/189 (100%)	188 (100%)	1 (0%)	92	97
3	G	189/189 (100%)	186 (98%)	3 (2%)	70	90
3	K	189/189 (100%)	186 (98%)	3 (2%)	70	90
3	O	189/189 (100%)	187 (99%)	2 (1%)	80	92
4	D	192/192 (100%)	192 (100%)	0	100	100
4	H	192/192 (100%)	192 (100%)	0	100	100
4	L	192/192 (100%)	192 (100%)	0	100	100
4	P	192/192 (100%)	190 (99%)	2 (1%)	82	93
All	All	2276/3220 (71%)	2254 (99%)	22 (1%)	82	93

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
2	B	570	LEU
2	B	574	LEU
3	C	38	TYR
1	E	79	LYS
2	F	540	ILE
2	F	543	LEU
2	F	570	LEU
3	G	95	GLN
3	G	122	THR
3	G	219	GLN
2	J	548	LEU
2	J	570	LEU
3	K	95	GLN
3	K	106	GLN
3	K	222	ARG

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Mol	Chain	Res	Type
2	N	519	TRP
2	N	548	LEU
3	O	28	VAL
3	O	38	TYR
4	P	117	VAL
4	P	206	THR

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

Mol	Chain	Res	Type
3	G	95	GLN
3	K	40	ASN
4	L	214	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

16 carbohydrates 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	B	701	2,6	14,14,15	0.99	1 (7%)	15,19,21	1.16	1 (6%)
6	NAG	B	702	6	14,14,15	1.03	2 (14%)	15,19,21	1.27	2 (13%)
6	BMA	B	703	6	11,11,12	0.86	0	14,15,17	0.90	1 (7%)
6	MAN	B	704	6	11,11,12	1.64	2 (18%)	14,15,17	1.08	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	F	701	2,6	14,14,15	1.00	1 (7%)	15,19,21	0.99	0
6	NAG	F	702	6	14,14,15	1.03	2 (14%)	15,19,21	1.24	3 (20%)
6	BMA	F	703	6	11,11,12	0.88	0	14,15,17	0.96	1 (7%)
6	MAN	F	704	6	11,11,12	1.68	2 (18%)	14,15,17	1.18	1 (7%)
6	NAG	J	701	2,6	14,14,15	1.00	1 (7%)	15,19,21	1.05	0
6	NAG	J	702	6	14,14,15	1.06	2 (14%)	15,19,21	1.19	3 (20%)
6	BMA	J	703	6	11,11,12	0.84	0	14,15,17	0.94	1 (7%)
6	MAN	J	704	6	11,11,12	1.67	2 (18%)	14,15,17	1.05	1 (7%)
6	NAG	N	701	2,6	14,14,15	0.97	1 (7%)	15,19,21	1.19	1 (6%)
6	NAG	N	702	6	14,14,15	1.07	2 (14%)	15,19,21	1.19	1 (6%)
6	BMA	N	703	6	11,11,12	0.83	0	14,15,17	1.19	1 (7%)
6	MAN	N	704	6	11,11,12	1.66	2 (18%)	14,15,17	1.10	1 (7%)

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	B	701	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	702	6	-	0/6/23/26	0/1/1/1
6	BMA	B	703	6	-	0/2/19/22	0/1/1/1
6	MAN	B	704	6	-	0/2/19/22	0/1/1/1
6	NAG	F	701	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	702	6	-	0/6/23/26	0/1/1/1
6	BMA	F	703	6	-	0/2/19/22	0/1/1/1
6	MAN	F	704	6	-	0/2/19/22	0/1/1/1
6	NAG	J	701	2,6	-	0/6/23/26	0/1/1/1
6	NAG	J	702	6	-	0/6/23/26	0/1/1/1
6	BMA	J	703	6	-	0/2/19/22	0/1/1/1
6	MAN	J	704	6	-	0/2/19/22	0/1/1/1
6	NAG	N	701	2,6	-	0/6/23/26	0/1/1/1
6	NAG	N	702	6	-	0/6/23/26	0/1/1/1
6	BMA	N	703	6	-	0/2/19/22	0/1/1/1
6	MAN	N	704	6	-	0/2/19/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	704	MAN	C2-C3	-2.97	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	704	MAN	C2-C3	-2.96	1.48	1.52
6	B	704	MAN	C2-C3	-2.94	1.48	1.52
6	F	704	MAN	C2-C3	-2.94	1.48	1.52
6	N	702	NAG	C2-N2	-2.16	1.42	1.46
6	J	702	NAG	C2-N2	-2.15	1.42	1.46
6	B	702	NAG	C2-N2	-2.08	1.42	1.46
6	F	702	NAG	C2-N2	-2.03	1.42	1.46
6	B	702	NAG	C7-N2	2.04	1.42	1.34
6	N	702	NAG	C7-N2	2.06	1.42	1.34
6	F	702	NAG	C7-N2	2.12	1.42	1.34
6	J	702	NAG	C7-N2	2.13	1.42	1.34
6	B	701	NAG	C7-N2	2.15	1.42	1.34
6	N	701	NAG	C7-N2	2.19	1.42	1.34
6	J	701	NAG	C7-N2	2.22	1.42	1.34
6	F	701	NAG	C7-N2	2.24	1.42	1.34
6	B	704	MAN	O5-C1	3.76	1.50	1.43
6	N	704	MAN	O5-C1	3.85	1.50	1.43
6	J	704	MAN	O5-C1	3.86	1.50	1.43
6	F	704	MAN	O5-C1	3.92	1.50	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	702	NAG	C2-N2-C7	-2.62	119.67	123.04
6	J	702	NAG	C2-N2-C7	-2.51	119.81	123.04
6	N	702	NAG	C2-N2-C7	-2.43	119.92	123.04
6	F	702	NAG	C2-N2-C7	-2.12	120.31	123.04
6	J	702	NAG	C8-C7-N2	2.05	120.03	116.11
6	F	702	NAG	C8-C7-N2	2.12	120.17	116.11
6	F	703	BMA	C1-O5-C5	2.13	114.95	112.25
6	J	702	NAG	C1-O5-C5	2.13	114.95	112.25
6	J	703	BMA	C1-O5-C5	2.18	115.01	112.25
6	B	703	BMA	C1-O5-C5	2.18	115.02	112.25
6	F	702	NAG	C1-O5-C5	2.25	115.10	112.25
6	B	701	NAG	C1-O5-C5	2.26	115.12	112.25
6	J	704	MAN	C1-C2-C3	2.48	112.48	109.54
6	N	704	MAN	C1-C2-C3	2.53	112.53	109.54
6	N	701	NAG	C3-C4-C5	2.56	114.66	110.20
6	B	704	MAN	C1-C2-C3	2.61	112.62	109.54
6	B	702	NAG	C1-O5-C5	2.64	115.60	112.25
6	F	704	MAN	C1-C2-C3	3.01	113.10	109.54
6	N	703	BMA	C1-O5-C5	3.36	116.51	112.25



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

5 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
5	NAG	A	701	1	14,14,15	1.07	2 (14%)	15,19,21	1.14	2 (13%)
5	NAG	A	702	1	14,14,15	1.00	1 (7%)	15,19,21	1.45	2 (13%)
5	NAG	E	701	1	14,14,15	1.02	2 (14%)	15,19,21	1.12	2 (13%)
5	NAG	I	701	1	14,14,15	1.06	2 (14%)	15,19,21	0.94	0
5	NAG	M	701	1	14,14,15	1.04	2 (14%)	15,19,21	0.91	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
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	NAG	A	702	1	-	0/6/23/26	0/1/1/1
5	NAG	E	701	1	-	0/6/23/26	0/1/1/1
5	NAG	I	701	1	-	0/6/23/26	0/1/1/1
5	NAG	M	701	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	702	NAG	C2-N2	-2.26	1.42	1.46
5	I	701	NAG	C2-N2	-2.17	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	701	NAG	C2-N2	-2.10	1.42	1.46
5	E	701	NAG	C2-N2	-2.06	1.42	1.46
5	A	701	NAG	C2-N2	-2.05	1.42	1.46
5	A	701	NAG	C7-N2	2.09	1.42	1.34
5	M	701	NAG	C7-N2	2.10	1.42	1.34
5	I	701	NAG	C7-N2	2.11	1.42	1.34
5	E	701	NAG	C7-N2	2.13	1.42	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	NAG	C2-N2-C7	-2.52	119.80	123.04
5	A	702	NAG	C2-N2-C7	-2.40	119.95	123.04
5	E	701	NAG	C2-N2-C7	-2.05	120.41	123.04
5	A	701	NAG	C8-C7-N2	2.05	120.04	116.11
5	E	701	NAG	C8-C7-N2	2.15	120.21	116.11
5	A	702	NAG	C1-O5-C5	3.68	116.91	112.25

There are no chirality outliers.

There are no torsion outliers.

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	A	156/250 (62%)	0.17	0 100 100	57, 82, 114, 126	0
1	E	154/250 (61%)	0.47	3 (1%) 70 56	73, 93, 135, 142	0
1	I	152/250 (60%)	0.42	1 (0%) 89 81	73, 93, 140, 160	0
1	M	152/250 (60%)	0.64	7 (4%) 36 26	93, 116, 147, 160	0
2	B	83/237 (35%)	0.32	0 100 100	72, 95, 109, 122	0
2	F	83/237 (35%)	0.56	4 (4%) 34 24	83, 118, 139, 149	0
2	J	83/237 (35%)	0.55	3 (3%) 46 33	84, 115, 138, 162	0
2	N	83/237 (35%)	0.47	4 (4%) 34 24	96, 123, 150, 157	0
3	C	211/211 (100%)	0.48	8 (3%) 44 32	72, 113, 140, 158	0
3	G	211/211 (100%)	0.53	8 (3%) 44 32	72, 100, 129, 153	0
3	K	211/211 (100%)	0.43	3 (1%) 78 65	68, 91, 111, 136	0
3	O	211/211 (100%)	0.53	19 (9%) 12 8	116, 147, 166, 173	0
4	D	226/226 (100%)	0.33	10 (4%) 38 27	57, 82, 140, 167	0
4	H	226/226 (100%)	0.37	7 (3%) 52 38	60, 80, 121, 173	0
4	L	226/226 (100%)	0.28	3 (1%) 79 66	52, 76, 124, 151	0
4	P	226/226 (100%)	0.41	10 (4%) 38 27	103, 129, 168, 185	0
All	All	2694/3696 (72%)	0.43	90 (3%) 50 36	52, 102, 151, 185	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	P	152	ALA	6.8
4	H	145	SER	6.7
3	O	1	ASP	6.5
3	C	1	ASP	6.2
4	L	144	LYS	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	D	145	SER	4.8
4	P	198	THR	4.7
4	P	145	SER	4.6
4	D	146	THR	4.4
4	P	197	VAL	4.4
3	K	219	GLN	4.2
3	K	1	ASP	3.8
2	N	510	ASN	3.6
3	O	125	ASP	3.6
3	C	131	ALA	3.6
3	G	1	ASP	3.5
2	J	583	PHE	3.5
1	M	137	LEU	3.4
4	D	147	SER	3.3
4	L	145	SER	3.3
4	L	146	THR	3.3
4	H	146	THR	3.2
4	P	153	LEU	3.2
3	G	219	GLN	3.1
3	O	155	LEU	3.1
1	I	39	GLY	3.0
1	E	50	MET	3.0
3	K	223	SER	3.0
4	P	151	ALA	2.9
3	C	219	GLN	2.8
4	P	1	GLN	2.8
3	O	53	LEU	2.8
4	D	144	LYS	2.8
3	C	155	LEU	2.8
2	N	578	THR	2.8
3	O	12	SER	2.7
2	F	516	LEU	2.7
1	M	41	LEU	2.7
4	H	147	SER	2.7
3	C	128	ARG	2.6
2	F	514	ALA	2.6
4	H	228	PRO	2.6
3	C	151	SER	2.6
3	G	169	LYS	2.6
4	H	144	LYS	2.5
1	M	67	SER	2.5
3	O	11	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	155	TYR	2.5
3	O	76	PHE	2.4
3	O	216	VAL	2.4
4	D	143	SER	2.4
4	H	116	ASP	2.4
3	G	13	ALA	2.4
3	G	216	VAL	2.4
2	F	577	THR	2.4
3	O	136	PHE	2.3
2	J	584	SER	2.3
2	N	516	LEU	2.2
3	O	39	LEU	2.2
1	M	128	GLN	2.2
1	M	154	MET	2.2
2	F	583	PHE	2.2
3	C	135	VAL	2.2
4	D	148	GLY	2.2
4	D	197	VAL	2.2
3	O	122	THR	2.2
4	P	50	LEU	2.2
3	C	132	ALA	2.2
4	P	144	LYS	2.1
3	O	8	PRO	2.1
3	O	166	VAL	2.1
4	D	154	GLY	2.1
4	D	195	SER	2.1
3	G	168	TRP	2.1
3	O	168	TRP	2.1
2	J	582	THR	2.1
1	E	52	PHE	2.1
3	G	43	GLN	2.1
4	D	151	ALA	2.1
4	H	115	MET	2.1
3	O	137	ILE	2.1
2	N	515	GLU	2.1
4	P	196	VAL	2.1
3	O	226	THR	2.1
1	M	93	TYR	2.1
1	E	25	ALA	2.1
3	O	219	GLN	2.1
3	G	115	GLN	2.0
3	O	54	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	O	229	PHE	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. 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	J	701	14/15	0.92	0.27	-1.05	95,102,115,118	0
6	NAG	N	701	14/15	0.88	0.23	-1.18	105,116,129,130	0
6	NAG	B	701	14/15	0.94	0.24	-1.27	73,83,93,106	0
6	NAG	F	701	14/15	0.88	0.26	-1.28	91,106,121,126	0
6	MAN	B	704	11/12	0.79	0.27	-	121,132,140,147	0
6	MAN	N	704	11/12	0.73	0.25	-	130,142,146,147	0
6	BMA	B	703	11/12	0.82	0.25	-	112,121,138,139	0
6	NAG	F	702	14/15	0.90	0.28	-	98,105,116,122	0
6	BMA	N	703	11/12	0.86	0.18	-	128,136,140,145	0
6	MAN	J	704	11/12	0.60	0.30	-	143,152,158,158	0
6	NAG	N	702	14/15	0.94	0.21	-	107,116,122,126	0
6	MAN	F	704	11/12	0.61	0.30	-	109,126,133,135	0
6	NAG	J	702	14/15	0.92	0.22	-	97,102,114,115	0
6	BMA	F	703	11/12	0.88	0.19	-	96,103,110,113	0
6	BMA	J	703	11/12	0.84	0.19	-	107,129,142,153	0
6	NAG	B	702	14/15	0.90	0.26	-	88,95,102,103	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. 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( $\text{\AA}^2$ )	Q<0.9
5	NAG	E	701	14/15	0.84	0.29	0.92	102,107,112,117	0
5	NAG	I	701	14/15	0.82	0.38	0.69	94,116,126,127	0
5	NAG	A	701	14/15	0.89	0.28	0.60	90,94,109,130	0
5	NAG	M	701	14/15	0.62	0.30	-0.48	116,129,135,138	0
5	NAG	A	702	14/15	0.77	0.23	-	125,135,142,143	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.