



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 12:29 AM EDT

PDB ID : 3JWD  
Title : Structure of HIV-1 gp120 with gp41-Interactive Region: Layered Architecture and Basis of Conformational Mobility  
Authors : Pancera, M.; Majeed, S.; Ban, Y.A.; Chen, L.; Huang, C.C.; Kong, L.; Kwon, Y.D.; Stuckey, J.; Zhou, T.; Robinson, J.E.; Schief, W.R.; Sodroski, J.; Wyatt, R.; Kwong, P.D.  
Deposited on : 2009-09-18  
Resolution : 2.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

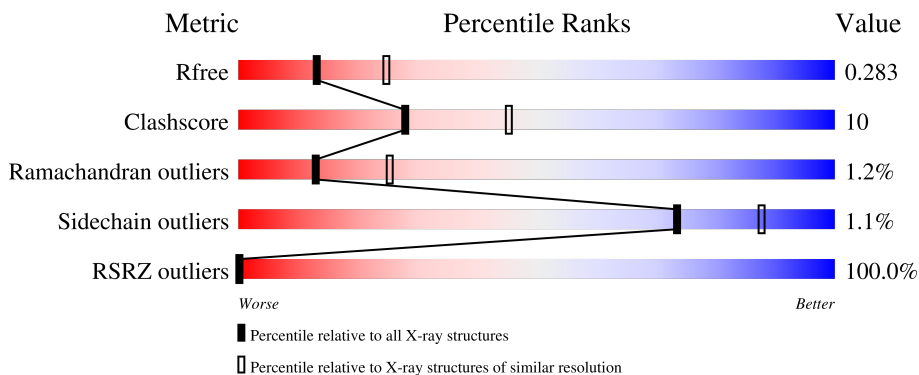
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	379	
1	B	379	
2	C	184	
2	D	184	

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Mol	Chain	Length	Quality of chain
3	L	213	
3	O	213	
4	H	220	
4	P	220	

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
3	YCM	L	214	-	-	-	X
5	NAG	A	588	-	-	-	X
5	NAG	A	734	X	-	-	X
5	NAG	A	741	-	-	-	X
5	NAG	A	762	-	-	-	X
5	NAG	A	776	-	-	-	X
5	NAG	A	789	-	-	-	X
5	NAG	A	886	-	-	-	X
5	NAG	A	892	-	-	-	X
5	NAG	A	897	-	-	-	X
5	NAG	A	948	X	-	-	X
5	NAG	B	588	X	-	-	X
5	NAG	B	734	-	-	-	X
5	NAG	B	762	-	-	-	X
5	NAG	B	776	-	-	-	X
5	NAG	B	789	-	-	-	X
5	NAG	B	795	-	-	-	X
5	NAG	B	886	-	-	-	X
5	NAG	B	892	-	-	-	X
5	NAG	B	948	-	-	-	X
6	GOL	B	1	-	-	-	X
6	GOL	P	215	-	-	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 15697 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 HIV-1 GP120 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	Total	C	N	O	S	0	0	0
			2800	1769	480	531	20			
1	B	354	Total	C	N	O	S	0	0	0
			2756	1744	472	520	20			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	184	Total	C	N	O	S	0	0	0
			1432	896	250	281	5			
2	D	183	Total	C	N	O	S	0	0	0
			1424	891	249	280	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1000	MET	-	initiating methionine	UNP P01730
D	1000	MET	-	initiating methionine	UNP P01730

- Molecule 3 is a protein called FAB 48D LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	213	Total	C	N	O	S	0	0	0
			1635	1022	274	333	6			
3	O	212	Total	C	N	O	S	0	0	0
			1624	1017	272	330	5			

- Molecule 4 is a protein called FAB 48D HEAVY CHAIN.

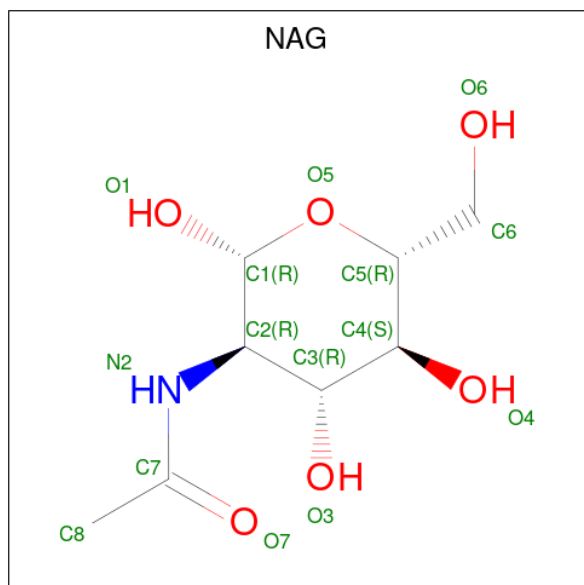
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	220	Total	C	N	O	S	0	0	0
			1654	1048	267	332	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	P	219	1644	1042	265	330	7	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



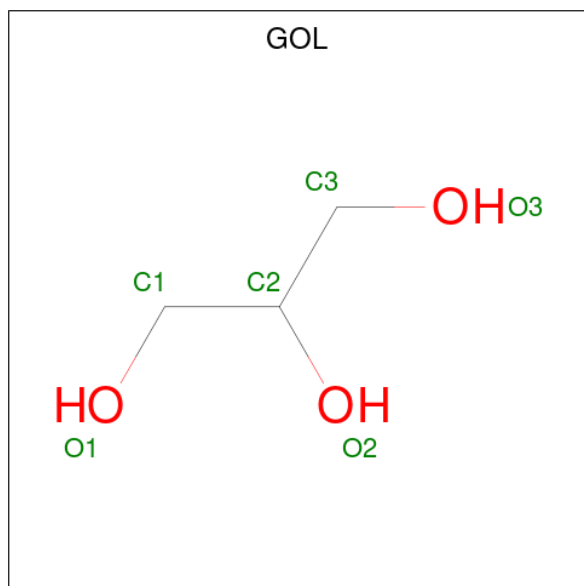
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0

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

- 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	P	1	Total	C	O	0	0
			6	3	3		

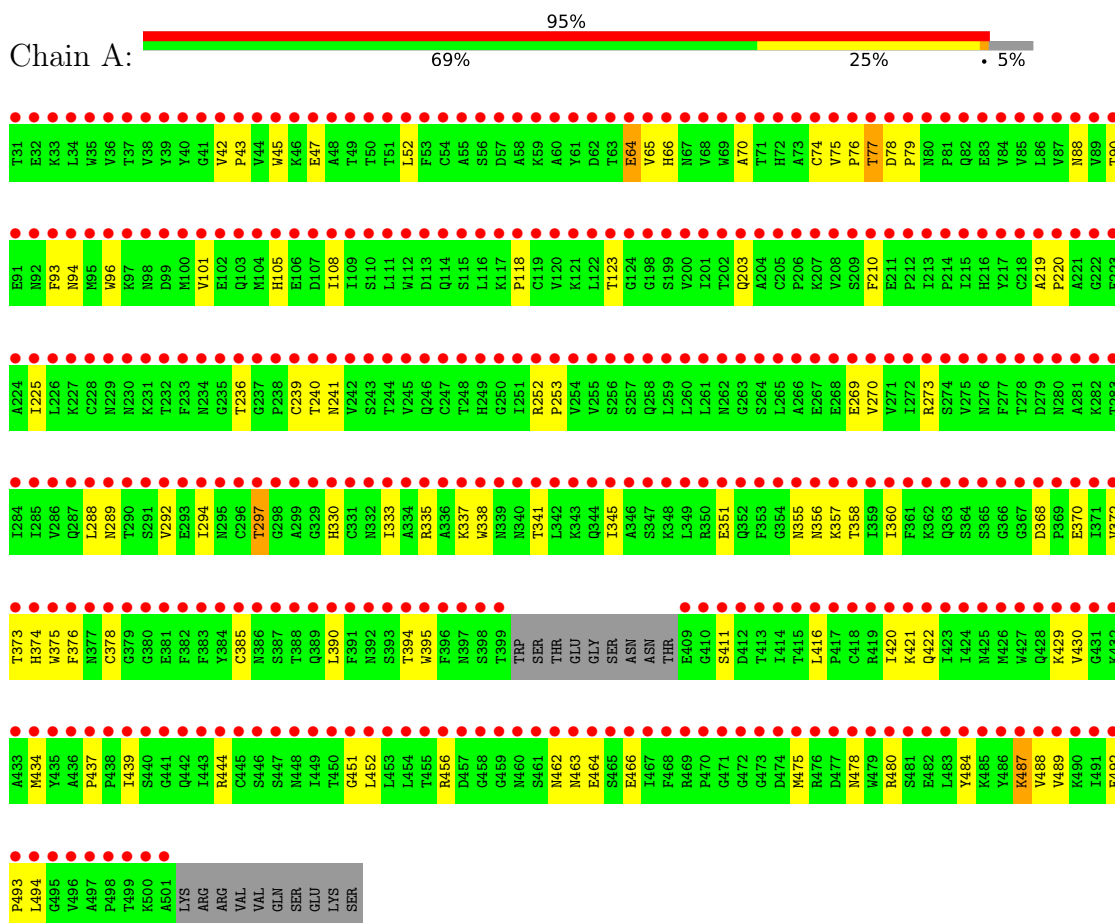
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	135	Total 135	O 135	0	0
7	C	50	Total 50	O 50	0	0
7	L	54	Total 54	O 54	0	0
7	H	47	Total 47	O 47	0	0
7	B	68	Total 68	O 68	0	0
7	D	34	Total 34	O 34	0	0
7	O	23	Total 23	O 23	0	0
7	P	39	Total 39	O 39	0	0

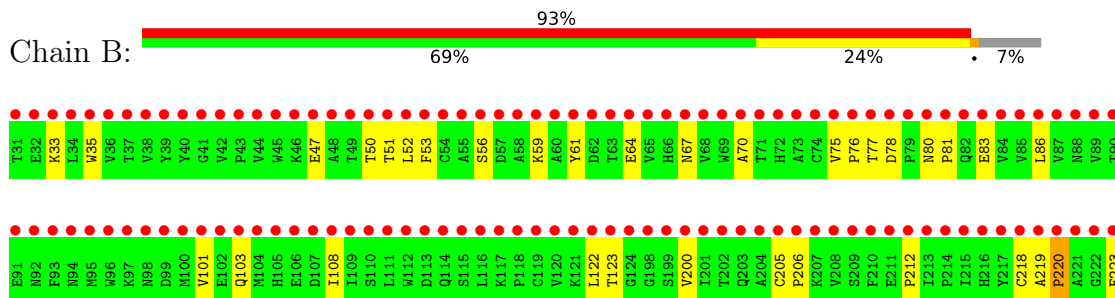
### 3 Residue-property plots

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

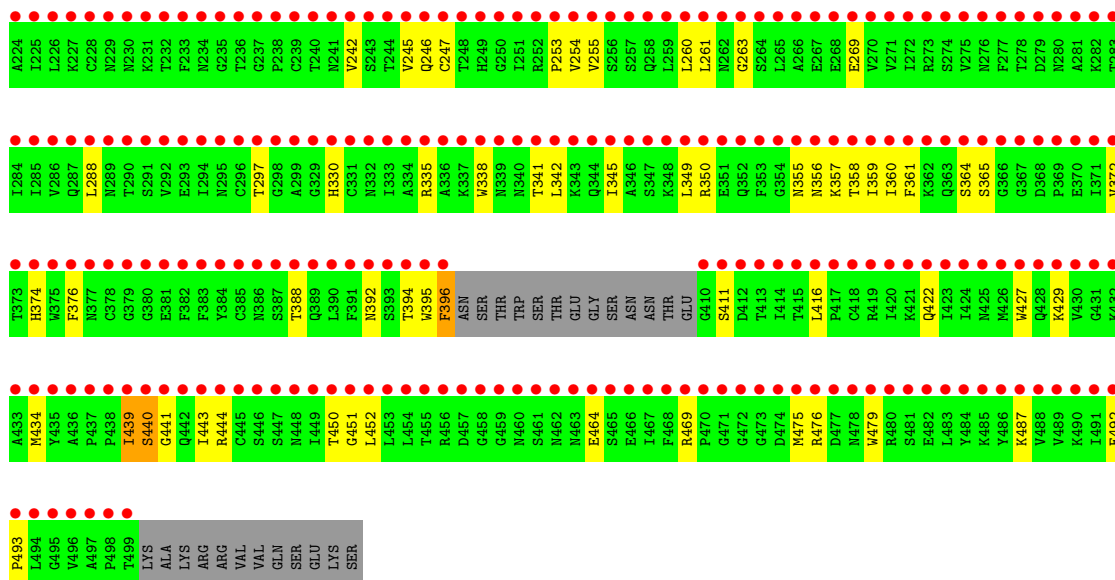
- Molecule 1: HIV-1 GP120 ENVELOPE GLYCOPROTEIN



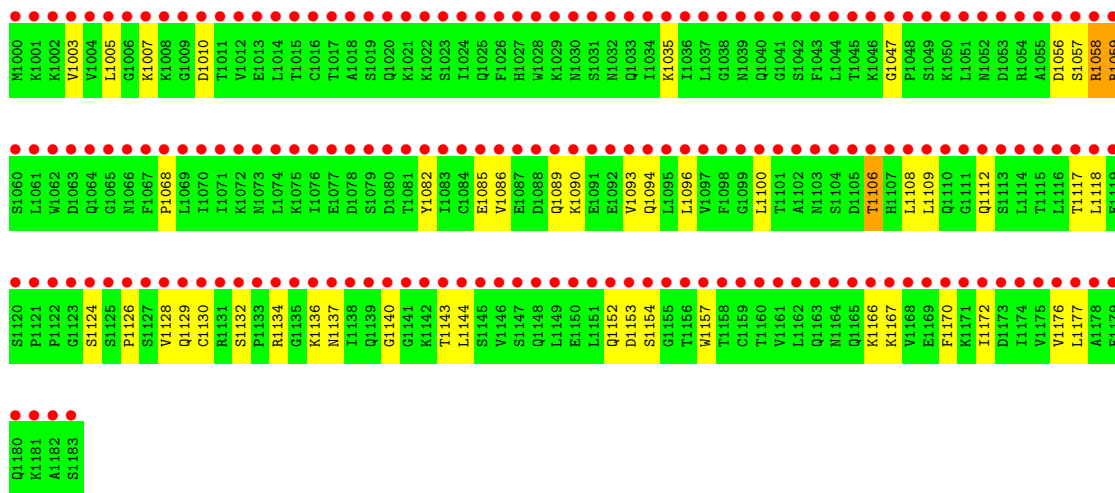
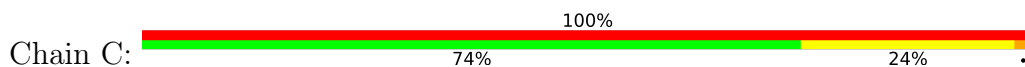
- Molecule 1: HIV-1 GP120 ENVELOPE GLYCOPROTEIN



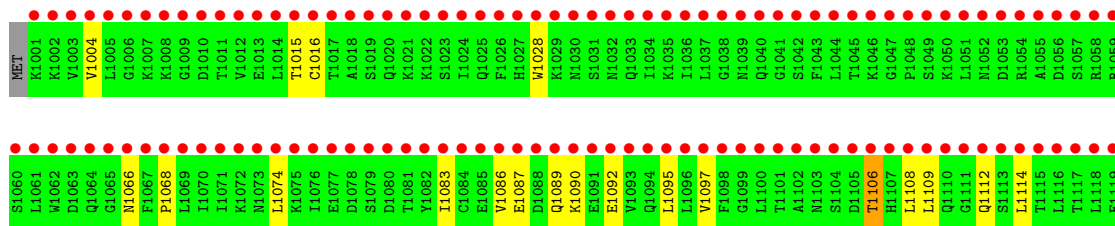
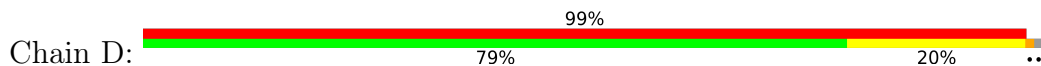




• Molecule 2: T-cell surface glycoprotein CD4

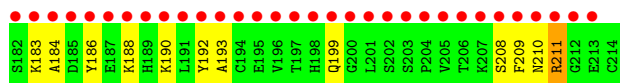
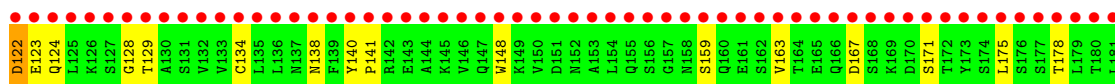
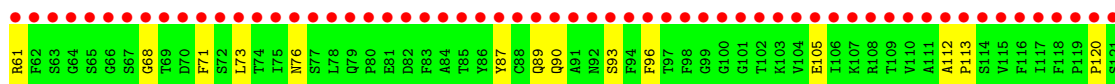
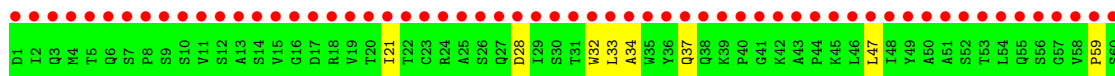
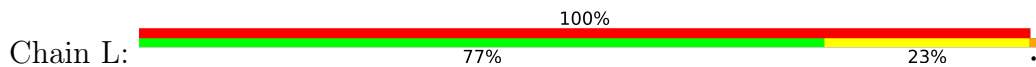


• Molecule 2: T-cell surface glycoprotein CD4

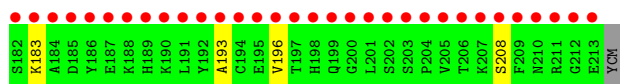
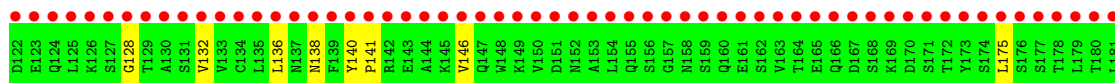
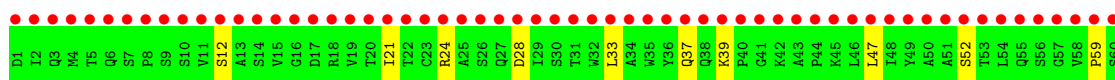
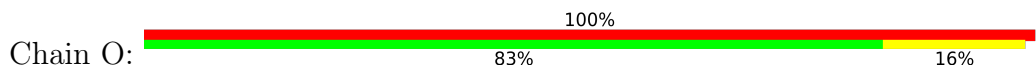




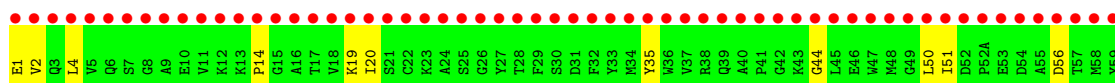
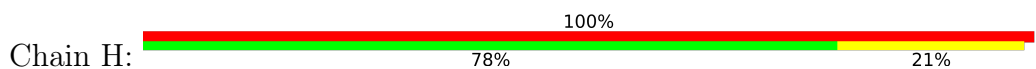
● Molecule 3: FAB 48D LIGHT CHAIN

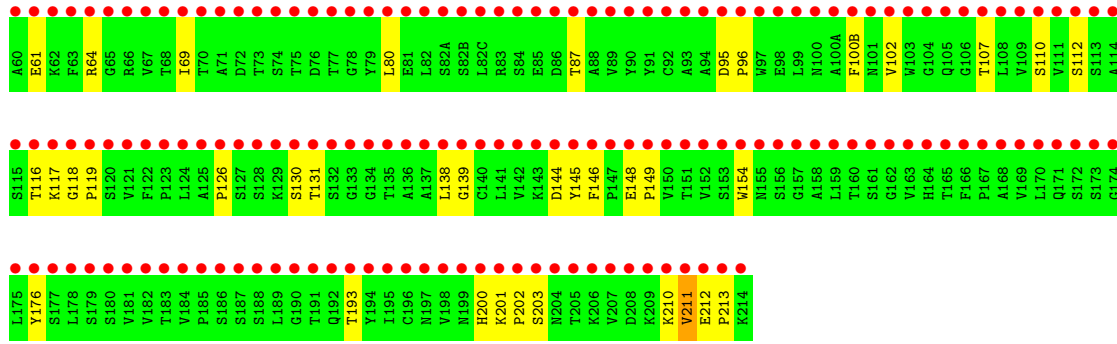


● Molecule 3: FAB 48D LIGHT CHAIN

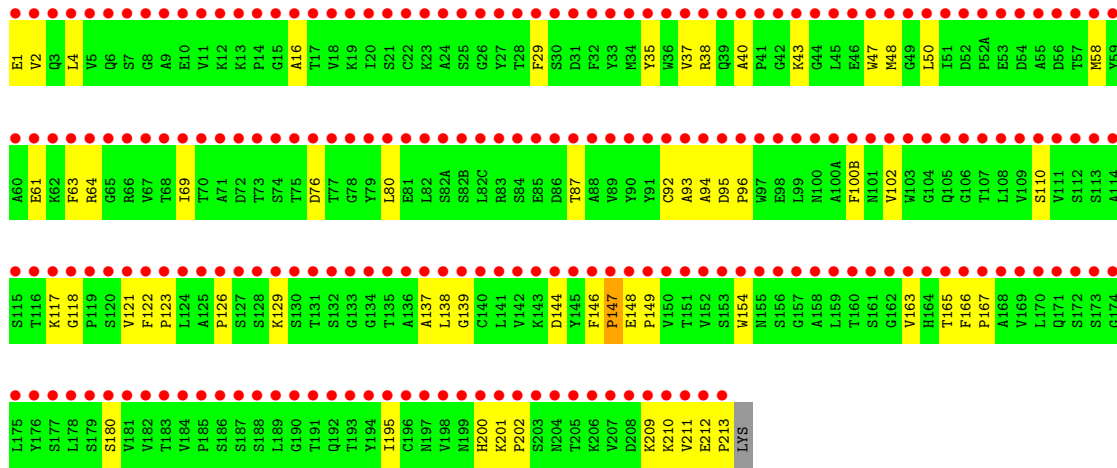
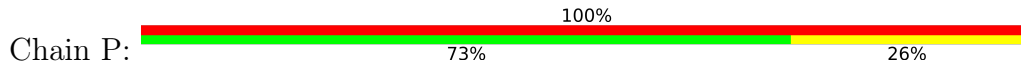


● Molecule 4: FAB 48D HEAVY CHAIN





● Molecule 4: FAB 48D HEAVY CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.11Å 172.95Å 193.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.86 – 2.61 43.86 – 2.61	Depositor EDS
% Data completeness (in resolution range)	63.8 (43.86-2.61) 63.9 (43.86-2.61)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.04 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (CCI APPS 2007_04_06_1210)	Depositor
R, $R_{free}$	0.201 , 0.275 0.203 , 0.283	Depositor DCC
$R_{free}$ test set	6030 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	-10.7	Xtrriage
Anisotropy	-7.799	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: NAG, GOL, YCM

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	0.24	0/2865	0.42	0/3900
1	B	0.22	0/2821	0.39	0/3841
2	C	0.23	0/1452	0.43	0/1955
2	D	0.22	0/1444	0.38	0/1945
3	L	0.23	0/1659	0.40	0/2252
3	O	0.21	0/1659	0.38	0/2252
4	H	0.22	0/1695	0.42	0/2311
4	P	0.21	0/1685	0.39	0/2300
All	All	0.22	0/15280	0.40	0/20756

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	2800	0	2724	67	0
1	B	2756	0	2683	68	0
2	C	1432	0	1460	35	0
2	D	1424	0	1451	21	0
3	L	1635	0	1582	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	1624	0	1574	19	0
4	H	1654	0	1613	30	0
4	P	1644	0	1600	37	0
5	A	140	0	130	2	0
5	B	126	0	117	2	0
6	B	6	0	8	3	0
6	P	6	0	8	0	0
7	A	135	0	0	1	0
7	B	68	0	0	0	0
7	C	50	0	0	1	0
7	D	34	0	0	0	0
7	H	47	0	0	0	0
7	L	54	0	0	1	0
7	O	23	0	0	0	0
7	P	39	0	0	0	0
All	All	15697	0	14950	299	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 10.

All (299) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:VAL:HB	6:B:1:GOL:H11	1.43	1.00
1:A:492:GLU:HB2	1:A:493:PRO:HD2	1.55	0.88
4:H:126:PRO:HD3	4:H:138:LEU:HD13	1.54	0.88
2:C:1085:GLU:HG2	2:C:1090:LYS:HG3	1.57	0.84
1:B:342:LEU:HB3	1:B:395:TRP:HE1	1.42	0.84
2:C:1058:ARG:HH12	2:C:1059:ARG:HH11	1.24	0.83
2:C:1058:ARG:NH1	2:C:1059:ARG:HH11	1.79	0.81
1:B:357:LYS:HD3	1:B:464:GLU:HA	1.62	0.81
1:A:45:TRP:CD1	1:A:489:VAL:HG21	2.16	0.80
1:B:51:THR:HA	1:B:103:GLN:HE22	1.48	0.78
2:C:1166:LYS:HD3	2:C:1167:LYS:H	1.49	0.76
3:O:21:ILE:HG21	3:O:102:THR:HG21	1.70	0.74
2:D:1106:THR:HB	2:D:1112:GLN:HG3	1.70	0.72
2:C:1106:THR:HB	2:C:1112:GLN:HG3	1.72	0.71
3:L:89:GLN:NE2	3:L:96:PHE:HB3	2.05	0.71
4:P:40:ALA:HB3	4:P:43:LYS:HB2	1.71	0.71
2:D:1131:ARG:HH21	2:D:1135:GLY:HA2	1.55	0.70
1:B:77:THR:HG22	1:B:78:ASP:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLU:HG2	1:B:487:LYS:HE3	1.73	0.69
3:L:190:LYS:HD2	3:L:211:ARG:HG2	1.74	0.69
2:D:1083:ILE:HG12	2:D:1092:GLU:HG3	1.75	0.69
4:H:20:ILE:HG21	4:H:107:THR:HG21	1.75	0.69
1:A:430:VAL:HG11	2:C:1059:ARG:HB2	1.75	0.68
4:P:93:ALA:HB1	4:P:100(B):PHE:HB3	1.75	0.68
3:L:89:GLN:HE21	3:L:96:PHE:HB3	1.60	0.67
1:B:78:ASP:HB3	1:B:81:PRO:CD	2.25	0.67
4:H:200:HIS:CE1	4:H:202:PRO:HB2	2.30	0.67
1:B:360:ILE:HG12	1:B:394:THR:HG23	1.76	0.66
1:B:123:THR:HG21	1:B:429:LYS:HE3	1.77	0.66
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.77	0.66
1:A:335:ARG:NH2	1:A:411:SER:HB3	2.11	0.66
2:C:1058:ARG:HH12	2:C:1059:ARG:NH1	1.94	0.65
1:A:64:GLU:OE2	1:A:66:HIS:HB2	1.96	0.65
1:A:77:THR:HG22	1:A:78:ASP:H	1.60	0.65
1:B:492:GLU:HB2	1:B:493:PRO:HD2	1.78	0.65
1:B:254:VAL:CB	6:B:1:GOL:H11	2.24	0.64
3:O:59:PRO:HB2	3:O:61:ARG:HG2	1.78	0.64
3:O:89:GLN:NE2	3:O:96:PHE:HB3	2.12	0.64
1:B:83:GLU:HB3	1:B:245:VAL:HG12	1.81	0.63
2:C:1100:LEU:HD21	2:C:1172:ILE:HD11	1.79	0.63
1:A:269:GLU:HA	1:A:289:ASN:HD22	1.64	0.63
4:P:61:GLU:HA	4:P:64:ARG:NH1	2.14	0.62
4:H:61:GLU:HA	4:H:64:ARG:NH1	2.15	0.62
1:A:420:ILE:HD12	1:A:420:ILE:H	1.64	0.61
1:A:360:ILE:HG12	1:A:394:THR:HG23	1.81	0.61
4:H:87:THR:HG23	4:H:110:SER:HA	1.82	0.61
4:H:138:LEU:HD11	4:H:211:VAL:HG11	1.82	0.61
1:A:492:GLU:HB2	1:A:493:PRO:CD	2.27	0.61
2:C:1132:SER:HB3	2:C:1136:LYS:HB3	1.82	0.61
4:P:69:ILE:HG12	4:P:80:LEU:HD12	1.83	0.61
4:P:121:VAL:HB	4:P:209:LYS:HG3	1.82	0.61
1:A:78:ASP:HB2	1:A:79:PRO:HA	1.82	0.61
1:B:75:VAL:HG13	1:B:76:PRO:HD2	1.83	0.61
2:D:1114:LEU:HB3	2:D:1146:VAL:HB	1.81	0.61
3:L:193:ALA:HB2	3:L:208:SER:HB3	1.82	0.60
3:O:193:ALA:HB2	3:O:208:SER:HB3	1.82	0.60
1:A:335:ARG:CZ	1:A:411:SER:HB3	2.32	0.60
2:C:1086:VAL:O	2:C:1089:GLN:HG2	2.01	0.60
2:C:1134:ARG:HD3	2:C:1152:GLN:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:HG13	1:B:475:MET:SD	2.43	0.58
1:A:108:ILE:HD12	1:A:253:PRO:HB3	1.84	0.58
2:C:1057:SER:HB2	2:C:1068:PRO:O	2.03	0.58
2:C:1140:GLY:HA3	2:C:1144:LEU:HG	1.85	0.58
1:B:338:TRP:NE1	1:B:342:LEU:HD11	2.19	0.58
2:C:1134:ARG:HH21	2:C:1136:LYS:HE2	1.69	0.58
1:A:45:TRP:HD1	1:A:489:VAL:HG21	1.66	0.58
2:C:1003:VAL:HG22	2:C:1094:GLN:HB3	1.86	0.58
1:B:78:ASP:HB3	1:B:81:PRO:HD2	1.86	0.57
4:P:200:HIS:CE1	4:P:202:PRO:HB2	2.40	0.57
1:B:330:HIS:HA	1:B:416:LEU:O	2.05	0.57
2:C:1108:LEU:HA	7:C:166:HOH:O	2.06	0.56
4:H:1:GLU:HG3	4:H:2:VAL:H	1.70	0.56
3:L:128:GLY:HA2	3:L:183:LYS:HD2	1.88	0.56
4:P:165:THR:HG23	4:P:180:SER:HB2	1.86	0.56
1:A:78:ASP:HB2	1:A:79:PRO:CA	2.36	0.55
1:B:52:LEU:HD12	1:B:52:LEU:H	1.71	0.55
1:B:64:GLU:HG3	1:B:67:ASN:H	1.72	0.55
1:B:80:ASN:N	1:B:81:PRO:HD3	2.21	0.55
4:P:117:LYS:HD3	4:P:118:GLY:O	2.05	0.55
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.42	0.55
4:P:87:THR:HG23	4:P:110:SER:HA	1.89	0.55
1:A:335:ARG:NE	1:A:411:SER:HB3	2.23	0.54
2:C:1118:LEU:HD22	2:C:1128:VAL:HG22	1.90	0.54
3:O:89:GLN:HE21	3:O:96:PHE:HB3	1.73	0.53
1:A:451:GLY:C	1:A:452:LEU:HD12	2.29	0.53
3:L:192:TYR:HB2	3:L:209:PHE:CE2	2.44	0.53
3:O:37:GLN:HB2	3:O:47:LEU:HD11	1.89	0.53
2:C:1154:SER:HB2	2:C:1176:VAL:HG12	1.90	0.53
1:B:108:ILE:HD13	1:B:253:PRO:HB3	1.91	0.52
1:B:350:ARG:O	1:B:355:ASN:HA	2.09	0.52
4:H:138:LEU:HD11	4:H:211:VAL:CG1	2.39	0.52
3:O:146:VAL:HG22	3:O:196:VAL:HG22	1.91	0.52
4:H:4:LEU:HD11	4:H:102:VAL:HG23	1.91	0.52
3:O:39:LYS:HG2	3:O:84:ALA:HB2	1.91	0.52
3:O:140:TYR:CG	3:O:141:PRO:HA	2.44	0.52
1:A:430:VAL:CG1	2:C:1059:ARG:HB2	2.40	0.51
1:B:297:THR:HA	1:B:443:ILE:O	2.10	0.51
2:D:1086:VAL:O	2:D:1089:GLN:HG2	2.10	0.51
2:D:1158:THR:HG22	2:D:1171:LYS:HG2	1.91	0.51
3:L:59:PRO:HB3	3:L:61:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1130:CYS:SG	2:C:1144:LEU:HD22	2.50	0.51
1:B:395:TRP:HA	1:B:395:TRP:CE3	2.45	0.51
1:A:90:THR:OG1	1:A:240:THR:HG22	2.12	0.50
1:B:361:PHE:HE2	1:B:395:TRP:HD1	1.59	0.50
2:D:1154:SER:HB2	2:D:1176:VAL:HB	1.93	0.50
4:H:117:LYS:HD3	4:H:118:GLY:N	2.26	0.50
1:B:388:THR:O	1:B:392:ASN:HB2	2.11	0.50
2:D:1066:ASN:O	2:D:1068:PRO:HD3	2.11	0.50
2:C:1089:GLN:C	2:C:1090:LYS:HD2	2.32	0.50
1:B:342:LEU:HB3	1:B:395:TRP:NE1	2.21	0.50
1:A:236:THR:O	5:A:734:NAG:H2	2.12	0.49
4:P:29:PHE:CD2	4:P:76:ASP:HA	2.47	0.49
4:P:195:ILE:CD1	4:P:210:LYS:HA	2.42	0.49
1:A:47:GLU:HG2	1:A:487:LYS:HE3	1.94	0.49
4:H:193:THR:HG23	4:H:210:LYS:HE3	1.93	0.49
3:L:184:ALA:O	3:L:188:LYS:HD3	2.12	0.49
2:C:1132:SER:CB	2:C:1136:LYS:HB3	2.42	0.49
3:O:136:LEU:HD13	3:O:175:LEU:HD22	1.93	0.49
3:O:89:GLN:HG2	3:O:90:GLN:O	2.12	0.49
2:C:1153:ASP:HB3	2:C:1157:TRP:HZ2	1.77	0.49
1:B:427:TRP:CE3	1:B:475:MET:HG3	2.47	0.49
2:D:1106:THR:HG21	2:D:1177:LEU:HD22	1.95	0.49
1:A:335:ARG:HH21	1:A:411:SER:HB3	1.78	0.49
1:A:351:GLU:HA	1:A:355:ASN:OD1	2.12	0.49
2:C:1166:LYS:CD	2:C:1167:LYS:H	2.24	0.49
1:A:294:ILE:HD12	1:A:333:ILE:HD11	1.94	0.48
1:A:420:ILE:HD12	1:A:420:ILE:N	2.26	0.48
1:B:77:THR:HG22	1:B:78:ASP:N	2.28	0.48
1:B:364:SER:OG	1:B:372:VAL:HA	2.13	0.48
2:D:1151:LEU:HD12	2:D:1176:VAL:HG11	1.95	0.48
3:O:28:ASP:OD1	3:O:68:GLY:HA2	2.12	0.48
1:A:70:ALA:O	1:A:74:CYS:HB2	2.13	0.48
3:L:167:ASP:O	3:L:171:SER:HA	2.12	0.48
1:B:342:LEU:HB2	1:B:395:TRP:HZ2	1.78	0.48
1:B:476:ARG:HA	1:B:479:TRP:CD1	2.49	0.48
4:H:200:HIS:HE1	4:H:202:PRO:HB2	1.78	0.48
1:B:59:LYS:HD3	1:B:61:TYR:OH	2.13	0.48
3:O:33:LEU:HD22	3:O:89:GLN:O	2.13	0.48
1:A:341:THR:O	1:A:345:ILE:HG13	2.12	0.48
3:L:90:GLN:O	3:L:96:PHE:HA	2.12	0.48
4:P:138:LEU:HD12	4:P:211:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:33:LEU:HG	3:L:34:ALA:N	2.29	0.48
4:H:148:GLU:HB3	4:H:149:PRO:HA	1.94	0.48
2:D:1132:SER:HB3	2:D:1136:LYS:HB3	1.95	0.48
1:A:77:THR:HG22	1:A:78:ASP:N	2.26	0.48
4:H:145:TYR:HD1	4:H:200:HIS:HE2	1.61	0.48
1:A:338:TRP:CE2	1:A:390:LEU:HD22	2.49	0.47
1:B:56:SER:OG	1:B:70:ALA:HB1	2.14	0.47
1:B:288:LEU:HD11	1:B:452:LEU:HD11	1.94	0.47
4:P:50:LEU:HG	4:P:58:MET:HB2	1.96	0.47
4:P:139:GLY:HA2	4:P:154:TRP:CH2	2.49	0.47
4:P:35:TYR:CG	4:P:100(B):PHE:CE1	3.02	0.47
4:P:195:ILE:HD13	4:P:210:LYS:HA	1.96	0.47
1:A:75:VAL:HG13	1:A:76:PRO:HD2	1.96	0.47
1:A:105:HIS:ND1	7:A:589:HOH:O	2.35	0.47
2:C:1082:TYR:O	2:C:1093:VAL:HG12	2.15	0.47
4:P:126:PRO:HG3	4:P:137:ALA:O	2.15	0.47
1:B:297:THR:HG21	1:B:330:HIS:NE2	2.30	0.47
4:H:14:PRO:HD3	4:H:112:SER:O	2.15	0.47
4:H:51:ILE:HA	4:H:56:ASP:O	2.15	0.47
1:A:43:PRO:HA	1:A:494:LEU:HD23	1.97	0.47
1:A:52:LEU:HD12	1:A:52:LEU:N	2.30	0.46
1:B:451:GLY:C	1:B:452:LEU:HD12	2.34	0.46
2:D:1108:LEU:O	2:D:1109:LEU:HB2	2.16	0.46
1:A:373:THR:HB	1:A:385:CYS:O	2.15	0.46
1:A:42:VAL:HG13	1:A:43:PRO:HD2	1.97	0.46
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.97	0.46
1:A:94:ASN:HA	1:A:236:THR:HG22	1.97	0.46
4:P:154:TRP:CD1	4:P:163:VAL:HG11	2.50	0.46
1:B:86:LEU:HB2	1:B:242:VAL:HG23	1.98	0.46
4:P:148:GLU:HB3	4:P:149:PRO:HA	1.98	0.46
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	0.46
3:L:183:LYS:HG3	7:L:247:HOH:O	2.15	0.46
4:H:212:GLU:HA	4:H:213:PRO:HD3	1.75	0.46
3:O:12:SER:HB3	3:O:105:GLU:OE1	2.16	0.46
4:P:47:TRP:HZ2	4:P:50:LEU:HD23	1.81	0.46
1:A:252:ARG:HA	1:A:253:PRO:HD3	1.76	0.45
1:A:357:LYS:HD3	1:A:466:GLU:HG2	1.98	0.45
4:P:48:MET:HG2	4:P:63:PHE:CE1	2.51	0.45
2:C:1007:LYS:HE3	2:C:1170:PHE:CE1	2.51	0.45
4:H:148:GLU:OE1	4:H:149:PRO:HA	2.16	0.45
1:B:59:LYS:HB3	1:B:61:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1089:GLN:C	2:D:1090:LYS:HD2	2.37	0.45
1:A:96:TRP:HD1	1:A:236:THR:HG21	1.81	0.45
3:L:159:SER:HA	3:L:178:THR:O	2.16	0.45
1:B:51:THR:HA	1:B:103:GLN:NE2	2.25	0.45
1:B:261:LEU:H	6:B:1:GOL:H12	1.81	0.45
2:D:1153:ASP:HB3	2:D:1157:TRP:HZ2	1.80	0.45
2:C:1129:GLN:NE2	2:C:1137:ASN:HB3	2.32	0.45
4:H:69:ILE:HG12	4:H:80:LEU:HD13	1.99	0.45
1:B:422:GLN:O	1:B:434:MET:HA	2.17	0.45
2:D:1086:VAL:HG22	2:D:1087:GLU:HG2	1.97	0.45
3:O:90:GLN:O	3:O:96:PHE:HA	2.17	0.45
4:H:116:THR:HG22	4:H:203:SER:HB3	1.97	0.45
1:A:270:VAL:HG22	1:A:288:LEU:HA	1.98	0.45
1:B:101:VAL:HG13	1:B:479:TRP:HB2	1.99	0.45
1:B:108:ILE:CD1	1:B:253:PRO:HB3	2.46	0.45
1:B:297:THR:HB	1:B:444:ARG:NH1	2.32	0.45
4:P:94:ALA:HB3	4:P:102:VAL:HG22	1.99	0.45
3:L:163:VAL:HG22	3:L:175:LEU:HD12	1.99	0.44
1:A:108:ILE:CD1	1:A:253:PRO:HB3	2.46	0.44
2:D:1128:VAL:HB	2:D:1144:LEU:HD11	1.98	0.44
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.79	0.44
1:A:358:THR:HG23	1:A:395:TRP:O	2.18	0.44
1:A:420:ILE:HG22	1:A:421:LYS:N	2.32	0.44
2:C:1124:SER:O	2:C:1126:PRO:HD3	2.17	0.44
2:C:1117:THR:HG23	2:C:1143:THR:HG22	2.00	0.44
2:C:1154:SER:HB2	2:C:1176:VAL:CG1	2.47	0.44
3:L:124:GLN:HG2	3:L:129:THR:O	2.18	0.44
4:H:95:ASP:N	4:H:96:PRO:HD3	2.33	0.44
1:B:205:CYS:N	1:B:206:PRO:HD3	2.33	0.44
4:P:129:LYS:HD3	4:P:129:LYS:C	2.38	0.44
3:L:128:GLY:CA	3:L:183:LYS:HD2	2.47	0.44
1:B:200:VAL:HG21	4:P:64:ARG:CZ	2.48	0.44
3:O:120:PRO:HD3	3:O:132:VAL:HG22	2.00	0.44
1:A:101:VAL:HG21	1:A:480:ARG:HG2	2.00	0.44
1:B:358:THR:HG23	1:B:396:PHE:CD1	2.53	0.44
1:A:118:PRO:HD2	1:A:203:GLN:NE2	2.32	0.44
2:C:1005:LEU:CD2	2:C:1096:LEU:HB2	2.48	0.44
1:B:33:LYS:HG3	1:B:35:TRP:H	1.83	0.44
4:P:4:LEU:HD12	4:P:102:VAL:HG23	2.00	0.44
3:L:210:ASN:HB3	3:L:211:ARG:H	1.47	0.43
4:H:145:TYR:CZ	4:H:176:TYR:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PRO:HG2	5:B:762:NAG:O7	2.18	0.43
1:A:422:GLN:O	1:A:434:MET:HA	2.18	0.43
1:B:439:ILE:HB	1:B:440:SER:H	1.57	0.43
1:A:88:ASN:HB2	5:A:588:NAG:O5	2.17	0.43
3:L:122:ASP:OD2	3:L:123:GLU:HG3	2.18	0.43
1:A:437:PRO:HB2	3:L:32:TRP:CZ2	2.54	0.43
1:B:492:GLU:HB2	1:B:493:PRO:CD	2.47	0.43
1:B:50:THR:HG21	1:B:223:PHE:CZ	2.53	0.43
2:D:1106:THR:HB	2:D:1112:GLN:CG	2.44	0.43
4:P:148:GLU:OE1	4:P:149:PRO:HA	2.18	0.43
3:O:24:ARG:HA	3:O:69:THR:O	2.18	0.43
1:B:53:PHE:CE2	1:B:218:CYS:HB2	2.53	0.43
4:H:116:THR:HA	4:H:146:PHE:O	2.19	0.43
1:B:246:GLN:HG3	1:B:247:CYS:SG	2.59	0.43
2:D:1074:LEU:HB3	2:D:1097:VAL:HG11	2.00	0.43
4:P:37:VAL:HG12	4:P:38:ARG:N	2.34	0.43
2:C:1118:LEU:HD22	2:C:1128:VAL:CG2	2.48	0.43
1:B:122:LEU:CD2	1:B:200:VAL:HG22	2.49	0.43
1:B:349:LEU:HB2	1:B:359:ILE:HD13	2.00	0.43
4:H:50:LEU:HD12	4:H:50:LEU:C	2.40	0.42
4:P:212:GLU:HA	4:P:213:PRO:HD3	1.92	0.42
1:A:65:VAL:HG21	1:A:210:PHE:CD1	2.54	0.42
1:B:358:THR:OG1	1:B:396:PHE:HE1	2.02	0.42
1:A:123:THR:HG21	1:A:429:LYS:HE3	2.02	0.42
1:A:475:MET:HA	1:A:478:ASN:OD1	2.19	0.42
4:P:95:ASP:N	4:P:96:PRO:HD3	2.34	0.42
1:A:376:PHE:HE2	1:A:378:CYS:HB2	1.84	0.42
1:B:335:ARG:NH2	1:B:411:SER:HB2	2.34	0.42
1:A:292:VAL:HG13	1:A:337:LYS:HE3	2.00	0.42
1:B:263:GLY:C	1:B:450:THR:HG21	2.40	0.42
4:P:201:LYS:N	4:P:202:PRO:CD	2.81	0.42
1:A:294:ILE:O	1:A:294:ILE:HG23	2.19	0.42
1:A:421:LYS:HE2	1:A:421:LYS:HB3	1.80	0.42
3:L:28:ASP:OD1	3:L:68:GLY:HA2	2.20	0.42
1:A:297:THR:HB	1:A:444:ARG:NH2	2.34	0.42
1:B:260:LEU:HD12	1:B:451:GLY:HA3	2.02	0.42
1:A:456:ARG:HD2	1:A:466:GLU:OE1	2.19	0.42
1:A:463:ASN:O	1:A:464:GLU:HB2	2.20	0.42
4:P:146:PHE:HA	4:P:147:PRO:HA	1.71	0.42
1:B:219:ALA:HA	1:B:220:PRO:HD3	1.86	0.42
1:A:368:ASP:O	1:A:372:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:120:PRO:HG2	3:L:186:TYR:CZ	2.55	0.41
1:B:269:GLU:HG2	5:B:789:NAG:HN2	1.85	0.41
1:A:330:HIS:HA	1:A:416:LEU:O	2.20	0.41
1:B:341:THR:O	1:B:345:ILE:HG13	2.20	0.41
3:L:134:CYS:HB2	3:L:148:TRP:CZ2	2.55	0.41
4:P:1:GLU:HG3	4:P:2:VAL:H	1.85	0.41
1:A:93:PHE:HE2	1:A:239:CYS:HB3	1.85	0.41
1:A:273:ARG:NH2	1:A:484:TYR:CE2	2.89	0.41
1:B:200:VAL:HG11	4:P:64:ARG:NH2	2.35	0.41
2:D:1004:VAL:O	2:D:1095:LEU:HD12	2.20	0.41
4:P:4:LEU:HD13	4:P:92:CYS:O	2.19	0.41
4:P:93:ALA:CB	4:P:100(B):PHE:HB3	2.47	0.41
3:L:112:ALA:HA	3:L:113:PRO:HD3	1.84	0.41
2:C:1134:ARG:NH1	2:C:1152:GLN:HB2	2.35	0.41
4:H:19:LYS:HA	4:H:80:LEU:O	2.21	0.41
1:B:365:SER:HB2	1:B:469:ARG:HD3	2.03	0.41
3:L:87:TYR:OH	4:H:44:GLY:HA2	2.21	0.41
1:A:370:GLU:HA	1:A:375:TRP:HB2	2.01	0.41
2:C:1035:LYS:O	2:C:1047:GLY:HA3	2.20	0.41
3:L:21:ILE:HD11	3:L:73:LEU:HD23	2.03	0.41
4:H:118:GLY:HA2	4:H:119:PRO:HD3	1.91	0.41
3:O:112:ALA:HA	3:O:113:PRO:HD3	1.80	0.41
4:P:122:PHE:HA	4:P:123:PRO:HD3	1.82	0.41
2:C:1108:LEU:O	2:C:1109:LEU:HB2	2.20	0.41
4:H:139:GLY:HA2	4:H:154:TRP:CH2	2.55	0.41
4:H:201:LYS:N	4:H:202:PRO:CD	2.83	0.41
3:O:128:GLY:HA2	3:O:183:LYS:HB2	2.02	0.41
4:H:35:TYR:CG	4:H:100(B):PHE:CE1	3.09	0.41
1:A:480:ARG:O	1:A:484:TYR:HB3	2.20	0.40
2:D:1016:CYS:HB2	2:D:1028:TRP:CZ2	2.57	0.40
4:P:166:PHE:HA	4:P:167:PRO:HD3	1.97	0.40
1:A:96:TRP:CD1	1:A:236:THR:HG21	2.56	0.40
1:B:374:HIS:CE1	1:B:376:PHE:CD1	3.10	0.40
2:D:1124:SER:HB2	2:D:1163:GLN:NE2	2.37	0.40
1:B:52:LEU:HD12	1:B:52:LEU:N	2.36	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	356/379 (94%)	311 (87%)	40 (11%)	5 (1%)	11	21
1	B	350/379 (92%)	314 (90%)	31 (9%)	5 (1%)	11	21
2	C	182/184 (99%)	168 (92%)	13 (7%)	1 (0%)	29	50
2	D	181/184 (98%)	159 (88%)	22 (12%)	0	100	100
3	L	211/213 (99%)	194 (92%)	14 (7%)	3 (1%)	11	21
3	O	210/213 (99%)	181 (86%)	26 (12%)	3 (1%)	11	21
4	H	218/220 (99%)	193 (88%)	22 (10%)	3 (1%)	11	21
4	P	217/220 (99%)	194 (89%)	20 (9%)	3 (1%)	11	21
All	All	1925/1992 (97%)	1714 (89%)	188 (10%)	23 (1%)	13	25

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	76	ASN
3	L	138	ASN
1	B	439	ILE
1	B	440	SER
1	A	356	ASN
4	H	130	SER
4	H	144	ASP
1	B	220	PRO
3	O	52	SER
4	P	144	ASP
1	A	241	ASN
1	A	439	ILE
2	C	1056	ASP
3	L	93	SER
4	H	131	THR
1	B	356	ASN
1	B	441	GLY

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Mol	Chain	Res	Type
4	P	16	ALA
3	O	138	ASN
1	A	462	ASN
1	A	487	LYS
3	O	100	GLY
4	P	147	PRO

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	315/333 (95%)	310 (98%)	5 (2%)	62 81
1	B	310/333 (93%)	309 (100%)	1 (0%)	92 97
2	C	166/166 (100%)	161 (97%)	5 (3%)	41 66
2	D	165/166 (99%)	162 (98%)	3 (2%)	59 79
3	L	184/184 (100%)	180 (98%)	4 (2%)	52 74
3	O	184/184 (100%)	184 (100%)	0	100 100
4	H	185/185 (100%)	184 (100%)	1 (0%)	88 95
4	P	184/185 (100%)	184 (100%)	0	100 100
All	All	1693/1736 (98%)	1674 (99%)	19 (1%)	73 88

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLU
1	A	77	THR
1	A	297	THR
1	A	374	HIS
1	A	488	VAL
2	C	1010	ASP
2	C	1058	ARG
2	C	1059	ARG
2	C	1106	THR

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Mol	Chain	Res	Type
2	C	1177	LEU
3	L	105	GLU
3	L	122	ASP
3	L	199	GLN
3	L	211	ARG
4	H	211	VAL
1	B	396	PHE
2	D	1015	THR
2	D	1106	THR
2	D	1168	VAL

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

Mol	Chain	Res	Type
3	O	27	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](#)

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
3	YCM	L	214	3	8,10,10	1.07	0	8,12,12	0.92	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
3	YCM	L	214	3	-	3/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	214	YCM	O-C-CA-N
3	L	214	YCM	CE-CD-SG-CB
3	L	214	YCM	OXT-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

21 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	B	734	1	14,14,15	0.51	0	17,19,21	0.75	0
5	NAG	A	762	1	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
5	NAG	B	588	1	14,14,15	0.51	0	17,19,21	0.75	1 (5%)
5	NAG	B	892	1	14,14,15	0.54	0	17,19,21	0.69	0
5	NAG	A	892	1	14,14,15	0.60	0	17,19,21	1.37	2 (11%)
6	GOL	P	215	-	5,5,5	0.39	0	5,5,5	0.25	0
5	NAG	B	886	1	14,14,15	0.50	0	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	795	1	14,14,15	0.47	0	17,19,21	0.83	1 (5%)
5	NAG	A	948	1	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
5	NAG	A	741	1	14,14,15	0.48	0	17,19,21	0.91	1 (5%)
5	NAG	B	789	1	14,14,15	0.52	0	17,19,21	0.92	1 (5%)
5	NAG	B	776	1	14,14,15	0.50	0	17,19,21	0.84	1 (5%)
5	NAG	A	897	1	14,14,15	0.55	0	17,19,21	0.78	0
5	NAG	A	734	1	14,14,15	0.54	0	17,19,21	0.79	0
5	NAG	B	948	1	14,14,15	0.52	0	17,19,21	0.76	0
5	NAG	A	588	1	14,14,15	0.53	0	17,19,21	0.98	1 (5%)
6	GOL	B	1	-	5,5,5	0.39	0	5,5,5	0.26	0
5	NAG	A	886	1	14,14,15	0.51	0	17,19,21	0.82	1 (5%)
5	NAG	B	762	1	14,14,15	0.54	0	17,19,21	0.87	1 (5%)
5	NAG	A	776	1	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
5	NAG	A	789	1	14,14,15	0.58	0	17,19,21	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	B	734	1	-	3/6/23/26	0/1/1/1
5	NAG	A	762	1	-	2/6/23/26	0/1/1/1
5	NAG	B	588	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	B	892	1	-	4/6/23/26	0/1/1/1
5	NAG	A	892	1	-	3/6/23/26	0/1/1/1
6	GOL	P	215	-	-	2/4/4/4	-
5	NAG	B	886	1	-	2/6/23/26	0/1/1/1
5	NAG	B	795	1	-	2/6/23/26	0/1/1/1
5	NAG	A	948	1	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	A	741	1	-	2/6/23/26	0/1/1/1
5	NAG	B	789	1	-	2/6/23/26	0/1/1/1
5	NAG	B	776	1	-	0/6/23/26	0/1/1/1
5	NAG	A	897	1	-	3/6/23/26	0/1/1/1
5	NAG	A	734	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	B	948	1	-	2/6/23/26	0/1/1/1
5	NAG	A	588	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	1	-	-	0/4/4/4	-
5	NAG	A	886	1	-	4/6/23/26	0/1/1/1
5	NAG	B	762	1	-	3/6/23/26	0/1/1/1
5	NAG	A	776	1	-	2/6/23/26	0/1/1/1
5	NAG	A	789	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	892	NAG	C1-O5-C5	3.76	117.29	112.19
5	A	892	NAG	O5-C1-C2	3.34	116.56	111.29
5	A	588	NAG	C1-O5-C5	3.07	116.35	112.19
5	B	886	NAG	C1-O5-C5	2.90	116.12	112.19
5	A	741	NAG	C1-O5-C5	2.83	116.02	112.19
5	B	762	NAG	C1-O5-C5	2.51	115.59	112.19
5	A	776	NAG	C1-O5-C5	2.38	115.42	112.19
5	A	948	NAG	O5-C1-C2	2.27	114.87	111.29
5	A	886	NAG	C1-O5-C5	2.23	115.22	112.19
5	B	795	NAG	C1-O5-C5	2.23	115.21	112.19
5	A	762	NAG	C1-O5-C5	2.19	115.16	112.19
5	B	776	NAG	C1-O5-C5	2.19	115.16	112.19
5	B	588	NAG	C1-O5-C5	2.17	115.13	112.19
5	B	789	NAG	C1-O5-C5	2.12	115.06	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	734	NAG	C1
5	A	948	NAG	C1
5	B	588	NAG	C1

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	588	NAG	C8-C7-N2-C2
5	A	588	NAG	O7-C7-N2-C2
5	A	734	NAG	C8-C7-N2-C2
5	A	734	NAG	O7-C7-N2-C2
5	A	741	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	A	789	NAG	C8-C7-N2-C2
5	A	789	NAG	O7-C7-N2-C2
5	A	886	NAG	C8-C7-N2-C2
5	A	886	NAG	O7-C7-N2-C2
5	A	897	NAG	C3-C2-N2-C7
5	A	897	NAG	C8-C7-N2-C2
5	A	897	NAG	O7-C7-N2-C2
5	B	588	NAG	C8-C7-N2-C2
5	B	588	NAG	O7-C7-N2-C2
5	B	734	NAG	C1-C2-N2-C7
5	B	734	NAG	C8-C7-N2-C2
5	B	734	NAG	O7-C7-N2-C2
5	B	789	NAG	C8-C7-N2-C2
5	B	789	NAG	O7-C7-N2-C2
5	B	795	NAG	C8-C7-N2-C2
5	B	795	NAG	O7-C7-N2-C2
5	B	892	NAG	C8-C7-N2-C2
5	B	892	NAG	O7-C7-N2-C2
6	P	215	GOL	O1-C1-C2-C3
5	A	741	NAG	C8-C7-N2-C2
5	B	948	NAG	C8-C7-N2-C2
5	A	776	NAG	C8-C7-N2-C2
5	B	948	NAG	O7-C7-N2-C2
5	A	734	NAG	C1-C2-N2-C7
5	A	886	NAG	O5-C5-C6-O6
5	B	892	NAG	O5-C5-C6-O6
5	A	776	NAG	O7-C7-N2-C2
5	B	762	NAG	C8-C7-N2-C2
5	A	762	NAG	O5-C5-C6-O6
5	B	886	NAG	O5-C5-C6-O6
5	A	886	NAG	C4-C5-C6-O6
5	B	762	NAG	O7-C7-N2-C2
5	B	762	NAG	O5-C5-C6-O6
6	P	215	GOL	O1-C1-C2-O2
5	B	892	NAG	C4-C5-C6-O6
5	A	892	NAG	C8-C7-N2-C2
5	A	892	NAG	O7-C7-N2-C2
5	A	892	NAG	O5-C5-C6-O6
5	A	762	NAG	C4-C5-C6-O6
5	A	948	NAG	C8-C7-N2-C2
5	B	886	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	789	NAG	1	0
5	A	734	NAG	1	0
5	A	588	NAG	1	0
6	B	1	GOL	3	0
5	B	762	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	360/379 (94%)	13.35	360 (100%) 0 0	45, 78, 151, 254	0
1	B	354/379 (93%)	13.06	354 (100%) 0 0	66, 113, 190, 233	0
2	C	184/184 (100%)	13.62	184 (100%) 0 0	56, 83, 125, 144	0
2	D	183/184 (99%)	13.21	183 (100%) 0 0	74, 127, 165, 188	0
3	L	212/213 (99%)	13.88	212 (100%) 0 0	59, 101, 179, 240	0
3	O	212/213 (99%)	12.92	212 (100%) 0 0	91, 147, 189, 220	0
4	H	220/220 (100%)	14.05	220 (100%) 0 0	70, 121, 179, 251	0
4	P	219/220 (99%)	13.54	219 (100%) 0 0	66, 121, 195, 243	0
All	All	1944/1992 (97%)	13.42	1944 (100%) 0 0	45, 110, 180, 254	0

All (1944) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	41	GLY	26.9
1	B	385	CYS	24.7
4	H	88	ALA	24.6
4	P	26	GLY	23.8
1	A	228	CYS	23.7
1	A	388	THR	23.5
1	A	54	CYS	23.1
1	A	235	GLY	23.1
2	C	1133	PRO	23.1
1	A	447	SER	22.6
1	A	230	ASN	22.4
2	D	1133	PRO	22.1
4	P	145	TYR	22.0
2	C	1159	CYS	22.0
1	B	222	GLY	21.9
4	P	28	THR	21.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	240	THR	21.6
1	A	84	VAL	21.6
2	D	1028	TRP	21.6
2	C	1006	GLY	21.6
3	L	178	THR	21.5
4	H	186	SER	21.5
2	C	1028	TRP	21.3
1	B	259	LEU	21.3
4	H	162	GLY	21.3
3	L	88	CYS	21.3
1	B	220	PRO	21.2
1	A	210	PHE	21.1
1	B	369	PRO	21.1
1	A	41	GLY	21.1
3	L	52	SER	21.0
1	B	244	THR	21.0
1	A	74	CYS	21.0
4	H	17	THR	20.9
1	A	55	ALA	20.9
3	L	180	THR	20.8
4	P	92	CYS	20.8
2	D	1006	GLY	20.8
1	A	296	CYS	20.6
3	O	43	ALA	20.6
4	H	109	VAL	20.6
3	O	112	ALA	20.4
2	C	1084	CYS	20.2
4	P	111	VAL	20.2
3	L	82	ASP	20.2
2	D	1111	GLY	20.2
1	A	48	ALA	20.1
3	L	68	GLY	20.1
2	C	1125	SER	20.1
4	P	115	SER	20.1
4	H	196	CYS	20.1
2	C	1102	ALA	20.1
4	H	82(C)	LEU	20.0
4	P	17	THR	20.0
3	O	130	ALA	20.0
1	A	331	CYS	20.0
4	H	165	THR	19.9
4	P	188	SER	19.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	H	20	ILE	19.9
1	A	219	ALA	19.8
1	B	119	CYS	19.8
4	H	185	PRO	19.8
4	P	88	ALA	19.8
1	B	72	HIS	19.7
1	A	385	CYS	19.7
4	H	204	ASN	19.7
3	O	40	PRO	19.7
3	L	67	SER	19.7
2	D	1047	GLY	19.7
2	C	1005	LEU	19.6
3	O	111	ALA	19.5
1	A	57	ASP	19.5
3	L	191	LEU	19.5
4	H	208	ASP	19.5
4	P	120	SER	19.4
3	L	168	SER	19.4
3	O	60	SER	19.3
1	A	68	VAL	19.3
2	C	1120	SER	19.3
4	H	111	VAL	19.2
4	P	113	SER	19.2
3	L	176	SER	19.2
4	H	86	ASP	19.2
1	A	112	TRP	19.1
4	H	76	ASP	19.1
4	H	112	SER	19.1
1	B	488	VAL	19.1
4	H	126	PRO	19.1
2	C	1009	GLY	19.0
2	D	1084	CYS	19.0
3	O	150	VAL	18.9
3	L	72	SER	18.9
4	H	170	LEU	18.8
1	B	54	CYS	18.8
4	P	172	SER	18.8
3	L	51	ALA	18.8
4	P	100	ASN	18.8
3	L	101	GLY	18.7
4	H	163	VAL	18.7
4	H	30	SER	18.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	373	THR	18.6
4	H	40	ALA	18.6
3	L	47	LEU	18.6
3	O	46	LEU	18.6
1	A	218	CYS	18.6
4	H	180	SER	18.6
2	C	1061	LEU	18.5
2	D	1175	VAL	18.5
4	H	77	THR	18.5
1	B	110	SER	18.4
4	P	8	GLY	18.4
3	L	60	SER	18.4
4	P	52(A)	PRO	18.4
1	A	443	ILE	18.4
1	A	465	SER	18.4
1	B	218	CYS	18.4
2	C	1130	CYS	18.3
4	H	137	ALA	18.3
4	P	203	SER	18.3
2	C	1122	PRO	18.3
4	H	188	SER	18.3
3	O	182	SER	18.2
3	L	91	ALA	18.2
1	A	216	HIS	18.2
1	B	359	ILE	18.2
1	A	94	ASN	18.2
1	A	105	HIS	18.2
2	D	1125	SER	18.2
2	C	1095	LEU	18.2
2	D	1103	ASN	18.2
4	H	9	ALA	18.1
1	A	448	ASN	18.1
2	D	1099	GLY	18.1
1	B	120	VAL	18.1
4	P	184	VAL	18.1
1	A	70	ALA	18.0
2	D	1154	SER	18.0
2	C	1129	GLN	18.0
3	L	177	SER	18.0
1	A	446	SER	18.0
2	D	1170	PHE	18.0
4	P	76	ASP	18.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	338	TRP	17.9
4	H	187	SER	17.9
1	B	122	LEU	17.9
3	L	80	PRO	17.9
3	L	37	GLN	17.9
1	A	436	ALA	17.9
2	C	1111	GLY	17.9
1	A	122	LEU	17.9
1	B	354	GLY	17.9
4	H	178	LEU	17.9
4	H	156	SER	17.8
1	B	329	GLY	17.8
4	P	90	TYR	17.8
2	C	1113	SER	17.8
3	O	14	SER	17.7
4	P	149	PRO	17.7
2	C	1078	ASP	17.7
1	B	45	TRP	17.7
1	A	236	THR	17.7
1	B	414	ILE	17.7
4	H	100	ASN	17.7
4	H	149	PRO	17.7
4	P	156	SER	17.7
4	P	153	SER	17.7
2	C	1010	ASP	17.7
1	A	459	GLY	17.7
2	C	1037	LEU	17.6
3	O	85	THR	17.7
2	D	1116	LEU	17.6
3	O	22	THR	17.6
3	L	173	TYR	17.6
1	B	253	PRO	17.6
4	H	96	PRO	17.6
1	B	87	VAL	17.5
1	A	119	CYS	17.5
3	L	198	HIS	17.5
3	O	177	SER	17.5
3	L	113	PRO	17.5
3	O	73	LEU	17.5
1	A	431	GLY	17.5
1	A	479	TRP	17.5
2	C	1183	SER	17.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	134	CYS	17.4
3	O	1	ASP	17.4
1	B	374	HIS	17.4
2	D	1132	SER	17.4
4	H	16	ALA	17.4
4	H	52(A)	PRO	17.3
1	A	205	CYS	17.3
3	L	84	ALA	17.3
1	A	413	THR	17.3
4	H	193	THR	17.3
2	D	1130	CYS	17.3
1	B	208	VAL	17.3
3	L	111	ALA	17.3
2	C	1011	THR	17.3
3	O	35	TRP	17.3
1	B	333	ILE	17.2
4	P	73	THR	17.2
3	L	204	PRO	17.2
2	D	1128	VAL	17.2
1	A	118	PRO	17.2
4	H	140	CYS	17.2
1	B	230	ASN	17.1
2	C	1153	ASP	17.1
3	O	59	PRO	17.1
3	L	102	THR	17.1
1	B	251	ILE	17.1
3	L	40	PRO	17.1
2	D	1127	SER	17.1
1	A	72	HIS	17.1
1	A	79	PRO	17.1
4	P	102	VAL	17.0
3	L	41	GLY	17.0
1	A	491	ILE	17.0
1	B	111	LEU	17.0
4	H	157	GLY	17.0
2	C	1156	THR	17.0
4	H	36	TRP	16.9
3	O	69	THR	16.9
1	B	366	GLY	16.9
2	C	1040	GLN	16.9
3	L	132	VAL	16.9
1	A	375	TRP	16.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	O	101	GLY	16.9
3	L	194	CYS	16.9
3	L	172	THR	16.9
2	C	1055	ALA	16.9
1	A	332	ASN	16.8
1	A	445	CYS	16.8
1	B	458	GLY	16.8
4	P	139	GLY	16.8
3	O	87	TYR	16.8
2	C	1097	VAL	16.8
2	C	1081	THR	16.8
3	O	72	SER	16.8
2	D	1161	VAL	16.8
3	L	69	THR	16.8
3	O	30	SER	16.8
3	L	10	SER	16.7
1	A	384	TYR	16.7
4	H	15	GLY	16.7
2	D	1079	SER	16.6
3	L	71	PHE	16.6
2	C	1036	ILE	16.6
1	A	393	SER	16.6
4	P	101	ASN	16.6
1	B	475	MET	16.6
3	L	21	ILE	16.6
4	H	181	VAL	16.6
4	H	174	GLY	16.6
3	L	36	TYR	16.6
1	B	107	ASP	16.5
2	C	1031	SER	16.5
3	L	114	SER	16.5
4	P	187	SER	16.5
3	L	19	VAL	16.5
2	C	1182	ALA	16.5
3	L	79	GLN	16.5
4	H	89	VAL	16.5
1	B	360	ILE	16.5
2	D	1146	VAL	16.5
4	H	160	THR	16.5
1	A	213	ILE	16.5
3	L	116	PHE	16.5
2	D	1162	LEU	16.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	22	THR	16.5
2	C	1103	ASN	16.4
3	O	36	TYR	16.4
1	A	495	GLY	16.4
1	A	99	ASP	16.4
2	D	1153	ASP	16.4
2	C	1079	SER	16.4
4	P	134	GLY	16.4
4	P	180	SER	16.4
3	O	98	PHE	16.4
4	H	47	TRP	16.4
1	A	104	MET	16.4
2	C	1146	VAL	16.4
1	B	70	ALA	16.4
4	H	24	ALA	16.4
1	A	425	ASN	16.4
1	B	223	PHE	16.4
4	H	138	LEU	16.4
4	H	166	PHE	16.4
4	P	160	THR	16.4
1	A	203	GLN	16.4
4	H	207	VAL	16.4
3	O	80	PRO	16.3
1	A	295	ASN	16.3
1	A	77	THR	16.3
3	L	25	ALA	16.3
2	C	1048	PRO	16.3
3	L	98	PHE	16.3
1	B	77	THR	16.3
3	O	178	THR	16.3
4	P	19	LYS	16.3
4	P	31	ASP	16.3
3	L	163	VAL	16.3
1	B	393	SER	16.3
3	L	74	THR	16.3
4	H	161	SER	16.3
4	H	194	TYR	16.3
1	A	52	LEU	16.3
2	D	1069	LEU	16.3
4	H	34	MET	16.3
4	H	121	VAL	16.3
2	C	1117	THR	16.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	181	LEU	16.3
3	L	11	VAL	16.3
1	B	384	TYR	16.2
4	P	50	LEU	16.2
2	D	1083	ILE	16.2
3	O	53	THR	16.2
3	L	119	PRO	16.2
4	H	95	ASP	16.2
4	P	84	SER	16.2
4	H	70	THR	16.2
1	A	85	VAL	16.2
1	B	55	ALA	16.2
4	H	203	SER	16.2
3	O	64	GLY	16.2
4	P	44	GLY	16.2
1	A	412	ASP	16.2
2	D	1010	ASP	16.2
4	H	103	TRP	16.2
3	O	102	THR	16.1
3	L	77	SER	16.1
3	O	135	LEU	16.1
2	D	1055	ALA	16.1
3	L	106	ILE	16.1
3	L	70	ASP	16.1
1	A	204	ALA	16.1
1	A	426	MET	16.1
4	H	11	VAL	16.1
1	A	71	THR	16.1
1	A	398	SER	16.1
4	H	84	SER	16.1
3	O	104	VAL	16.0
3	O	127	SER	16.0
4	H	94	ALA	16.0
4	P	109	VAL	16.0
4	P	157	GLY	16.0
1	A	333	ILE	16.0
4	H	119	PRO	16.0
1	B	426	MET	16.0
1	B	68	VAL	16.0
3	O	134	CYS	16.0
1	B	206	PRO	16.0
3	L	83	PHE	16.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	276	ASN	16.0
1	B	436	ALA	16.0
3	O	15	VAL	16.0
1	B	81	PRO	16.0
4	P	179	SER	16.0
1	B	484	TYR	16.0
3	L	179	LEU	16.0
4	P	91	TYR	16.0
1	B	410	GLY	16.0
2	C	1049	SER	16.0
2	D	1017	THR	15.9
4	P	137	ALA	15.9
4	H	134	GLY	15.9
4	P	151	THR	15.9
3	L	170	ASP	15.9
4	P	69	ILE	15.9
1	A	249	HIS	15.9
3	L	43	ALA	15.9
3	O	129	THR	15.9
1	A	245	VAL	15.9
1	A	69	TRP	15.9
2	D	1051	LEU	15.8
3	O	144	ALA	15.8
3	O	209	PHE	15.8
2	C	1054	ARG	15.8
3	L	203	SER	15.8
1	A	272	ILE	15.8
1	B	109	ILE	15.8
2	C	1076	ILE	15.8
2	C	1069	LEU	15.8
4	H	22	CYS	15.8
1	A	239	CYS	15.8
1	A	357	LYS	15.8
4	H	87	THR	15.8
1	B	486	TYR	15.8
1	B	92	ASN	15.8
2	D	1159	CYS	15.8
1	B	495	GLY	15.8
2	C	1032	ASN	15.8
2	C	1155	GLY	15.7
4	H	21	SER	15.7
1	A	63	THR	15.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	H	32	PHE	15.7
1	B	105	HIS	15.7
2	D	1102	ALA	15.7
4	H	151	THR	15.7
3	L	137	ASN	15.7
4	P	175	LEU	15.7
3	L	7	SER	15.7
4	P	34	MET	15.7
4	H	71	ALA	15.7
2	C	1124	SER	15.7
3	L	139	PHE	15.7
4	H	82(A)	SER	15.7
3	O	138	ASN	15.7
1	B	345	ILE	15.7
3	L	14	SER	15.7
1	A	43	PRO	15.7
1	A	120	VAL	15.7
1	B	71	THR	15.7
4	H	136	ALA	15.6
1	A	418	CYS	15.6
2	D	1158	THR	15.6
3	L	81	GLU	15.6
3	O	97	THR	15.6
1	B	228	CYS	15.6
2	D	1140	GLY	15.6
4	P	200	HIS	15.6
3	L	93	SER	15.6
3	L	32	TRP	15.6
2	D	1117	THR	15.6
4	P	74	SER	15.6
4	P	165	THR	15.6
1	B	336	ALA	15.6
3	L	29	ILE	15.6
4	H	197	ASN	15.6
1	B	394	THR	15.6
3	O	7	SER	15.6
4	P	87	THR	15.6
4	P	135	THR	15.6
1	A	40	TYR	15.6
2	C	1114	LEU	15.6
4	H	177	SER	15.5
1	A	95	MET	15.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	497	ALA	15.5
3	L	53	THR	15.5
4	P	33	TYR	15.5
1	A	369	PRO	15.5
3	O	167	ASP	15.5
1	A	374	HIS	15.5
1	B	210	PHE	15.5
2	C	1160	THR	15.5
4	H	175	LEU	15.5
1	B	264	SER	15.5
1	A	262	ASN	15.5
1	B	296	CYS	15.5
2	C	1062	TRP	15.5
2	D	1156	THR	15.5
3	O	114	SER	15.5
1	A	275	VAL	15.5
3	O	204	PRO	15.5
1	B	49	THR	15.4
2	C	1148	GLN	15.4
3	O	4	MET	15.4
4	P	80	LEU	15.4
4	P	186	SER	15.4
3	L	5	THR	15.4
2	D	1138	ILE	15.4
2	D	1080	ASP	15.4
1	B	270	VAL	15.4
1	A	53	PHE	15.4
1	B	44	VAL	15.4
1	A	206	PRO	15.4
1	A	438	PRO	15.4
4	H	100(B)	PHE	15.4
1	B	438	PRO	15.4
2	C	1063	ASP	15.3
3	L	136	LEU	15.3
3	O	181	LEU	15.3
1	B	67	ASN	15.3
1	B	283	THR	15.3
4	P	20	ILE	15.3
1	B	434	MET	15.3
4	P	138	LEU	15.3
3	L	87	TYR	15.3
1	A	392	ASN	15.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	O	86	TYR	15.3
1	B	295	ASN	15.3
1	A	330	HIS	15.3
1	B	50	THR	15.3
1	B	271	VAL	15.3
2	D	1037	LEU	15.3
3	O	132	VAL	15.3
4	P	178	LEU	15.3
2	D	1015	THR	15.2
1	A	81	PRO	15.2
1	B	493	PRO	15.2
4	H	81	GLU	15.2
1	B	375	TRP	15.2
1	B	225	ILE	15.2
3	O	125	LEU	15.2
4	P	170	LEU	15.2
3	L	202	SER	15.2
1	A	96	TRP	15.2
1	A	209	SER	15.2
4	H	31	ASP	15.2
2	C	1143	THR	15.2
3	O	75	ILE	15.2
1	B	379	GLY	15.1
3	L	30	SER	15.1
3	O	88	CYS	15.1
4	H	195	ILE	15.1
2	C	1154	SER	15.1
3	O	31	THR	15.1
4	H	28	THR	15.1
4	P	107	THR	15.1
4	P	18	VAL	15.1
3	L	58	VAL	15.1
2	C	1158	THR	15.1
2	C	1051	LEU	15.1
1	A	76	PRO	15.1
2	C	1012	VAL	15.1
2	D	1119	GLU	15.1
2	C	1093	VAL	15.1
1	A	217	TYR	15.1
4	P	86	ASP	15.1
2	C	1162	LEU	15.0
3	L	99	GLY	15.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	219	ALA	15.0
1	A	36	VAL	15.0
2	D	1073	ASN	15.0
1	A	75	VAL	15.0
1	A	276	ASN	15.0
4	P	130	SER	15.0
4	P	176	TYR	15.0
4	H	45	LEU	15.0
4	H	172	SER	15.0
2	D	1109	LEU	15.0
1	B	368	ASP	15.0
1	B	433	ALA	15.0
2	C	1112	GLN	15.0
3	L	46	LEU	15.0
3	L	206	THR	15.0
2	D	1086	VAL	14.9
3	O	12	SER	14.9
4	H	74	SER	14.9
1	B	80	ASN	14.9
3	L	120	PRO	14.9
2	D	1145	SER	14.9
4	P	71	ALA	14.9
4	P	89	VAL	14.9
1	B	450	THR	14.9
3	O	44	PRO	14.9
3	L	156	SER	14.9
1	B	443	ILE	14.9
4	P	211	VAL	14.9
1	B	388	THR	14.9
2	D	1082	TYR	14.9
1	A	60	ALA	14.9
3	L	164	THR	14.9
4	P	93	ALA	14.9
3	L	167	ASP	14.9
2	D	1113	SER	14.9
3	L	174	SER	14.9
3	L	130	ALA	14.9
4	H	176	TYR	14.9
2	D	1068	PRO	14.9
4	P	41	PRO	14.9
3	L	86	TYR	14.8
4	H	27	TYR	14.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	P	47	TRP	14.8
4	H	182	VAL	14.8
1	B	239	CYS	14.8
1	B	449	ILE	14.8
1	A	115	SER	14.8
1	B	492	GLU	14.8
1	A	222	GLY	14.8
2	D	1067	PHE	14.8
2	C	1083	ILE	14.8
2	C	1014	LEU	14.8
2	C	1019	SER	14.8
4	P	58	MET	14.8
2	C	1043	PHE	14.8
3	O	83	PHE	14.8
1	A	498	PRO	14.8
4	P	59	TYR	14.8
1	B	250	GLY	14.7
4	H	49	GLY	14.7
1	A	233	PHE	14.7
2	C	1157	TRP	14.7
1	A	259	LEU	14.7
2	D	1070	ILE	14.7
4	P	114	ALA	14.7
2	D	1114	LEU	14.7
3	O	176	SER	14.7
2	C	1080	ASP	14.7
2	D	1052	ASN	14.7
1	B	427	TRP	14.7
1	B	479	TRP	14.7
1	A	387	SER	14.7
1	B	447	SER	14.7
1	B	66	HIS	14.7
3	O	17	ASP	14.7
1	B	202	THR	14.7
2	C	1174	ILE	14.7
1	A	246	GLN	14.7
1	B	245	VAL	14.7
2	C	1116	LEU	14.7
1	B	365	SER	14.7
4	H	179	SER	14.7
3	L	148	TRP	14.7
4	H	79	TYR	14.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	1098	PHE	14.7
2	D	1003	VAL	14.7
2	D	1104	SER	14.7
2	C	1068	PRO	14.7
4	H	100(A)	ALA	14.7
4	P	140	CYS	14.7
2	D	1089	GLN	14.7
4	H	142	VAL	14.7
2	C	1052	ASN	14.6
4	H	116	THR	14.6
3	L	144	ALA	14.6
4	P	55	ALA	14.6
1	A	223	PHE	14.6
1	A	462	ASN	14.6
1	A	435	TYR	14.6
4	H	29	PHE	14.6
1	B	112	TRP	14.6
4	H	154	TRP	14.6
2	D	1120	SER	14.6
4	P	142	VAL	14.6
1	B	377	ASN	14.6
1	A	241	ASN	14.6
1	B	76	PRO	14.6
1	B	299	ALA	14.6
4	P	121	VAL	14.6
2	D	1040	GLN	14.6
3	L	171	SER	14.6
3	L	23	CYS	14.6
3	L	73	LEU	14.6
1	A	214	PRO	14.5
4	P	123	PRO	14.5
3	L	131	SER	14.5
1	A	229	ASN	14.5
3	L	24	ARG	14.5
1	B	474	ASP	14.5
3	L	17	ASP	14.5
1	A	422	GLN	14.5
3	O	202	SER	14.5
1	A	486	TYR	14.5
3	L	59	PRO	14.5
1	A	449	ILE	14.5
4	H	57	THR	14.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	O	208	SER	14.5
4	H	141	LEU	14.5
2	C	1030	ASN	14.5
1	A	107	ASP	14.5
3	O	141	PRO	14.5
1	A	215	ILE	14.5
1	A	299	ALA	14.5
1	B	281	ALA	14.5
3	O	154	LEU	14.5
3	O	140	TYR	14.5
3	L	112	ALA	14.4
1	A	73	ALA	14.4
1	B	413	THR	14.4
2	D	1173	ASP	14.4
4	P	42	GLY	14.4
4	P	27	TYR	14.4
2	C	1131	ARG	14.4
1	A	432	LYS	14.4
1	A	364	SER	14.4
1	B	212	PRO	14.4
2	D	1031	SER	14.4
3	L	104	VAL	14.4
4	H	37	VAL	14.4
1	B	459	GLY	14.4
1	A	421	LYS	14.4
4	H	115	SER	14.4
1	A	111	LEU	14.4
1	B	367	GLY	14.4
3	O	84	ALA	14.4
2	D	1097	VAL	14.4
1	B	339	ASN	14.4
4	H	63	PHE	14.4
2	C	1110	GLN	14.4
2	C	1145	SER	14.4
3	L	44	PRO	14.4
4	H	51	ILE	14.4
3	L	6	GLN	14.3
4	P	161	SER	14.3
1	A	474	ASP	14.3
1	B	457	ASP	14.3
1	B	496	VAL	14.3
2	D	1143	THR	14.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	427	TRP	14.3
4	P	97	TRP	14.3
2	C	1038	GLY	14.3
3	L	159	SER	14.3
4	H	78	GLY	14.3
2	D	1118	LEU	14.3
1	A	497	ALA	14.3
4	H	91	TYR	14.3
1	B	123	THR	14.3
3	L	197	THR	14.3
1	B	95	MET	14.3
2	D	1177	LEU	14.3
1	A	199	SER	14.3
1	B	94	ASN	14.3
2	D	1094	GLN	14.3
1	B	205	CYS	14.3
1	A	473	GLY	14.3
3	L	38	GLN	14.3
3	O	38	GLN	14.3
3	O	96	PHE	14.3
4	H	106	GLY	14.3
1	A	61	TYR	14.3
1	A	256	SER	14.3
2	C	1082	TYR	14.3
1	A	467	ILE	14.3
1	B	118	PRO	14.2
1	B	437	PRO	14.2
2	D	1064	GLN	14.2
3	O	66	GLY	14.2
3	O	187	GLU	14.2
4	P	100(B)	PHE	14.2
3	O	74	THR	14.2
3	O	168	SER	14.2
1	A	201	ILE	14.2
2	D	1062	TRP	14.2
2	C	1086	VAL	14.2
1	A	247	CYS	14.2
3	L	50	ALA	14.2
4	H	60	ALA	14.2
4	H	107	THR	14.2
3	L	92	ASN	14.2
4	P	112	SER	14.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	O	89	GLN	14.2
2	C	1170	PHE	14.2
4	P	94	ALA	14.2
1	B	420	ILE	14.2
3	L	175	LEU	14.2
3	L	169	LYS	14.2
3	L	2	ILE	14.2
1	A	253	PRO	14.2
1	A	338	TRP	14.2
1	A	221	ALA	14.2
1	B	383	PHE	14.2
4	P	166	PHE	14.2
2	D	1011	THR	14.2
2	D	1157	TRP	14.2
4	P	136	ALA	14.2
2	D	1107	HIS	14.1
4	H	59	TYR	14.1
4	H	167	PRO	14.1
4	P	37	VAL	14.1
1	A	56	SER	14.1
1	A	123	THR	14.1
1	A	488	VAL	14.1
2	D	1063	ASP	14.1
1	B	61	TYR	14.1
2	C	1023	SER	14.1
4	H	75	THR	14.1
3	O	48	ILE	14.1
4	P	152	VAL	14.1
1	B	236	THR	14.1
4	H	200	HIS	14.1
4	P	177	SER	14.1
1	A	38	VAL	14.1
3	L	193	ALA	14.1
2	D	1095	LEU	14.1
1	B	294	ILE	14.1
3	O	67	SER	14.1
4	H	127	SER	14.1
2	D	1027	HIS	14.1
2	D	1009	GLY	14.1
1	A	455	THR	14.0
2	D	1101	THR	14.0
1	B	48	ALA	14.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	264	SER	14.0
2	D	1112	GLN	14.0
3	L	150	VAL	14.0
1	A	35	TRP	14.0
4	H	164	HIS	14.0
2	C	1121	PRO	14.0
1	B	378	CYS	14.0
2	C	1067	PHE	14.0
4	H	33	TYR	14.0
1	A	232	THR	14.0
4	P	183	THR	14.0
3	L	127	SER	14.0
4	H	110	SER	14.0
1	A	208	VAL	14.0
4	P	79	TYR	14.0
4	H	120	SER	14.0
1	B	108	ILE	14.0
1	B	73	ALA	14.0
1	A	108	ILE	13.9
1	B	213	ILE	13.9
1	B	90	THR	13.9
1	B	238	PRO	13.9
2	C	1013	GLU	13.9
2	D	1174	ILE	13.9
1	A	44	VAL	13.9
4	H	25	SER	13.9
2	C	1172	ILE	13.9
3	L	9	SER	13.9
3	O	20	THR	13.9
1	B	226	LEU	13.9
1	B	297	THR	13.9
3	L	57	GLY	13.9
1	A	274	SER	13.9
2	C	1027	HIS	13.9
1	A	58	ALA	13.8
4	P	82(C)	LEU	13.8
4	P	110	SER	13.8
2	C	1000	MET	13.8
1	B	43	PRO	13.8
1	B	217	TYR	13.8
3	L	48	ILE	13.8
4	P	21	SER	13.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	45	TRP	13.8
4	H	82(B)	SER	13.8
1	A	366	GLY	13.8
4	P	51	ILE	13.8
2	D	1081	THR	13.8
4	H	135	THR	13.8
4	P	116	THR	13.8
4	P	191	THR	13.8
1	B	376	PHE	13.8
4	P	24	ALA	13.8
4	P	141	LEU	13.8
1	A	463	ASN	13.8
4	P	146	PHE	13.8
1	A	458	GLY	13.8
3	L	34	ALA	13.8
1	B	242	VAL	13.8
2	C	1176	VAL	13.8
1	A	379	GLY	13.8
1	A	294	ILE	13.7
3	O	21	ILE	13.7
2	D	1030	ASN	13.7
2	D	1164	ASN	13.7
3	L	210	ASN	13.7
2	C	1123	GLY	13.7
1	B	96	TRP	13.7
2	D	1074	LEU	13.7
1	B	372	VAL	13.7
4	H	152	VAL	13.7
1	A	88	ASN	13.7
3	L	182	SER	13.7
2	C	1141	GLY	13.7
3	L	35	TRP	13.7
1	B	439	ILE	13.7
4	P	35	TYR	13.7
3	O	163	VAL	13.7
3	O	45	LYS	13.7
4	H	18	VAL	13.7
1	B	277	PHE	13.7
3	O	164	THR	13.7
4	H	153	SER	13.7
1	A	362	LYS	13.7
1	A	389	GLN	13.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	454	LEU	13.7
4	P	45	LEU	13.7
1	B	38	VAL	13.7
3	L	15	VAL	13.7
1	B	350	ARG	13.6
1	B	435	TYR	13.6
1	A	220	PRO	13.6
2	D	1087	GLU	13.6
1	A	476	ARG	13.6
3	O	91	ALA	13.6
4	P	196	CYS	13.6
3	L	8	PRO	13.6
1	A	336	ALA	13.6
4	P	56	ASP	13.6
2	C	1101	THR	13.6
2	D	1002	LYS	13.6
1	B	453	LEU	13.6
3	L	125	LEU	13.6
1	A	212	PRO	13.6
1	A	468	PHE	13.6
1	B	116	LEU	13.6
3	L	12	SER	13.6
2	C	1118	LEU	13.6
4	H	122	PHE	13.6
2	C	1053	ASP	13.6
4	H	93	ALA	13.6
1	A	395	TRP	13.6
1	B	278	THR	13.6
1	B	494	LEU	13.6
4	P	95	ASP	13.5
2	D	1029	LYS	13.5
1	B	37	THR	13.5
1	A	420	ILE	13.5
2	D	1038	GLY	13.5
2	D	1054	ARG	13.5
1	A	98	ASN	13.5
1	B	63	THR	13.5
3	L	97	THR	13.5
3	O	2	ILE	13.5
2	D	1050	LYS	13.5
1	B	204	ALA	13.5
1	B	249	HIS	13.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	200	VAL	13.5
1	A	345	ILE	13.5
1	B	275	VAL	13.5
3	L	76	ASN	13.5
3	O	210	ASN	13.5
2	D	1106	THR	13.5
1	A	39	TYR	13.5
2	D	1066	ASN	13.5
2	C	1064	GLN	13.5
3	O	192	TYR	13.5
1	A	110	SER	13.5
1	A	483	LEU	13.5
1	B	418	CYS	13.4
1	A	399	THR	13.4
1	B	415	THR	13.4
4	H	68	THR	13.4
1	A	382	PHE	13.4
1	B	93	PHE	13.4
3	O	34	ALA	13.4
4	P	60	ALA	13.4
3	L	28	ASP	13.4
1	B	65	VAL	13.4
1	A	359	ILE	13.4
1	B	102	GLU	13.4
3	L	49	TYR	13.4
1	A	240	THR	13.4
1	B	60	ALA	13.4
2	C	1104	SER	13.4
1	A	417	PRO	13.4
4	P	124	LEU	13.4
1	A	480	ARG	13.4
4	P	81	GLU	13.4
1	A	67	ASN	13.4
4	H	80	LEU	13.4
4	P	29	PHE	13.3
1	B	89	VAL	13.3
2	C	1016	CYS	13.3
2	C	1039	ASN	13.3
4	P	185	PRO	13.3
2	C	1177	LEU	13.3
1	B	35	TRP	13.3
1	B	203	GLN	13.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	1041	GLY	13.3
1	A	347	SER	13.3
1	A	339	ASN	13.3
4	P	202	PRO	13.3
4	P	205	THR	13.3
3	O	137	ASN	13.3
1	A	456	ARG	13.3
2	C	1144	LEU	13.3
1	A	365	SER	13.3
3	L	18	ARG	13.3
1	A	225	ILE	13.3
1	A	433	ALA	13.3
2	D	1144	LEU	13.3
3	O	8	PRO	13.3
1	A	50	THR	13.3
3	O	152	ASN	13.3
1	B	272	ILE	13.3
2	C	1126	PRO	13.3
1	A	283	THR	13.2
2	D	1093	VAL	13.2
4	H	145	TYR	13.2
4	P	104	GLY	13.2
1	A	266	ALA	13.2
3	L	56	SER	13.2
2	C	1094	GLN	13.2
1	A	250	GLY	13.2
3	L	154	LEU	13.2
2	C	1026	PHE	13.2
4	P	118	GLY	13.2
3	O	133	VAL	13.2
1	A	106	GLU	13.2
1	B	419	ARG	13.2
3	O	196	VAL	13.2
4	P	108	LEU	13.2
4	P	67	VAL	13.2
1	B	40	TYR	13.2
1	A	490	LYS	13.2
1	B	425	ASN	13.2
3	O	189	HIS	13.1
1	A	82	GLN	13.1
3	O	136	LEU	13.1
1	B	386	ASN	13.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	P	155	ASN	13.1
1	B	489	VAL	13.1
4	H	118	GLY	13.1
1	A	281	ALA	13.1
4	H	55	ALA	13.1
4	P	36	TRP	13.1
3	L	89	GLN	13.1
4	H	192	GLN	13.1
2	D	1092	GLU	13.1
2	D	1049	SER	13.1
4	P	5	VAL	13.1
2	D	1151	LEU	13.1
3	O	110	VAL	13.1
1	A	288	LEU	13.1
2	D	1126	PRO	13.1
3	L	186	TYR	13.1
2	D	1022	LYS	13.1
1	B	261	LEU	13.1
2	D	1060	SER	13.1
1	A	62	ASP	13.1
4	H	52	ASP	13.1
1	A	386	ASN	13.0
4	H	54	ASP	13.0
4	H	146	PHE	13.0
4	P	131	THR	13.0
4	P	3	GLN	13.0
1	A	397	ASN	13.0
3	O	58	VAL	13.0
3	O	25	ALA	13.0
3	L	66	GLY	13.0
1	B	448	ASN	13.0
1	B	491	ILE	13.0
4	P	199	ASN	13.0
1	B	104	MET	13.0
4	H	211	VAL	13.0
4	H	102	VAL	13.0
4	P	181	VAL	13.0
1	A	289	ASN	13.0
1	B	468	PHE	13.0
3	O	193	ALA	13.0
1	A	424	ILE	12.9
2	C	1003	VAL	12.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	280	ASN	12.9
1	A	37	THR	12.9
4	H	183	THR	12.9
1	A	493	PRO	12.9
2	C	1096	LEU	12.9
4	P	6	GLN	12.9
1	B	114	GLN	12.9
1	B	389	GLN	12.9
2	C	1098	PHE	12.9
1	A	42	VAL	12.9
3	O	113	PRO	12.9
3	L	121	SER	12.9
3	O	52	SER	12.9
2	D	1016	CYS	12.9
4	P	4	LEU	12.9
4	P	98	GLU	12.9
3	O	212	GLY	12.9
1	A	244	THR	12.9
1	A	437	PRO	12.9
4	P	103	TRP	12.9
3	L	155	GLN	12.9
4	H	61	GLU	12.9
1	B	342	LEU	12.9
2	C	1151	LEU	12.9
2	D	1078	ASP	12.9
3	O	205	VAL	12.9
3	O	174	SER	12.8
4	H	69	ILE	12.8
4	P	173	SER	12.8
4	H	5	VAL	12.8
4	H	83	ARG	12.8
3	L	55	GLN	12.8
4	H	2	VAL	12.8
4	H	41	PRO	12.8
4	H	133	GLY	12.8
1	A	261	LEU	12.8
1	B	258	GLN	12.8
2	C	1050	LYS	12.8
2	C	1173	ASP	12.8
3	L	31	THR	12.8
4	H	213	PRO	12.8
1	B	113	ASP	12.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	391	PHE	12.8
3	L	117	ILE	12.8
1	A	49	THR	12.8
1	B	340	ASN	12.8
4	H	50	LEU	12.8
3	L	142	ARG	12.8
1	B	115	SER	12.8
3	L	26	SER	12.8
1	B	284	ILE	12.8
1	B	355	ASN	12.8
2	D	1012	VAL	12.7
1	A	411	SER	12.7
4	H	201	LYS	12.7
3	O	90	GLN	12.7
2	C	1018	ALA	12.7
1	B	100	MET	12.7
4	H	130	SER	12.7
1	B	99	ASP	12.7
3	L	109	THR	12.7
2	C	1128	VAL	12.7
1	B	353	PHE	12.7
4	P	63	PHE	12.7
2	D	1034	ILE	12.7
2	D	1071	ILE	12.7
2	C	1090	LYS	12.7
1	B	74	CYS	12.7
1	A	380	GLY	12.7
1	A	116	LEU	12.7
2	D	1032	ASN	12.7
2	C	1070	ILE	12.7
2	D	1160	THR	12.7
3	L	85	THR	12.7
1	B	266	ALA	12.7
1	A	430	VAL	12.7
1	B	265	LEU	12.7
1	B	199	SER	12.7
1	B	243	SER	12.7
4	H	123	PRO	12.7
4	P	16	ALA	12.7
2	D	1046	LYS	12.7
3	L	190	LYS	12.7
1	A	109	ILE	12.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	1042	SER	12.6
1	A	349	LEU	12.6
1	B	483	LEU	12.6
3	O	166	GLN	12.6
4	H	205	THR	12.6
4	P	68	THR	12.6
3	O	51	ALA	12.6
4	H	23	LYS	12.6
2	D	1122	PRO	12.6
3	O	143	GLU	12.6
1	A	87	VAL	12.6
1	A	292	VAL	12.6
2	D	1163	GLN	12.6
1	A	207	LYS	12.6
1	A	278	THR	12.6
1	B	201	ILE	12.6
2	C	1106	THR	12.6
1	B	98	ASN	12.6
1	A	286	VAL	12.6
3	O	29	ILE	12.6
2	C	1137	ASN	12.6
4	H	199	ASN	12.6
1	B	124	GLY	12.6
1	B	431	GLY	12.6
3	O	65	SER	12.6
4	P	70	THR	12.6
1	A	254	VAL	12.6
1	A	489	VAL	12.6
2	D	1056	ASP	12.6
1	A	114	GLN	12.5
2	C	1171	LYS	12.5
3	L	105	GLU	12.5
3	O	109	THR	12.5
2	D	1045	THR	12.5
3	O	82	ASP	12.5
1	B	480	ARG	12.5
3	L	140	TYR	12.5
4	P	163	VAL	12.5
4	P	169	VAL	12.5
2	D	1121	PRO	12.5
1	B	216	HIS	12.5
4	H	92	CYS	12.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	496	VAL	12.5
1	B	286	VAL	12.5
4	P	1	GLU	12.5
4	P	85	GLU	12.5
3	O	5	THR	12.5
4	H	38	ARG	12.5
4	P	167	PRO	12.5
3	O	197	THR	12.5
1	A	414	ILE	12.5
1	A	383	PHE	12.5
1	A	350	ARG	12.5
1	B	234	ASN	12.5
4	P	197	ASN	12.5
3	O	206	THR	12.5
1	B	86	LEU	12.5
1	A	242	VAL	12.5
1	B	53	PHE	12.5
1	A	475	MET	12.5
4	P	148	GLU	12.4
3	O	13	ALA	12.4
3	O	78	LEU	12.4
3	L	108	ARG	12.4
2	D	1043	PHE	12.4
3	L	45	LYS	12.4
3	O	194	CYS	12.4
4	P	57	THR	12.4
2	C	1138	ILE	12.4
1	B	422	GLN	12.4
2	C	1089	GLN	12.4
3	O	23	CYS	12.4
1	A	265	LEU	12.4
2	D	1178	ALA	12.4
1	A	89	VAL	12.4
2	C	1065	GLY	12.4
4	H	35	TYR	12.4
1	B	392	ASN	12.4
2	D	1169	GLU	12.4
2	D	1044	LEU	12.4
2	D	1182	ALA	12.4
3	O	201	LEU	12.4
4	H	108	LEU	12.4
1	B	84	VAL	12.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	1061	LEU	12.3
2	D	1096	LEU	12.3
1	A	285	ILE	12.3
2	C	1105	ASP	12.3
4	P	164	HIS	12.3
2	C	1015	THR	12.3
3	O	92	ASN	12.3
1	B	442	GLN	12.3
1	B	207	LYS	12.3
1	B	411	SER	12.3
3	O	56	SER	12.3
2	D	1115	THR	12.3
1	B	36	VAL	12.3
4	H	184	VAL	12.3
4	P	182	VAL	12.3
4	H	85	GLU	12.3
3	O	119	PRO	12.3
1	A	390	LEU	12.3
1	A	334	ALA	12.3
1	B	280	ASN	12.3
3	L	54	LEU	12.3
2	D	1171	LYS	12.3
1	A	93	PHE	12.3
3	L	110	VAL	12.3
2	C	1132	SER	12.3
1	A	32	GLU	12.3
1	A	464	GLU	12.3
1	A	423	ILE	12.3
1	A	83	GLU	12.2
1	B	412	ASP	12.2
1	B	344	GLN	12.2
2	C	1165	GLN	12.2
2	D	1025	GLN	12.2
2	C	1074	LEU	12.2
2	C	1175	VAL	12.2
2	D	1180	GLN	12.2
1	B	331	CYS	12.2
1	A	297	THR	12.2
3	O	180	THR	12.2
1	A	481	SER	12.2
4	H	4	LEU	12.2
1	B	293	GLU	12.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	373	THR	12.2
1	A	238	PRO	12.2
4	H	97	TRP	12.2
4	P	39	GLN	12.2
1	B	221	ALA	12.2
1	B	69	TRP	12.2
2	C	1058	ARG	12.2
1	B	291	SER	12.1
3	L	78	LEU	12.1
1	B	31	THR	12.1
1	B	33	LYS	12.1
1	B	395	TRP	12.1
1	B	209	SER	12.1
3	O	203	SER	12.1
2	C	1034	ILE	12.1
2	C	1109	LEU	12.1
2	C	1092	GLU	12.1
1	B	430	VAL	12.1
2	C	1024	ILE	12.1
3	O	151	ASP	12.1
4	H	148	GLU	12.1
1	B	229	ASN	12.1
1	B	356	ASN	12.1
3	L	65	SER	12.1
3	O	57	GLY	12.1
4	H	99	LEU	12.1
3	L	3	GLN	12.1
3	O	26	SER	12.1
4	H	90	TYR	12.1
2	C	1139	GLN	12.1
3	O	32	TRP	12.1
2	C	1001	LYS	12.1
1	B	224	ALA	12.1
1	B	465	SER	12.1
4	P	2	VAL	12.0
1	A	492	GLU	12.0
4	P	212	GLU	12.0
1	A	257	SER	12.0
3	L	4	MET	12.0
3	O	175	LEU	12.0
1	B	424	ILE	12.0
4	P	9	ALA	12.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	20	THR	12.0
4	H	144	ASP	12.0
4	P	52	ASP	12.0
4	P	143	LYS	12.0
1	A	341	THR	12.0
1	A	277	PHE	12.0
3	O	159	SER	12.0
1	A	434	MET	12.0
1	A	269	GLU	12.0
1	B	52	LEU	12.0
2	C	1046	LYS	12.0
2	D	1014	LEU	12.0
3	O	120	PRO	12.0
1	A	410	GLY	12.0
3	L	138	ASN	12.0
3	L	160	GLN	12.0
4	P	75	THR	12.0
1	A	372	VAL	12.0
3	L	33	LEU	12.0
3	O	148	TRP	12.0
4	H	159	LEU	12.0
3	O	18	ARG	12.0
1	B	462	ASN	11.9
1	B	477	ASP	11.9
1	A	444	ARG	11.9
2	C	1115	THR	11.9
3	O	173	TYR	11.9
3	L	195	GLU	11.9
3	O	186	TYR	11.9
2	D	1134	ARG	11.9
4	P	83	ARG	11.9
1	A	270	VAL	11.9
2	D	1172	ILE	11.9
3	L	157	GLY	11.9
1	A	271	VAL	11.9
1	B	117	LYS	11.9
4	H	202	PRO	11.9
3	L	63	SER	11.9
2	D	1110	GLN	11.9
4	P	54	ASP	11.9
3	O	158	ASN	11.9
4	P	22	CYS	11.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	H	132	SER	11.9
4	P	30	SER	11.9
4	H	168	ALA	11.9
4	P	40	ALA	11.9
1	A	342	LEU	11.9
1	B	341	THR	11.9
2	D	1023	SER	11.9
4	H	150	VAL	11.9
1	B	262	ASN	11.8
3	O	47	LEU	11.8
1	B	279	ASP	11.8
1	B	51	THR	11.8
1	B	254	VAL	11.8
4	P	65	GLY	11.8
4	P	207	VAL	11.8
1	B	215	ILE	11.8
4	P	82(A)	SER	11.8
3	L	42	LYS	11.8
4	P	12	LYS	11.8
1	B	91	GLU	11.8
4	P	96	PRO	11.8
1	A	346	ALA	11.8
3	O	155	GLN	11.8
2	D	1137	ASN	11.8
1	B	330	HIS	11.8
1	B	260	LEU	11.8
1	B	381	GLU	11.8
1	B	476	ARG	11.8
4	H	67	VAL	11.8
2	C	1108	LEU	11.8
3	L	135	LEU	11.8
3	O	126	LYS	11.8
3	O	139	PHE	11.8
4	P	99	LEU	11.8
4	P	82(B)	SER	11.8
2	C	1066	ASN	11.8
3	O	71	PHE	11.7
1	A	90	THR	11.7
1	B	499	THR	11.7
4	H	44	GLY	11.7
4	P	122	PHE	11.7
3	L	211	ARG	11.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	P	213	PRO	11.7
4	P	125	ALA	11.7
2	C	1060	SER	11.7
2	C	1147	SER	11.7
3	O	142	ARG	11.7
4	H	131	THR	11.7
2	C	1033	GLN	11.7
3	O	184	ALA	11.7
2	D	1141	GLY	11.7
1	B	211	GLU	11.7
2	D	1139	GLN	11.7
1	B	255	VAL	11.7
4	H	13	LYS	11.7
2	D	1088	ASP	11.7
3	L	141	PRO	11.7
1	B	363	GLN	11.7
1	B	421	LYS	11.7
2	C	1100	LEU	11.7
2	D	1004	VAL	11.7
4	P	100(A)	ALA	11.7
4	P	159	LEU	11.7
3	O	68	GLY	11.7
3	O	190	LYS	11.7
1	B	263	GLY	11.7
1	A	65	VAL	11.6
1	B	78	ASP	11.7
4	H	58	MET	11.6
1	B	349	LEU	11.6
4	P	209	LYS	11.6
2	C	1119	GLU	11.6
3	O	213	GLU	11.6
1	B	473	GLY	11.6
1	B	440	SER	11.6
3	L	94	PHE	11.6
3	L	162	SER	11.6
3	L	61	ARG	11.6
4	H	139	GLY	11.6
1	A	457	ASP	11.6
1	A	477	ASP	11.6
4	P	32	PHE	11.6
3	O	106	ILE	11.6
1	B	214	PRO	11.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	1161	VAL	11.6
1	A	66	HIS	11.6
1	A	469	ARG	11.6
3	L	115	VAL	11.6
1	A	113	ASP	11.6
3	O	172	THR	11.6
4	H	191	THR	11.6
1	A	298	GLY	11.5
1	A	340	ASN	11.5
3	L	118	PHE	11.5
4	P	174	GLY	11.5
1	B	274	SER	11.5
4	H	19	LYS	11.5
2	D	1176	VAL	11.5
4	H	198	VAL	11.5
4	P	38	ARG	11.5
1	A	454	LEU	11.5
2	D	1108	LEU	11.5
4	H	7	SER	11.5
2	D	1152	GLN	11.5
1	A	470	PRO	11.5
1	B	64	GLU	11.5
1	B	256	SER	11.5
3	O	100	GLY	11.5
2	C	1056	ASP	11.5
1	B	246	GLN	11.5
3	O	146	VAL	11.5
1	A	484	TYR	11.5
4	H	143	LYS	11.5
2	D	1057	SER	11.5
4	H	171	GLN	11.5
1	B	446	SER	11.5
1	A	260	LEU	11.5
1	B	463	ASN	11.4
3	O	49	TYR	11.4
1	A	358	THR	11.4
1	A	251	ILE	11.4
2	C	1168	VAL	11.4
1	A	202	THR	11.4
4	H	158	ALA	11.4
1	A	255	VAL	11.4
4	P	62	LYS	11.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	1	ASP	11.4
3	O	94	PHE	11.4
3	L	64	GLY	11.4
3	O	93	SER	11.4
4	P	127	SER	11.4
1	B	466	GLU	11.4
2	C	1021	LYS	11.4
1	B	75	VAL	11.4
1	A	353	PHE	11.4
1	B	382	PHE	11.4
2	C	1127	SER	11.3
3	L	145	LYS	11.3
4	P	144	ASP	11.3
4	P	7	SER	11.3
1	A	415	THR	11.3
4	P	192	GLN	11.3
1	A	279	ASP	11.3
4	H	114	ALA	11.3
4	P	154	TRP	11.3
2	C	1073	ASN	11.3
1	A	378	CYS	11.3
4	P	48	MET	11.3
3	L	75	ILE	11.3
3	L	96	PHE	11.3
2	D	1168	VAL	11.3
3	O	123	GLU	11.3
3	O	170	ASP	11.3
3	O	79	GLN	11.3
3	O	116	PHE	11.3
1	B	444	ARG	11.3
1	B	288	LEU	11.3
4	P	133	GLY	11.2
2	D	1021	LYS	11.2
1	B	464	GLU	11.2
4	H	64	ARG	11.2
4	H	101	ASN	11.2
1	B	41	GLY	11.2
2	C	1035	LYS	11.2
1	B	347	SER	11.2
1	A	391	PHE	11.2
1	A	368	ASP	11.2
1	B	62	ASP	11.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	1100	LEU	11.2
3	L	185	ASP	11.2
1	B	289	ASN	11.2
1	A	198	GLY	11.2
1	A	100	MET	11.2
1	A	377	ASN	11.2
3	O	76	ASN	11.2
1	B	58	ALA	11.2
4	H	14	PRO	11.2
2	C	1150	GLU	11.1
2	C	1140	GLY	11.1
3	O	121	SER	11.1
1	A	376	PHE	11.1
1	B	417	PRO	11.1
4	P	11	VAL	11.1
3	L	152	ASN	11.1
1	A	252	ARG	11.1
2	D	1036	ILE	11.1
4	H	56	ASP	11.1
4	H	189	LEU	11.1
4	H	147	PRO	11.1
4	P	14	PRO	11.1
1	A	248	THR	11.1
1	A	226	LEU	11.1
2	C	1025	GLN	11.1
4	H	39	GLN	11.1
1	B	416	LEU	11.1
4	P	189	LEU	11.1
4	P	208	ASP	11.0
2	C	1045	THR	11.0
2	C	1169	GLU	11.0
1	B	467	ILE	11.0
3	O	10	SER	11.0
1	B	85	VAL	11.0
2	C	1017	THR	11.0
2	D	1059	ARG	11.0
3	O	55	GLN	11.0
3	L	184	ALA	11.0
1	A	92	ASN	11.0
1	A	409	GLU	11.0
2	C	1044	LEU	11.0
1	A	371	ILE	11.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	196	VAL	11.0
3	O	11	VAL	11.0
1	A	441	GLY	11.0
1	B	396	PHE	11.0
1	B	432	LYS	11.0
2	D	1018	ALA	11.0
3	L	153	ALA	11.0
3	O	153	ALA	11.0
3	O	115	VAL	11.0
4	P	194	TYR	11.0
3	O	6	GLN	11.0
1	B	455	THR	11.0
4	H	66	ARG	11.0
2	D	1148	GLN	11.0
3	O	27	GLN	11.0
1	B	257	SER	11.0
1	B	470	PRO	11.0
1	B	237	GLY	10.9
1	B	247	CYS	10.9
3	O	195	GLU	10.9
1	A	234	ASN	10.9
4	H	155	ASN	10.9
1	B	472	GLY	10.9
2	D	1150	GLU	10.9
4	P	46	GLU	10.9
2	C	1072	LYS	10.9
4	H	206	LYS	10.9
1	B	248	THR	10.9
1	B	233	PHE	10.9
1	A	291	SER	10.9
2	C	1029	LYS	10.9
3	L	205	VAL	10.9
1	A	452	LEU	10.9
2	C	1149	LEU	10.9
3	L	143	GLU	10.9
4	P	66	ARG	10.9
1	A	485	LYS	10.9
2	D	1091	GLU	10.9
2	D	1001	LYS	10.9
1	B	380	GLY	10.9
3	O	156	SER	10.9
1	B	290	THR	10.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	1179	PHE	10.8
4	P	147	PRO	10.8
1	A	478	ASN	10.8
2	C	1004	VAL	10.8
2	D	1129	GLN	10.8
1	A	461	SER	10.8
2	C	1091	GLU	10.8
1	A	344	GLN	10.8
2	D	1147	SER	10.8
1	B	39	TYR	10.8
1	B	241	ASN	10.8
3	O	160	GLN	10.8
3	L	90	GLN	10.8
1	A	381	GLU	10.8
2	D	1085	GLU	10.8
2	D	1042	SER	10.8
1	A	78	ASP	10.8
1	A	363	GLN	10.8
1	B	82	GLN	10.8
1	A	450	THR	10.8
4	H	8	GLY	10.7
1	B	34	LEU	10.7
2	D	1026	PHE	10.7
1	A	102	GLU	10.7
3	O	81	GLU	10.7
2	D	1005	LEU	10.7
1	B	445	CYS	10.7
2	C	1135	GLY	10.7
3	L	62	PHE	10.7
4	P	77	THR	10.7
1	A	211	GLU	10.7
1	B	106	GLU	10.7
2	C	1047	GLY	10.7
4	P	168	ALA	10.7
4	P	162	GLY	10.7
4	H	10	GLU	10.7
2	C	1107	HIS	10.7
4	P	201	LYS	10.7
3	L	189	HIS	10.6
3	O	183	LYS	10.6
2	D	1135	GLY	10.6
4	H	124	LEU	10.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	361	PHE	10.6
1	A	282	LYS	10.6
1	A	268	GLU	10.6
1	A	419	ARG	10.6
3	L	192	TYR	10.6
4	H	46	GLU	10.6
4	H	104	GLY	10.6
1	A	224	ALA	10.6
4	P	190	GLY	10.6
1	A	117	LYS	10.6
1	B	358	THR	10.6
4	P	119	PRO	10.6
1	B	292	VAL	10.6
1	B	452	LEU	10.6
1	A	80	ASN	10.6
4	H	214	LYS	10.6
2	D	1179	PHE	10.6
4	P	128	SER	10.5
3	L	146	VAL	10.5
2	D	1008	LYS	10.5
1	A	482	GLU	10.5
1	B	361	PHE	10.5
3	L	161	GLU	10.5
4	H	73	THR	10.5
1	B	42	VAL	10.5
3	L	209	PHE	10.5
4	P	105	GLN	10.5
3	L	103	LYS	10.5
4	P	23	LYS	10.5
2	C	1057	SER	10.5
3	O	50	ALA	10.5
1	A	428	GLN	10.5
1	B	46	LYS	10.5
2	D	1024	ILE	10.5
4	P	198	VAL	10.5
2	C	1142	LYS	10.5
3	O	122	ASP	10.4
1	B	357	LYS	10.4
1	B	471	GLY	10.4
1	A	352	GLN	10.4
4	H	98	GLU	10.4
1	B	390	LEU	10.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	360	ILE	10.4
2	C	1075	LYS	10.4
2	D	1058	ARG	10.4
1	B	198	GLY	10.4
3	O	117	ILE	10.4
3	L	128	GLY	10.4
1	B	79	PRO	10.4
2	D	1041	GLY	10.3
2	C	1178	ALA	10.3
1	A	103	GLN	10.3
4	P	195	ILE	10.3
3	L	123	GLU	10.3
2	C	1007	LYS	10.3
3	L	16	GLY	10.3
1	B	487	LYS	10.3
2	D	1124	SER	10.3
4	H	105	GLN	10.3
1	A	351	GLU	10.3
3	O	169	LYS	10.3
2	C	1164	ASN	10.3
3	O	37	GLN	10.3
3	L	151	ASP	10.2
1	B	235	GLY	10.2
3	L	199	GLN	10.2
4	H	6	GLN	10.2
1	A	243	SER	10.2
3	O	161	GLU	10.2
4	P	72	ASP	10.2
3	L	200	GLY	10.2
1	A	263	GLY	10.2
3	L	212	GLY	10.2
1	B	32	GLU	10.2
1	A	440	SER	10.2
3	O	77	SER	10.2
4	H	3	GLN	10.1
3	O	9	SER	10.1
1	B	47	GLU	10.1
1	B	88	ASN	10.1
4	H	82	LEU	10.1
4	H	12	LYS	10.1
1	A	494	LEU	10.1
3	O	70	ASP	10.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	31	THR	10.1
1	B	298	GLY	10.1
2	C	1002	LYS	10.1
2	D	1033	GLN	10.1
1	B	387	SER	10.1
3	L	133	VAL	10.1
3	L	27	GLN	10.1
1	B	282	LYS	10.1
1	B	428	GLN	10.1
2	C	1088	ASP	10.1
1	A	284	ILE	10.1
1	B	461	SER	10.1
2	D	1183	SER	10.0
3	O	179	LEU	10.0
1	A	59	LYS	10.0
2	C	1008	LYS	10.0
1	B	469	ARG	10.0
1	A	396	PHE	10.0
1	B	423	ILE	10.0
4	H	169	VAL	10.0
3	L	201	LEU	10.0
4	P	64	ARG	10.0
2	D	1090	LYS	10.0
4	H	212	GLU	10.0
1	A	453	LEU	10.0
4	P	53	GLU	10.0
4	P	210	LYS	10.0
1	B	351	GLU	10.0
1	A	501	ALA	10.0
3	O	108	ARG	9.9
1	B	332	ASN	9.9
4	P	171	GLN	9.9
1	A	416	LEU	9.9
2	D	1048	PRO	9.9
3	L	165	GLU	9.9
2	C	1071	ILE	9.9
3	L	207	LYS	9.9
4	P	78	GLY	9.8
2	C	1163	GLN	9.8
3	O	62	PHE	9.8
1	A	348	LYS	9.8
1	B	121	LYS	9.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	129	THR	9.8
2	D	1065	GLY	9.8
4	H	42	GLY	9.8
1	B	362	LYS	9.8
1	B	268	GLU	9.8
1	B	57	ASP	9.8
1	A	124	GLY	9.8
2	D	1155	GLY	9.8
1	B	231	LYS	9.8
4	P	150	VAL	9.8
1	B	478	ASN	9.7
3	O	198	HIS	9.7
3	L	187	GLU	9.7
1	A	64	GLU	9.7
4	P	126	PRO	9.7
3	L	208	SER	9.7
3	O	171	SER	9.7
2	D	1039	ASN	9.7
1	B	371	ILE	9.7
1	B	460	ASN	9.7
2	D	1013	GLU	9.7
2	C	1020	GLN	9.7
3	O	28	ASP	9.6
1	B	101	VAL	9.6
1	A	354	GLY	9.6
4	H	190	GLY	9.6
1	B	287	GLN	9.6
3	L	183	LYS	9.6
4	H	113	SER	9.6
2	C	1022	LYS	9.6
1	B	97	LYS	9.6
1	A	367	GLY	9.6
1	B	456	ARG	9.6
2	D	1035	LYS	9.6
1	A	34	LEU	9.6
1	A	86	LEU	9.6
1	B	485	LYS	9.6
2	D	1136	LYS	9.6
3	L	126	LYS	9.6
3	L	213	GLU	9.6
3	O	42	LYS	9.6
3	O	149	LYS	9.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	1053	ASP	9.6
3	L	122	ASP	9.6
2	C	1181	LYS	9.6
3	L	100	GLY	9.6
3	O	54	LEU	9.6
2	C	1085	GLU	9.5
2	D	1149	LEU	9.5
4	P	15	GLY	9.5
1	A	273	ARG	9.5
1	B	273	ARG	9.5
4	H	173	SER	9.5
2	D	1167	LYS	9.5
4	P	10	GLU	9.5
2	D	1019	SER	9.5
1	A	394	THR	9.5
4	H	117	LYS	9.5
2	D	1123	GLY	9.5
3	L	166	GLN	9.5
4	P	158	ALA	9.5
1	A	97	LYS	9.4
3	O	207	LYS	9.4
3	O	200	GLY	9.4
4	H	43	LYS	9.4
4	H	62	LYS	9.4
2	D	1131	ARG	9.4
3	O	191	LEU	9.4
3	O	131	SER	9.4
4	H	210	LYS	9.4
4	P	206	LYS	9.4
1	B	334	ALA	9.4
1	B	267	GLU	9.4
1	A	121	LYS	9.3
1	B	364	SER	9.3
1	B	59	LYS	9.3
4	H	53	GLU	9.3
4	P	82	LEU	9.3
2	D	1105	ASP	9.3
1	A	460	ASN	9.3
2	C	1180	GLN	9.3
3	O	61	ARG	9.2
1	B	441	GLY	9.2
3	L	124	GLN	9.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	O	162	SER	9.2
4	H	1	GLU	9.2
1	A	237	GLY	9.2
1	A	471	GLY	9.2
1	B	498	PRO	9.2
3	O	3	GLN	9.2
3	O	188	LYS	9.2
1	B	285	ILE	9.1
1	B	348	LYS	9.1
4	H	26	GLY	9.1
2	D	1076	ILE	9.1
2	C	1059	ARG	9.1
4	H	125	ALA	9.1
2	D	1165	GLN	9.0
1	A	91	GLU	9.0
2	D	1181	LYS	9.0
3	O	211	ARG	9.0
4	P	117	LYS	9.0
1	B	232	THR	9.0
4	P	193	THR	9.0
3	L	188	LYS	9.0
3	L	147	GLN	9.0
2	C	1166	LYS	9.0
1	A	439	ILE	8.9
1	A	258	GLN	8.9
1	A	500	LYS	8.9
2	D	1007	LYS	8.9
3	O	199	GLN	8.9
4	H	48	MET	8.9
1	A	337	LYS	8.9
1	A	290	THR	8.9
3	O	157	GLY	8.8
1	A	46	LYS	8.8
3	O	118	PHE	8.8
2	D	1072	LYS	8.8
4	H	72	ASP	8.8
4	H	129	LYS	8.8
1	A	499	THR	8.8
3	O	24	ARG	8.8
1	A	356	ASN	8.7
3	O	105	GLU	8.7
4	P	49	GLY	8.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	P	43	LYS	8.7
1	B	370	GLU	8.7
1	B	490	LYS	8.7
3	O	107	LYS	8.7
4	P	25	SER	8.7
3	O	185	ASP	8.7
1	B	227	LYS	8.7
1	B	481	SER	8.6
4	P	106	GLY	8.6
3	O	63	SER	8.6
2	C	1087	GLU	8.6
3	L	149	LYS	8.6
1	A	287	GLN	8.6
4	P	132	SER	8.5
4	P	204	ASN	8.5
1	B	200	VAL	8.5
1	B	346	ALA	8.5
1	B	83	GLU	8.5
3	L	13	ALA	8.5
3	O	16	GLY	8.5
1	A	343	LYS	8.5
1	A	329	GLY	8.4
1	A	267	GLU	8.4
3	O	128	GLY	8.4
2	C	1077	GLU	8.4
1	B	269	GLU	8.4
3	O	124	GLN	8.3
1	B	451	GLY	8.3
1	A	466	GLU	8.3
1	A	370	GLU	8.3
3	O	165	GLU	8.3
1	A	442	GLN	8.3
3	O	103	LYS	8.3
1	A	472	GLY	8.2
2	D	1166	LYS	8.2
1	B	429	LYS	8.2
1	A	47	GLU	8.2
2	C	1152	GLN	8.1
2	C	1099	GLY	8.1
1	A	33	LYS	8.1
2	C	1167	LYS	8.1
4	P	61	GLU	8.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	1134	ARG	8.1
1	A	293	GLU	8.1
1	A	487	LYS	8.1
3	O	147	GLN	8.1
4	H	65	GLY	8.0
3	L	107	LYS	8.0
3	O	99	GLY	8.0
4	H	209	LYS	8.0
1	B	343	LYS	8.0
1	B	335	ARG	8.0
1	B	352	GLN	7.9
4	H	128	SER	7.8
2	D	1077	GLU	7.8
3	O	33	LEU	7.8
3	L	39	LYS	7.7
1	B	103	GLN	7.7
1	A	51	THR	7.7
3	O	19	VAL	7.7
2	D	1075	LYS	7.7
4	P	13	LYS	7.6
1	B	56	SER	7.6
1	A	101	VAL	7.6
2	D	1020	GLN	7.5
1	A	231	LYS	7.4
1	B	252	ARG	7.4
1	A	335	ARG	7.3
3	O	39	LYS	7.3
1	A	429	LYS	7.3
1	A	227	LYS	7.2
1	B	482	GLU	7.2
4	P	129	LYS	7.1
2	C	1136	LYS	7.0
3	O	145	LYS	6.8
1	A	355	ASN	6.5
3	L	158	ASN	6.4
1	A	451	GLY	5.8
2	D	1142	LYS	5.8
1	B	337	LYS	5.7

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
3	YCM	L	214	11/11	-0.30	1.01	180,198,236,238	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	734	14/15	-0.30	1.16	167,184,193,194	0
5	NAG	A	776	14/15	-0.23	1.20	80,95,117,119	0
5	NAG	B	948	14/15	-0.21	1.13	147,169,175,179	0
5	NAG	B	886	14/15	-0.20	1.06	105,122,143,147	0
5	NAG	A	948	14/15	-0.14	1.03	143,154,166,166	0
5	NAG	A	886	14/15	-0.14	1.31	70,97,131,139	0
5	NAG	B	795	14/15	-0.13	1.03	169,190,203,209	0
5	NAG	B	789	14/15	-0.12	1.19	139,187,198,202	0
5	NAG	B	588	14/15	-0.12	0.89	119,161,167,169	0
5	NAG	A	762	14/15	-0.10	1.09	70,75,96,97	0
5	NAG	A	789	14/15	-0.08	1.16	86,104,117,128	0
6	GOL	B	1	6/6	-0.05	0.87	127,132,138,143	0
5	NAG	A	897	14/15	-0.03	1.10	124,150,169,175	0
5	NAG	A	741	14/15	-0.02	1.01	141,160,164,166	0
5	NAG	A	892	14/15	-0.01	1.13	117,148,182,193	0
5	NAG	B	762	14/15	0.02	1.00	102,122,145,155	0
5	NAG	A	734	14/15	0.04	1.10	113,130,148,153	0
5	NAG	B	776	14/15	0.07	1.03	118,135,157,161	0
5	NAG	A	588	14/15	0.07	1.10	99,141,159,174	0
5	NAG	B	892	14/15	0.08	1.08	166,204,227,236	0
6	GOL	P	215	6/6	0.26	0.81	134,147,156,162	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.