



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:51 AM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

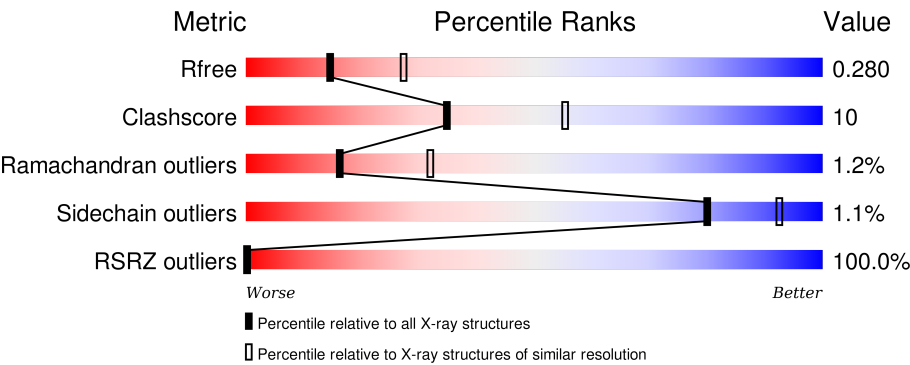
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

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}	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	379	<div><div>95%</div><div><div></div><div></div><div></div><div></div></div><div>69%25%• 5%</div></div>
1	B	379	<div><div>93%</div><div><div></div><div></div><div></div><div></div></div><div>69%24%• 7%</div></div>
2	C	184	<div><div>100%</div><div><div></div><div></div><div></div><div></div></div><div>74%24%•</div></div>
2	D	184	<div><div>99%</div><div><div></div><div></div><div></div><div></div></div><div>79%20%••</div></div>
3	L	213	<div><div>100%</div><div><div></div><div></div><div></div><div></div></div><div>77%23%•</div></div>

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Mol	Chain	Length	Quality of chain
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
5	NAG	A	734	X	-	-	X
5	NAG	A	762	-	-	-	X
5	NAG	A	776	-	-	-	X
5	NAG	A	789	-	-	-	X
5	NAG	A	886	-	-	-	X
5	NAG	A	897	-	-	-	X
5	NAG	A	948	X	-	-	X
5	NAG	B	588	X	-	-	-
5	NAG	B	734	-	-	-	X
5	NAG	B	762	-	-	-	X
5	NAG	B	776	-	-	-	X
5	NAG	B	789	-	-	-	X
6	GOL	B	1	-	-	-	X
6	GOL	P	215	-	-	-	X

2 Entry composition

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
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
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
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.

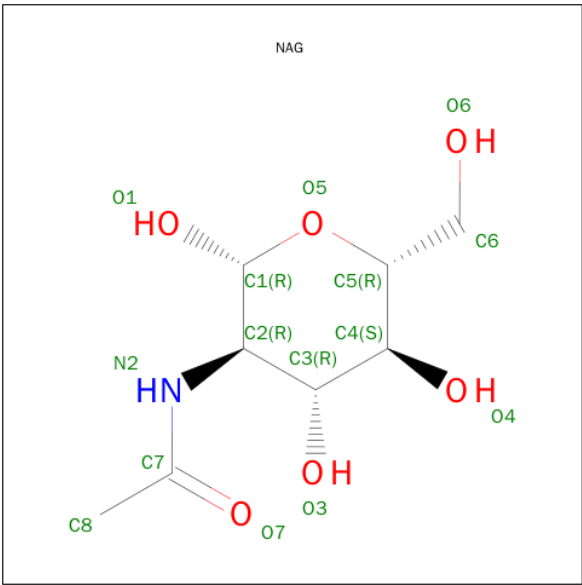
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	220	Total	C	N	O	S	0	0	0
			1654	1048	267	332	7			

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



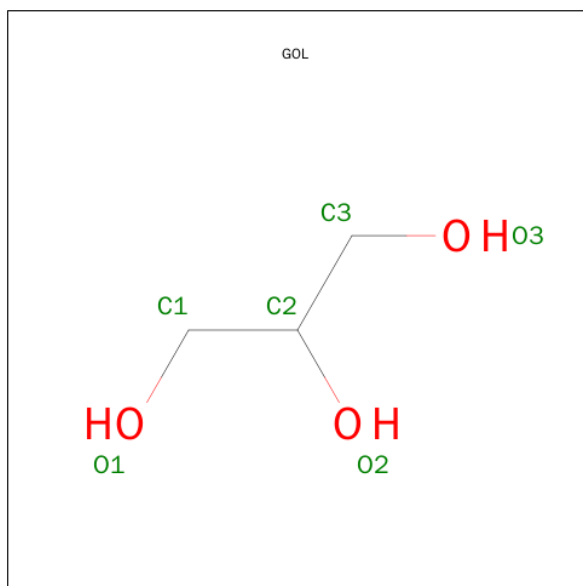
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14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

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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: C₃H₈O₃).



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		

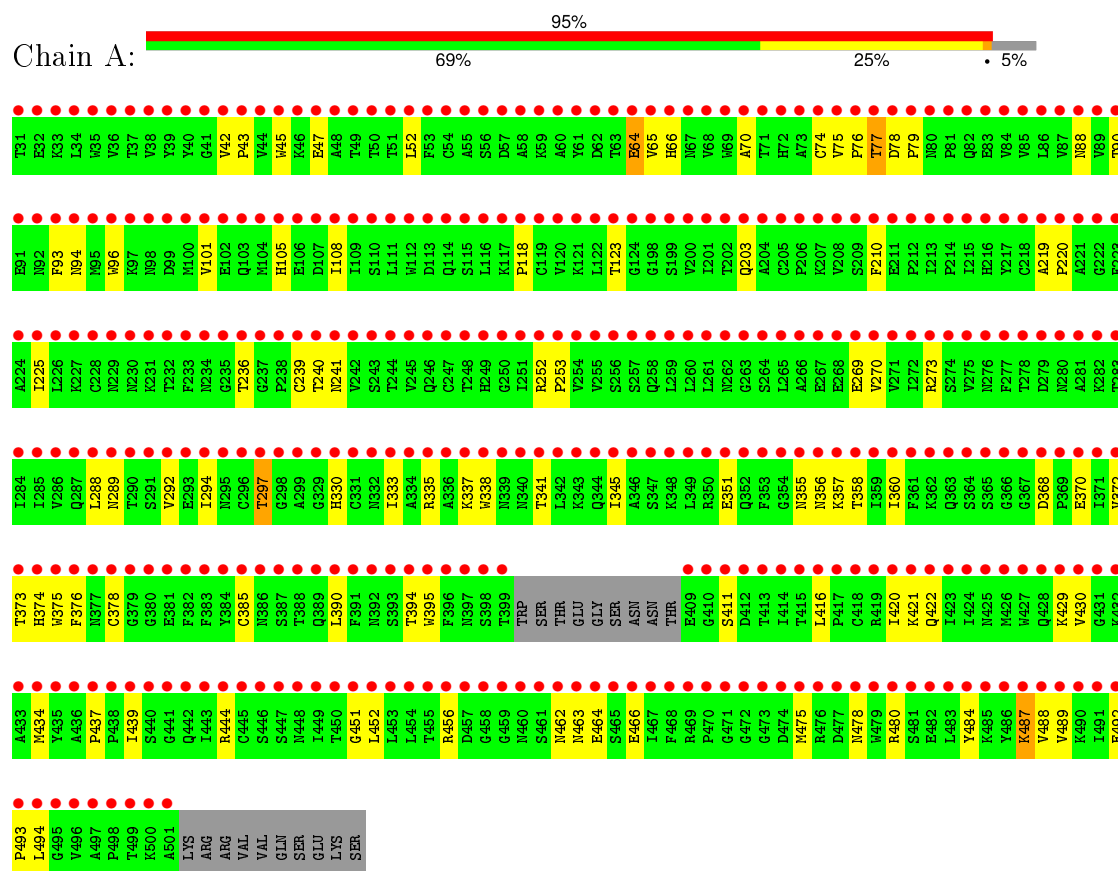
- Molecule 7 is water.

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

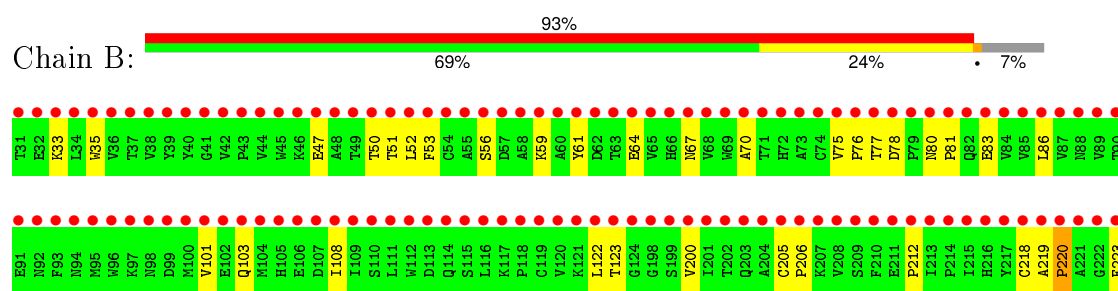
3 Residue-property plots

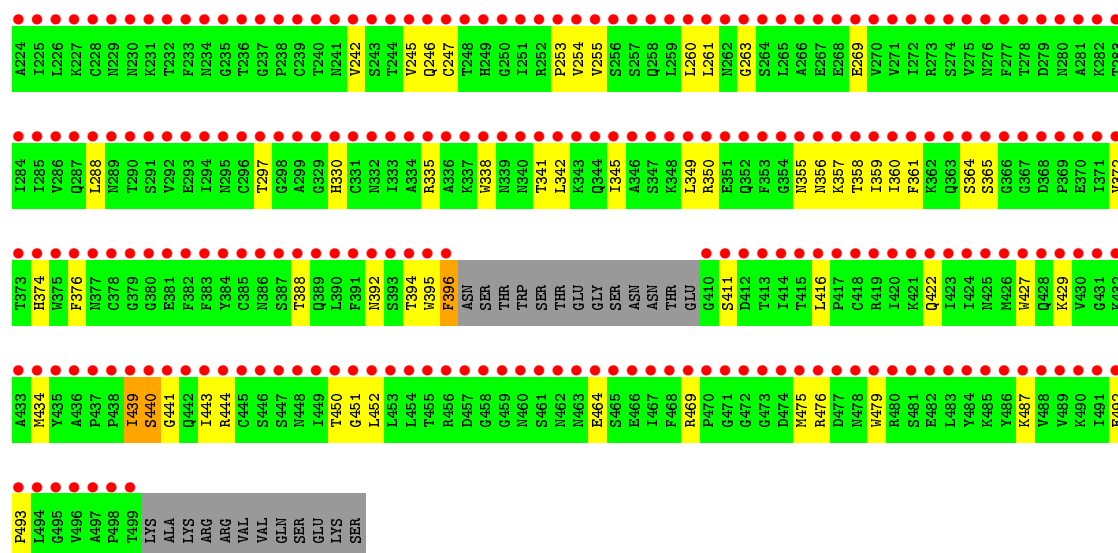
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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

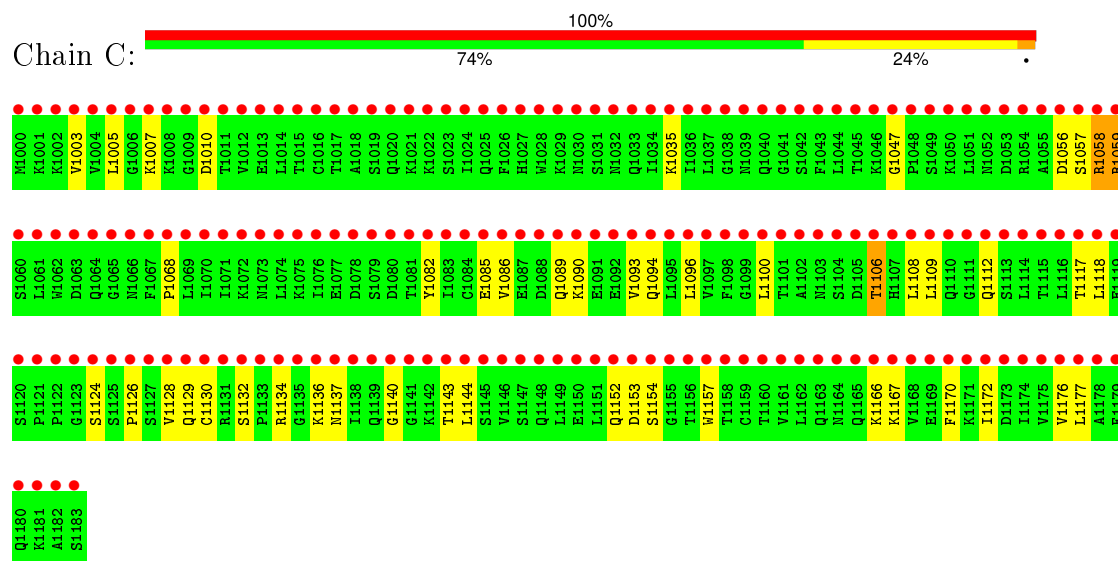


• Molecule 1: HIV-1 GP120 ENVELOPE GLYCOPROTEIN

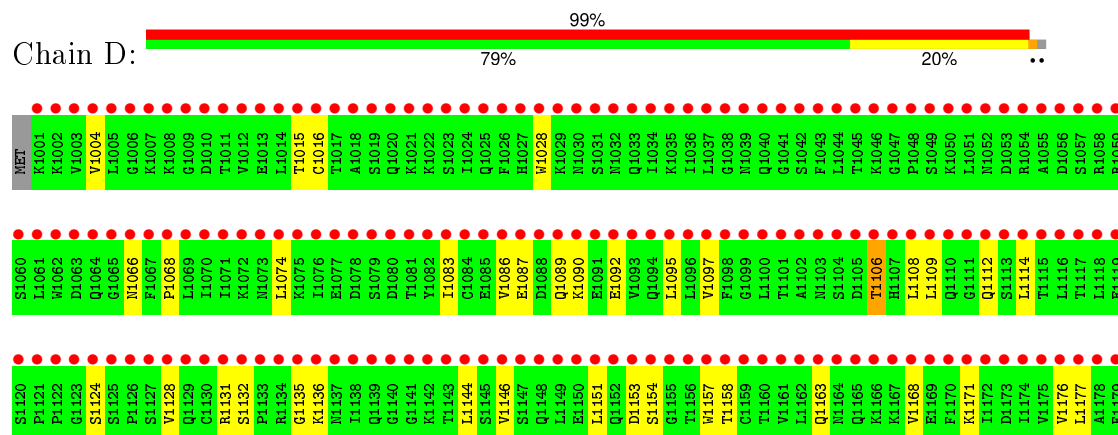




• Molecule 2: T-cell surface glycoprotein CD4



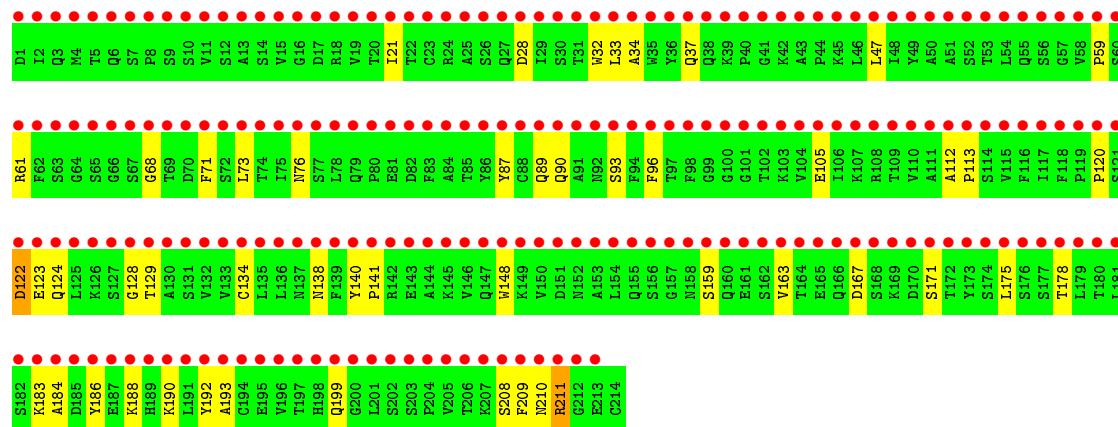
• Molecule 2: T-cell surface glycoprotein CD4




Q1180
K1181
A1182
S1183

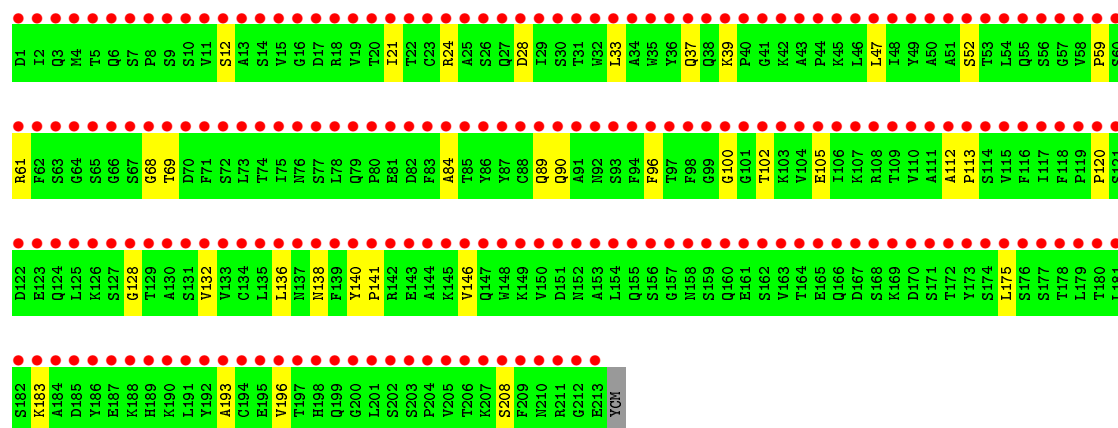
• Molecule 3: FAB 48D LIGHT CHAIN

Chain L:  100% 77% 23%




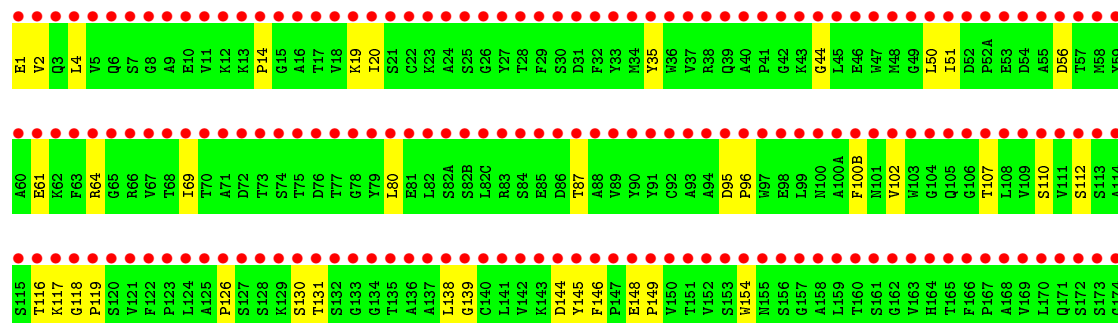
• Molecule 3: FAB 48D LIGHT CHAIN

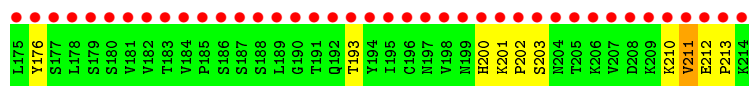
Chain O:  100% 83% 16%



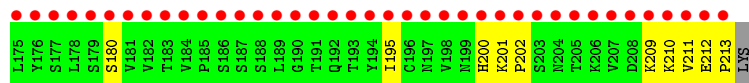
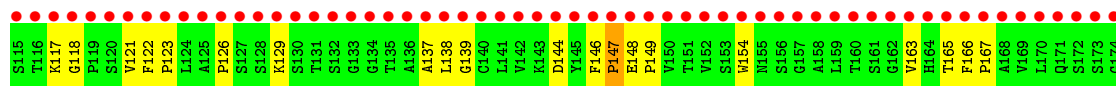
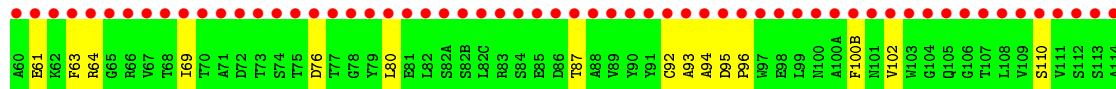
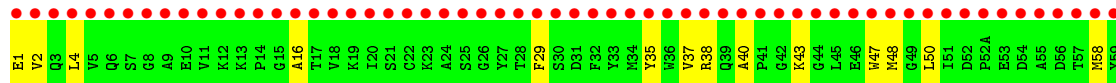
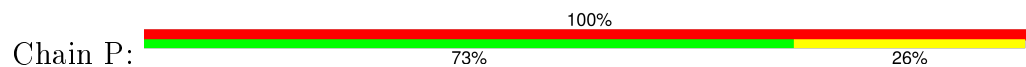
• Molecule 4: FAB 48D HEAVY CHAIN

Chain H:  100% 78% 21%





● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	0.04 (at 2.61Å)	Xtriage
Refinement program	PHENIX (CCI APPS 2007_04_06_1210)	Depositor
R, R_{free}	0.201 , 0.275 0.198 , 0.280	Depositor DCC
R_{free} test set	5577 reflections (10.14%)	DCC
Wilson B-factor (Å ²)	-10.7	Xtriage
Anisotropy	-7.799	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 62.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	23 of 59587 reflections (0.039%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15697	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, 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:H	1:A:420:ILE:HD12	1.64	0.61
4:H:138:LEU:HD11	4:H:211:VAL:HG11	1.82	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
1:A:492:GLU:HB2	1:A:493:PRO:CD	2.27	0.61
4:P:69:ILE:HG12	4:P:80:LEU:HD12	1.83	0.61
2:C:1132:SER:HB3	2:C:1136:LYS:HB3	1.82	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
2:C:1057:SER:HB2	2:C:1068:PRO:O	2.03	0.58
1:A:108:ILE:HD12	1:A:253:PRO:HB3	1.84	0.58
1:B:338:TRP:NE1	1:B:342:LEU:HD11	2.19	0.58
2:C:1140:GLY:HA3	2:C:1144:LEU:HG	1.85	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:80:ASN:N	1:B:81:PRO:HD3	2.21	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
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:140:TYR:CG	3:O:141:PRO:HA	2.44	0.52
3:O:39:LYS:HG2	3:O:84:ALA:HB2	1.91	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:B:361:PHE:HE2	1:B:395:TRP:HD1	1.59	0.50
1:A:90:THR:OG1	1:A:240:THR:HG22	2.12	0.50
2:D:1154:SER:HB2	2:D:1176:VAL:HB	1.93	0.50
2:D:1066:ASN:O	2:D:1068:PRO:HD3	2.11	0.50
1:B:388:THR:O	1:B:392:ASN:HB2	2.11	0.50
4:H:117:LYS:HD3	4:H:118:GLY:N	2.26	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
4:P:29:PHE:CD2	4:P:76:ASP:HA	2.47	0.49
1:A:236:THR:O	5:A:734:NAG:H2	2.12	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:D:1106:THR:HG21	2:D:1177:LEU:HD22	1.95	0.49
1:B:427:TRP:CE3	1:B:475:MET:HG3	2.47	0.49
2:C:1153:ASP:HB3	2:C:1157:TRP:HZ2	1.77	0.49
1:A:335:ARG:HH21	1:A:411:SER:HB3	1.78	0.49
2:C:1166:LYS:CD	2:C:1167:LYS:H	2.24	0.49
1:A:351:GLU:HA	1:A:355:ASN:OD1	2.12	0.49
1:B:77:THR:HG22	1:B:78:ASP:N	2.28	0.48
1:A:420:ILE:HD12	1:A:420:ILE:N	2.26	0.48
2:D:1151:LEU:HD12	2:D:1176:VAL:HG11	1.95	0.48
1:A:294:ILE:HD12	1:A:333:ILE:HD11	1.94	0.48
3:O:28:ASP:OD1	3:O:68:GLY:HA2	2.12	0.48
1:B:364:SER:OG	1:B:372:VAL:HA	2.13	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
3:O:33:LEU:HD22	3:O:89:GLN:O	2.13	0.48
1:B:59:LYS:HD3	1:B:61:TYR:OH	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
2:D:1132:SER:HB3	2:D:1136:LYS:HB3	1.95	0.48
4:H:148:GLU:HB3	4:H:149:PRO:HA	1.94	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
4:P:139:GLY:HA2	4:P:154:TRP:CH2	2.49	0.47
1:B:288:LEU:HD11	1:B:452:LEU:HD11	1.94	0.47
1:A:338:TRP:CE2	1:A:390:LEU:HD22	2.49	0.47
4:P:50:LEU:HG	4:P:58:MET:HB2	1.96	0.47
1:B:56:SER:OG	1:B:70:ALA:HB1	2.14	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:105:HIS:ND1	7:A:589:HOH:O	2.35	0.47
1:A:75:VAL:HG13	1:A:76:PRO:HD2	1.96	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:B:451:GLY:C	1:B:452:LEU:HD12	2.34	0.46
1:A:52:LEU:N	1:A:52:LEU:HD12	2.30	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
4:P:148:GLU:HB3	4:P:149:PRO:HA	1.98	0.46
1:B:86:LEU:HB2	1:B:242:VAL:HG23	1.98	0.46
3:L:183:LYS:HG3	7:L:247:HOH:O	2.15	0.46
4:P:47:TRP:HZ2	4:P:50:LEU:HD23	1.81	0.46
3:O:12:SER:HB3	3:O:105:GLU:OE1	2.16	0.46
4:H:212:GLU:HA	4:H:213:PRO:HD3	1.75	0.46
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	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:D:1089:GLN:C	2:D:1090:LYS:HD2	2.37	0.45
1:B:59:LYS:HB3	1:B:61:TYR:CE1	2.51	0.45
4:H:148:GLU:OE1	4:H:149:PRO:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1007:LYS:HE3	2:C:1170:PHE:CE1	2.51	0.45
1:B:261:LEU:H	6:B:1:GOL:H12	1.81	0.45
1:B:51:THR:HA	1:B:103:GLN:NE2	2.25	0.45
1:A:96:TRP:HD1	1:A:236:THR:HG21	1.81	0.45
2:D:1153:ASP:HB3	2:D:1157:TRP:HZ2	1.80	0.45
3:L:159:SER:HA	3:L:178:THR:O	2.16	0.45
4:H:69:ILE:HG12	4:H:80:LEU:HD13	1.99	0.45
2:C:1129:GLN:NE2	2:C:1137:ASN:HB3	2.32	0.45
3:O:90:GLN:O	3:O:96:PHE:HA	2.17	0.45
2:D:1086:VAL:HG22	2:D:1087:GLU:HG2	1.97	0.45
1:B:422:GLN:O	1:B:434:MET: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:108:ILE:CD1	1:B:253:PRO:HB3	2.46	0.45
1:B:101:VAL:HG13	1:B:479:TRP:HB2	1.99	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:420:ILE:HG22	1:A:421:LYS:N	2.32	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
2:C:1124:SER:O	2:C:1126:PRO:HD3	2.17	0.44
2:C:1154:SER:HB2	2:C:1176:VAL:CG1	2.47	0.44
2:C:1117:THR:HG23	2:C:1143:THR:HG22	2.00	0.44
3:L:124:GLN:HG2	3:L:129:THR:O	2.18	0.44
4:P:129:LYS:HD3	4:P:129:LYS:C	2.38	0.44
1:B:205:CYS:N	1:B:206:PRO:HD3	2.33	0.44
4:H:95:ASP:N	4:H:96:PRO:HD3	2.33	0.44
1:B:200:VAL:HG21	4:P:64:ARG:CZ	2.48	0.44
3:L:128:GLY:CA	3:L:183:LYS:HD2	2.47	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
4:P:4:LEU:HD12	4:P:102:VAL:HG23	2.00	0.44
1:B:33:LYS:HG3	1:B:35:TRP:H	1.83	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
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:B:439:ILE:HB	1:B:440:SER:H	1.57	0.43
1:A:422:GLN:O	1:A:434:MET:HA	2.18	0.43
3:L:122:ASP:OD2	3:L:123:GLU:HG3	2.18	0.43
1:A:88:ASN:HB2	5:A:588:NAG:O5	2.17	0.43
1:B:492:GLU:HB2	1:B:493:PRO:CD	2.47	0.43
1:A:437:PRO:HB2	3:L:32:TRP:CZ2	2.54	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
1:B:50:THR:HG21	1:B:223:PHE:CZ	2.53	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
1:B:122:LEU:CD2	1:B:200:VAL:HG22	2.49	0.43
2:C:1118:LEU:HD22	2:C:1128:VAL:CG2	2.48	0.43
1:B:349:LEU:HB2	1:B:359:ILE:HD13	2.00	0.43
4:H:50:LEU:C	4:H:50:LEU:HD12	2.40	0.42
4:P:212:GLU:HA	4:P:213:PRO:HD3	1.92	0.42
1:B:358:THR:OG1	1:B:396:PHE:HE1	2.02	0.42
1:A:65:VAL:HG21	1:A:210:PHE:CD1	2.54	0.42
4:P:95:ASP:N	4:P:96:PRO:HD3	2.34	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
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
4:P:201:LYS:N	4:P:202:PRO:CD	2.81	0.42
1:B:263:GLY:C	1:B:450:THR:HG21	2.40	0.42
1:A:292:VAL:HG13	1:A:337:LYS:HE3	2.00	0.42
1:A:421:LYS:HE2	1:A:421:LYS:HB3	1.80	0.42
1:A:294:ILE:O	1:A:294:ILE:HG23	2.19	0.42
3:L:28:ASP:OD1	3:L:68:GLY:HA2	2.20	0.42
1:B:260:LEU:HD12	1:B:451:GLY:HA3	2.02	0.42
1:A:297:THR:HB	1:A:444:ARG:NH2	2.34	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)
1:B:269:GLU:HG2	5:B:789:NAG:HN2	1.85	0.41
3:L:120:PRO:HG2	3:L:186:TYR:CZ	2.55	0.41
1:B:341:THR:O	1:B:345:ILE:HG13	2.20	0.41
1:A:330:HIS:HA	1:A:416:LEU:O	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
4:P:93:ALA:CB	4:P:100(B):PHE:HB3	2.47	0.41
1:B:200:VAL:HG11	4:P:64:ARG:NH2	2.35	0.41
4:P:4:LEU:HD13	4:P:92:CYS:O	2.19	0.41
1:A:273:ARG:NH2	1:A:484:TYR:CE2	2.89	0.41
2:D:1004:VAL:O	2:D:1095:LEU:HD12	2.20	0.41
1:A:93:PHE:HE2	1:A:239:CYS:HB3	1.85	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
4:H:118:GLY:HA2	4:H:119:PRO:HD3	1.91	0.41
1:A:370:GLU:HA	1:A:375:TRP:HB2	2.01	0.41
3:O:112:ALA:HA	3:O:113:PRO:HD3	1.80	0.41
3:L:21:ILE:HD11	3:L:73:LEU:HD23	2.03	0.41
2:C:1035:LYS:O	2:C:1047:GLY:HA3	2.20	0.41
4:P:122:PHE:HA	4:P:123:PRO:HD3	1.82	0.41
4:H:201:LYS:N	4:H:202:PRO:CD	2.83	0.41
2:C:1108:LEU:O	2:C:1109:LEU:HB2	2.20	0.41
3:O:128:GLY:HA2	3:O:183:LYS:HB2	2.02	0.41
4:H:139:GLY:HA2	4:H:154:TRP:CH2	2.55	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
4:P:166:PHE:HA	4:P:167:PRO:HD3	1.97	0.40
2:D:1016:CYS:HB2	2:D:1028:TRP:CZ2	2.57	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/379 (94%)	311 (87%)	40 (11%)	5 (1%)	14	26
1	B	350/379 (92%)	314 (90%)	31 (9%)	5 (1%)	14	26
2	C	182/184 (99%)	168 (92%)	13 (7%)	1 (0%)	34	58
2	D	181/184 (98%)	159 (88%)	22 (12%)	0	100	100
3	L	211/213 (99%)	194 (92%)	14 (7%)	3 (1%)	14	26
3	O	210/213 (99%)	181 (86%)	26 (12%)	3 (1%)	14	26
4	H	218/220 (99%)	193 (88%)	22 (10%)	3 (1%)	14	26
4	P	217/220 (99%)	194 (89%)	20 (9%)	3 (1%)	14	26
All	All	1925/1992 (97%)	1714 (89%)	188 (10%)	23 (1%)	16	32

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 ⓘ

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%)	70	88
1	B	310/333 (93%)	309 (100%)	1 (0%)	94	99
2	C	166/166 (100%)	161 (97%)	5 (3%)	48	75
2	D	165/166 (99%)	162 (98%)	3 (2%)	66	86
3	L	184/184 (100%)	180 (98%)	4 (2%)	60	83
3	O	184/184 (100%)	184 (100%)	0	100	100
4	H	185/185 (100%)	184 (100%)	1 (0%)	92	98
4	P	184/185 (100%)	184 (100%)	0	100	100
All	All	1693/1736 (98%)	1674 (99%)	19 (1%)	80	92

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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	7,10,10	1.30	2 (28%)	4,12,12	0.82	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	-	0/6/10/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	214	YCM	CB-SG	-2.37	1.76	1.81
3	L	214	YCM	CD-SG	-2.27	1.76	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	A	588	1	14,14,15	0.50	0	15,19,21	1.02	1 (6%)
5	NAG	A	734	1	14,14,15	0.51	0	15,19,21	0.75	0
5	NAG	A	741	1	14,14,15	0.46	0	15,19,21	0.98	1 (6%)
5	NAG	A	762	1	14,14,15	0.50	0	15,19,21	0.90	1 (6%)
5	NAG	A	776	1	14,14,15	0.47	0	15,19,21	0.92	1 (6%)
5	NAG	A	789	1	14,14,15	0.55	0	15,19,21	0.72	0
5	NAG	A	886	1	14,14,15	0.48	0	15,19,21	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	892	1	14,14,15	0.58	0	15,19,21	1.21	1 (6%)
5	NAG	A	897	1	14,14,15	0.53	0	15,19,21	0.74	0
5	NAG	A	948	1	14,14,15	0.52	0	15,19,21	0.75	0
6	GOL	B	1	-	5,5,5	0.38	0	5,5,5	0.20	0
5	NAG	B	588	1	14,14,15	0.48	0	15,19,21	0.80	1 (6%)
5	NAG	B	734	1	14,14,15	0.48	0	15,19,21	0.75	0
5	NAG	B	762	1	14,14,15	0.51	0	15,19,21	0.95	1 (6%)
5	NAG	B	776	1	14,14,15	0.47	0	15,19,21	0.88	1 (6%)
5	NAG	B	789	1	14,14,15	0.50	0	15,19,21	0.86	1 (6%)
5	NAG	B	795	1	14,14,15	0.45	0	15,19,21	0.88	1 (6%)
5	NAG	B	886	1	14,14,15	0.47	0	15,19,21	0.95	1 (6%)
5	NAG	B	892	1	14,14,15	0.51	0	15,19,21	0.70	0
5	NAG	B	948	1	14,14,15	0.49	0	15,19,21	0.70	0
6	GOL	P	215	-	5,5,5	0.38	0	5,5,5	0.24	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	588	1	-	0/6/23/26	0/1/1/1
5	NAG	A	734	1	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	A	741	1	-	0/6/23/26	0/1/1/1
5	NAG	A	762	1	-	0/6/23/26	0/1/1/1
5	NAG	A	776	1	-	0/6/23/26	0/1/1/1
5	NAG	A	789	1	-	1/6/23/26	0/1/1/1
5	NAG	A	886	1	-	0/6/23/26	0/1/1/1
5	NAG	A	892	1	-	0/6/23/26	0/1/1/1
5	NAG	A	897	1	-	0/6/23/26	0/1/1/1
5	NAG	A	948	1	1/1/5/7	0/6/23/26	0/1/1/1
6	GOL	B	1	-	-	0/4/4/4	0/0/0/0
5	NAG	B	588	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	734	1	-	1/6/23/26	0/1/1/1
5	NAG	B	762	1	-	0/6/23/26	0/1/1/1
5	NAG	B	776	1	-	0/6/23/26	0/1/1/1
5	NAG	B	789	1	-	0/6/23/26	0/1/1/1
5	NAG	B	795	1	-	0/6/23/26	0/1/1/1
5	NAG	B	886	1	-	0/6/23/26	0/1/1/1
5	NAG	B	892	1	-	1/6/23/26	0/1/1/1
5	NAG	B	948	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	P	215	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	789	NAG	C1-O5-C5	2.22	115.06	112.25
5	B	588	NAG	C1-O5-C5	2.27	115.13	112.25
5	B	776	NAG	C1-O5-C5	2.29	115.16	112.25
5	A	762	NAG	C1-O5-C5	2.29	115.16	112.25
5	B	795	NAG	C1-O5-C5	2.34	115.21	112.25
5	A	886	NAG	C1-O5-C5	2.34	115.22	112.25
5	A	776	NAG	C1-O5-C5	2.50	115.42	112.25
5	B	762	NAG	C1-O5-C5	2.63	115.59	112.25
5	A	741	NAG	C1-O5-C5	2.97	116.02	112.25
5	B	886	NAG	C1-O5-C5	3.05	116.12	112.25
5	A	588	NAG	C1-O5-C5	3.23	116.35	112.25
5	A	892	NAG	C1-O5-C5	3.97	117.29	112.25

All (3) chirality outliers are listed below:

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

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	734	NAG	O7-C7-N2-C2
5	B	892	NAG	O7-C7-N2-C2
5	A	789	NAG	O7-C7-N2-C2
5	B	734	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	762	NAG	1	0
5	B	789	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, 95th 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 ²)	Q<0.9
1	A	360/379 (94%)	13.52	360 (100%) 0 0	45, 78, 151, 254	0
1	B	354/379 (93%)	13.23	354 (100%) 0 0	66, 113, 190, 233	0
2	C	184/184 (100%)	13.79	184 (100%) 0 0	56, 83, 125, 144	0
2	D	183/184 (99%)	13.38	183 (100%) 0 0	74, 127, 165, 188	0
3	L	212/213 (99%)	14.03	212 (100%) 0 0	59, 101, 179, 240	0
3	O	212/213 (99%)	13.07	212 (100%) 0 0	91, 147, 189, 220	0
4	H	220/220 (100%)	14.19	220 (100%) 0 0	70, 121, 179, 251	0
4	P	219/220 (99%)	13.71	219 (100%) 0 0	66, 121, 195, 243	0
All	All	1944/1992 (97%)	13.58	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	27.1
4	H	88	ALA	24.9
1	B	385	CYS	24.6
4	P	26	GLY	24.2
1	A	228	CYS	23.9
1	A	388	THR	23.5
1	A	54	CYS	23.3
2	C	1133	PRO	23.3
1	A	235	GLY	23.1
1	A	230	ASN	22.7
1	A	447	SER	22.7
4	P	28	THR	22.6
1	B	222	GLY	22.6
2	D	1133	PRO	22.5
2	C	1159	CYS	22.3
4	H	186	SER	22.2

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Mol	Chain	Res	Type	RSRZ
4	P	145	TYR	22.0
3	L	88	CYS	22.0
1	B	240	THR	21.9
2	C	1006	GLY	21.9
1	A	84	VAL	21.9
4	H	162	GLY	21.9
3	L	178	THR	21.7
1	A	74	CYS	21.7
4	P	92	CYS	21.7
2	D	1028	TRP	21.5
2	D	1006	GLY	21.5
3	L	52	SER	21.3
3	O	43	ALA	21.2
1	B	369	PRO	21.2
2	C	1028	TRP	21.2
1	B	244	THR	21.2
1	B	259	LEU	21.2
1	A	210	PHE	21.0
1	B	220	PRO	21.0
3	L	68	GLY	20.9
1	A	55	ALA	20.9
3	L	180	THR	20.8
1	A	41	GLY	20.8
4	H	109	VAL	20.8
3	O	112	ALA	20.8
3	L	82	ASP	20.8
4	H	17	THR	20.6
1	A	296	CYS	20.6
1	A	331	CYS	20.6
2	C	1084	CYS	20.6
4	P	188	SER	20.5
1	B	72	HIS	20.4
1	A	385	CYS	20.4
2	D	1111	GLY	20.3
4	P	17	THR	20.3
2	C	1125	SER	20.3
4	P	115	SER	20.3
4	H	196	CYS	20.2
1	A	48	ALA	20.2
1	B	119	CYS	20.2
4	P	111	VAL	20.2
3	O	111	ALA	20.0

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Mol	Chain	Res	Type	RSRZ
4	H	165	THR	20.0
1	A	57	ASP	20.0
1	A	219	ALA	20.0
2	C	1102	ALA	20.0
4	H	204	ASN	20.0
3	O	130	ALA	19.9
4	H	82(C)	LEU	19.9
4	H	208	ASP	19.8
3	O	40	PRO	19.8
4	H	185	PRO	19.8
3	L	67	SER	19.7
2	D	1047	GLY	19.6
4	H	20	ILE	19.6
2	C	1120	SER	19.6
2	C	1009	GLY	19.6
4	H	112	SER	19.4
4	P	100	ASN	19.3
1	A	68	VAL	19.3
3	L	191	LEU	19.3
4	H	163	VAL	19.3
3	L	168	SER	19.3
1	A	112	TRP	19.3
4	P	120	SER	19.3
4	H	76	ASP	19.2
4	H	111	VAL	19.2
4	H	86	ASP	19.2
2	C	1005	LEU	19.2
3	L	176	SER	19.2
4	H	40	ALA	19.2
1	B	488	VAL	19.2
1	B	54	CYS	19.2
4	H	9	ALA	19.1
3	O	60	SER	19.1
4	P	88	ALA	19.1
2	D	1084	CYS	19.1
3	O	150	VAL	19.1
4	H	126	PRO	19.0
3	L	51	ALA	19.0
4	P	113	SER	19.0
1	A	465	SER	19.0
3	L	101	GLY	19.0
4	H	170	LEU	19.0

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Mol	Chain	Res	Type	RSRZ
2	D	1175	VAL	19.0
1	A	218	CYS	19.0
4	P	8	GLY	18.9
4	H	30	SER	18.9
2	D	1125	SER	18.9
4	P	184	VAL	18.8
2	C	1061	LEU	18.7
2	D	1170	PHE	18.7
3	L	91	ALA	18.6
3	L	47	LEU	18.6
3	O	46	LEU	18.6
4	P	172	SER	18.6
4	P	203	SER	18.6
1	A	216	HIS	18.5
4	H	137	ALA	18.5
2	C	1129	GLN	18.5
3	L	72	SER	18.5
1	A	373	THR	18.5
1	A	448	ASN	18.5
2	C	1122	PRO	18.5
1	B	120	VAL	18.4
2	D	1103	ASN	18.4
2	C	1130	CYS	18.4
3	L	60	SER	18.4
2	D	1099	GLY	18.4
2	D	1154	SER	18.4
4	H	188	SER	18.4
1	A	94	ASN	18.4
4	P	52(A)	PRO	18.4
4	H	77	THR	18.4
1	B	110	SER	18.3
4	H	180	SER	18.3
1	B	354	GLY	18.3
2	C	1095	LEU	18.3
1	A	436	ALA	18.3
1	B	329	GLY	18.3
2	C	1078	ASP	18.3
1	A	122	LEU	18.3
4	H	187	SER	18.3
1	A	236	THR	18.3
1	A	105	HIS	18.3
4	H	16	ALA	18.2

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Mol	Chain	Res	Type	RSRZ
1	A	70	ALA	18.2
2	C	1111	GLY	18.2
1	A	446	SER	18.2
3	O	182	SER	18.2
1	B	218	CYS	18.1
3	O	22	THR	18.1
1	B	338	TRP	18.1
1	B	253	PRO	18.1
3	L	177	SER	18.1
3	L	80	PRO	18.1
3	O	14	SER	18.1
1	B	122	LEU	18.0
2	D	1130	CYS	18.0
4	H	100	ASN	18.0
2	C	1113	SER	18.0
1	B	359	ILE	18.0
2	C	1010	ASP	18.0
4	P	90	TYR	18.0
1	B	87	VAL	18.0
3	L	37	GLN	18.0
1	A	443	ILE	18.0
1	A	119	CYS	18.0
3	O	73	LEU	17.9
3	O	1	ASP	17.9
4	P	76	ASP	17.9
1	A	459	GLY	17.9
4	H	178	LEU	17.8
4	P	153	SER	17.8
2	C	1037	LEU	17.8
3	L	198	HIS	17.8
1	B	333	ILE	17.8
4	H	193	THR	17.8
4	P	149	PRO	17.8
1	A	431	GLY	17.8
3	L	173	TYR	17.7
1	A	413	THR	17.7
2	C	1011	THR	17.7
4	P	156	SER	17.7
1	B	374	HIS	17.7
3	O	85	THR	17.7
4	H	96	PRO	17.7
4	P	73	THR	17.7

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Mol	Chain	Res	Type	RSRZ
1	B	45	TRP	17.7
4	H	52(A)	PRO	17.7
2	D	1132	SER	17.7
3	O	177	SER	17.7
1	A	445	CYS	17.6
2	D	1116	LEU	17.6
2	C	1153	ASP	17.6
3	L	113	PRO	17.6
1	A	479	TRP	17.6
3	L	134	CYS	17.6
1	A	205	CYS	17.5
3	L	111	ALA	17.5
2	C	1183	SER	17.4
3	O	59	PRO	17.4
3	L	172	THR	17.4
3	L	84	ALA	17.4
4	H	149	PRO	17.4
1	B	414	ILE	17.4
3	O	35	TRP	17.3
3	L	40	PRO	17.3
4	H	156	SER	17.3
2	C	1156	THR	17.3
1	A	118	PRO	17.3
4	H	36	TRP	17.3
4	P	102	VAL	17.2
3	O	69	THR	17.2
1	B	111	LEU	17.2
1	B	208	VAL	17.2
4	H	157	GLY	17.2
2	C	1055	ALA	17.2
1	A	72	HIS	17.2
1	B	251	ILE	17.2
4	P	160	THR	17.2
2	D	1127	SER	17.2
1	B	458	GLY	17.2
3	O	87	TYR	17.1
1	B	475	MET	17.1
2	C	1040	GLN	17.1
1	A	375	TRP	17.1
3	L	41	GLY	17.1
3	O	72	SER	17.1
3	L	194	CYS	17.1

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Mol	Chain	Res	Type	RSRZ
1	B	230	ASN	17.1
1	A	79	PRO	17.1
3	L	114	SER	17.0
4	P	101	ASN	17.0
2	C	1081	THR	17.0
1	A	99	ASP	17.0
1	A	384	TYR	17.0
1	A	393	SER	17.0
4	H	140	CYS	17.0
1	A	491	ILE	17.0
1	B	366	GLY	17.0
4	H	15	GLY	17.0
2	C	1146	VAL	17.0
2	D	1055	ALA	16.9
4	H	174	GLY	16.9
1	B	107	ASP	16.9
3	L	70	ASP	16.9
2	D	1128	VAL	16.9
3	L	10	SER	16.9
3	L	102	THR	16.9
2	D	1153	ASP	16.9
3	L	204	PRO	16.9
2	D	1161	VAL	16.9
2	D	1079	SER	16.9
3	O	30	SER	16.9
2	C	1036	ILE	16.9
3	L	36	TYR	16.9
3	L	79	GLN	16.8
3	L	132	VAL	16.8
3	O	101	GLY	16.8
4	H	160	THR	16.8
2	C	1097	VAL	16.8
1	B	70	ALA	16.8
1	A	332	ASN	16.8
2	C	1079	SER	16.8
2	C	1103	ASN	16.8
2	C	1182	ALA	16.8
1	A	104	MET	16.8
3	L	69	THR	16.8
1	B	77	THR	16.8
1	B	360	ILE	16.7
3	L	71	PHE	16.7

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Mol	Chain	Res	Type	RSRZ
4	H	84	SER	16.7
3	L	22	THR	16.7
1	A	213	ILE	16.7
4	P	187	SER	16.7
3	L	25	ALA	16.7
1	B	384	TYR	16.7
4	P	84	SER	16.7
4	H	181	VAL	16.7
4	P	31	ASP	16.7
4	H	34	MET	16.7
3	L	74	THR	16.6
4	H	194	TYR	16.6
1	A	412	ASP	16.6
3	L	116	PHE	16.6
3	L	119	PRO	16.6
4	P	139	GLY	16.6
1	A	204	ALA	16.6
3	O	36	TYR	16.6
1	A	77	THR	16.6
1	B	55	ALA	16.6
1	B	393	SER	16.6
4	P	180	SER	16.6
2	D	1162	LEU	16.6
4	H	70	THR	16.6
3	L	19	VAL	16.6
1	A	426	MET	16.5
4	H	24	ALA	16.5
1	A	495	GLY	16.5
4	H	207	VAL	16.5
2	C	1031	SER	16.5
4	P	19	LYS	16.5
2	D	1010	ASP	16.5
3	O	98	PHE	16.5
1	A	203	GLN	16.5
1	A	85	VAL	16.5
4	H	166	PHE	16.5
4	H	47	TRP	16.5
1	B	223	PHE	16.5
3	L	21	ILE	16.5
4	H	95	ASP	16.4
3	O	15	VAL	16.4
3	O	178	THR	16.4

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Mol	Chain	Res	Type	RSRZ
1	A	425	ASN	16.4
2	D	1083	ILE	16.4
4	H	138	LEU	16.4
2	C	1117	THR	16.4
2	C	1048	PRO	16.4
1	B	426	MET	16.4
4	P	109	VAL	16.4
3	L	170	ASP	16.4
1	B	436	ALA	16.4
3	L	163	VAL	16.4
4	H	89	VAL	16.4
1	A	52	LEU	16.4
3	L	181	LEU	16.4
1	B	497	ALA	16.4
4	P	50	LEU	16.4
2	D	1146	VAL	16.3
4	H	121	VAL	16.3
4	P	91	TYR	16.3
3	O	53	THR	16.3
3	L	98	PHE	16.3
2	D	1069	LEU	16.3
4	P	69	ILE	16.3
1	A	295	ASN	16.3
4	H	203	SER	16.3
3	L	77	SER	16.3
4	H	161	SER	16.3
3	O	80	PRO	16.3
1	B	484	TYR	16.3
3	O	102	THR	16.3
3	L	11	VAL	16.3
1	B	264	SER	16.3
3	O	129	THR	16.3
3	O	135	LEU	16.3
1	B	410	GLY	16.2
3	O	64	GLY	16.2
4	H	22	CYS	16.2
1	A	398	SER	16.2
2	C	1076	ILE	16.2
1	B	206	PRO	16.2
3	L	83	PHE	16.2
1	B	276	ASN	16.2
1	B	495	GLY	16.2

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Mol	Chain	Res	Type	RSRZ
1	A	71	THR	16.2
4	H	103	TRP	16.2
4	H	11	VAL	16.2
4	H	134	GLY	16.1
1	B	345	ILE	16.1
3	L	106	ILE	16.1
4	P	137	ALA	16.1
3	L	43	ALA	16.1
3	L	53	THR	16.1
3	O	209	PHE	16.1
3	O	104	VAL	16.1
4	P	34	MET	16.1
4	P	134	GLY	16.1
4	H	71	ALA	16.1
1	B	486	TYR	16.1
1	A	245	VAL	16.1
4	H	136	ALA	16.1
1	A	239	CYS	16.1
1	A	69	TRP	16.0
3	O	167	ASP	16.0
1	A	249	HIS	16.0
3	L	179	LEU	16.0
1	B	92	ASN	16.0
1	B	81	PRO	16.0
3	O	181	LEU	16.0
3	L	203	SER	16.0
2	C	1063	ASP	16.0
4	P	157	GLY	16.0
3	O	127	SER	16.0
2	C	1032	ASN	16.0
4	P	44	GLY	16.0
1	B	438	PRO	16.0
1	A	63	THR	16.0
3	L	7	SER	16.0
4	P	151	THR	16.0
4	P	200	HIS	16.0
4	H	82(A)	SER	16.0
4	P	179	SER	16.0
4	H	87	THR	16.0
1	A	272	ILE	15.9
4	P	165	THR	15.9
1	A	40	TYR	15.9

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Mol	Chain	Res	Type	RSRZ
4	H	151	THR	15.9
2	C	1054	ARG	15.9
1	B	109	ILE	15.9
1	A	95	MET	15.9
1	B	228	CYS	15.9
1	B	68	VAL	15.9
1	B	71	THR	15.9
2	D	1051	LEU	15.9
4	P	33	TYR	15.9
2	D	1140	GLY	15.9
4	H	94	ALA	15.9
3	L	139	PHE	15.9
1	B	49	THR	15.9
1	A	275	VAL	15.9
3	O	144	ALA	15.8
1	A	120	VAL	15.8
1	A	418	CYS	15.8
3	L	93	SER	15.8
3	O	114	SER	15.8
3	L	81	GLU	15.8
3	O	138	ASN	15.8
4	P	186	SER	15.8
1	B	296	CYS	15.8
4	H	32	PHE	15.8
4	P	87	THR	15.8
1	A	333	ILE	15.8
1	B	67	ASN	15.8
3	L	14	SER	15.8
4	H	177	SER	15.8
2	C	1069	LEU	15.8
1	B	105	HIS	15.8
2	D	1102	ALA	15.8
2	C	1155	GLY	15.8
1	A	357	LYS	15.7
1	B	295	ASN	15.7
3	L	137	ASN	15.7
1	A	262	ASN	15.7
1	A	438	PRO	15.7
2	D	1158	THR	15.7
4	H	21	SER	15.7
2	D	1080	ASP	15.7
1	A	374	HIS	15.7

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Mol	Chain	Res	Type	RSRZ
2	D	1156	THR	15.7
4	P	175	LEU	15.7
2	C	1049	SER	15.7
1	B	394	THR	15.7
2	D	1017	THR	15.7
3	O	97	THR	15.7
4	H	119	PRO	15.7
4	H	31	ASP	15.7
2	D	1159	CYS	15.7
3	O	31	THR	15.7
1	B	336	ALA	15.6
2	C	1148	GLN	15.6
3	L	29	ILE	15.6
4	H	195	ILE	15.6
1	A	43	PRO	15.6
4	P	135	THR	15.6
3	O	7	SER	15.6
3	L	32	TRP	15.6
3	O	125	LEU	15.6
2	D	1138	ILE	15.6
3	O	86	TYR	15.6
2	C	1062	TRP	15.6
1	A	81	PRO	15.6
1	A	330	HIS	15.6
1	B	270	VAL	15.6
4	P	121	VAL	15.6
1	B	50	THR	15.6
1	B	434	MET	15.6
2	C	1114	LEU	15.6
2	D	1015	THR	15.6
4	P	176	TYR	15.5
1	B	283	THR	15.5
1	A	392	ASN	15.5
1	B	219	ALA	15.5
1	A	53	PHE	15.5
4	P	80	LEU	15.5
3	L	5	THR	15.5
1	A	209	SER	15.5
1	B	210	PHE	15.5
4	P	138	LEU	15.5
2	C	1124	SER	15.5
1	A	76	PRO	15.5

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Mol	Chain	Res	Type	RSRZ
3	O	132	VAL	15.5
1	B	271	VAL	15.5
1	B	44	VAL	15.4
3	O	134	CYS	15.4
4	H	81	GLU	15.4
3	L	167	ASP	15.4
4	P	74	SER	15.4
1	B	368	ASP	15.4
4	H	175	LEU	15.4
3	L	202	SER	15.4
1	B	80	ASN	15.4
4	P	86	ASP	15.4
2	D	1037	LEU	15.4
1	B	379	GLY	15.4
2	C	1012	VAL	15.4
4	H	197	ASN	15.4
1	A	369	PRO	15.4
3	O	204	PRO	15.4
3	L	87	TYR	15.4
1	B	281	ALA	15.4
4	H	100(B)	PHE	15.3
1	A	96	TRP	15.3
1	B	225	ILE	15.3
2	C	1160	THR	15.3
3	O	4	MET	15.3
1	A	206	PRO	15.3
3	O	17	ASP	15.3
4	P	89	VAL	15.3
4	P	58	MET	15.3
4	P	20	ILE	15.3
1	A	36	VAL	15.3
4	H	28	THR	15.3
1	A	217	TYR	15.3
2	C	1051	LEU	15.3
3	L	136	LEU	15.3
1	B	375	TRP	15.3
1	A	299	ALA	15.3
4	P	18	VAL	15.3
3	O	88	CYS	15.3
3	O	75	ILE	15.2
2	C	1080	ASP	15.2
2	C	1158	THR	15.2

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Mol	Chain	Res	Type	RSRZ
2	C	1154	SER	15.2
1	B	443	ILE	15.2
4	P	114	ALA	15.2
1	A	246	GLN	15.2
3	L	59	PRO	15.2
3	L	164	THR	15.2
4	P	107	THR	15.2
1	A	60	ALA	15.2
2	D	1086	VAL	15.2
2	D	1119	GLU	15.2
1	B	493	PRO	15.2
3	L	120	PRO	15.2
2	D	1109	LEU	15.2
2	D	1113	SER	15.2
2	D	1117	THR	15.2
4	P	142	VAL	15.2
4	P	178	LEU	15.2
1	A	75	VAL	15.2
1	A	276	ASN	15.2
1	A	222	GLY	15.2
4	P	211	VAL	15.1
2	C	1143	THR	15.1
3	L	58	VAL	15.1
4	H	182	VAL	15.1
1	B	76	PRO	15.1
3	L	156	SER	15.1
1	B	450	THR	15.1
2	C	1112	GLN	15.1
4	H	27	TYR	15.1
1	B	212	PRO	15.1
2	D	1073	ASN	15.1
3	L	99	GLY	15.1
3	O	44	PRO	15.1
4	P	130	SER	15.1
2	C	1162	LEU	15.1
1	B	388	THR	15.1
3	L	86	TYR	15.1
4	P	93	ALA	15.1
3	L	17	ASP	15.1
1	B	202	THR	15.1
2	D	1082	TYR	15.1
2	D	1068	PRO	15.1

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Mol	Chain	Res	Type	RSRZ
4	P	59	TYR	15.0
1	B	447	SER	15.0
3	L	174	SER	15.0
4	P	71	ALA	15.0
1	A	115	SER	15.0
3	L	46	LEU	15.0
2	C	1093	VAL	15.0
2	D	1052	ASN	15.0
2	D	1003	VAL	15.0
3	L	23	CYS	15.0
3	L	30	SER	15.0
4	H	45	LEU	15.0
1	A	229	ASN	15.0
2	D	1040	GLN	15.0
1	B	433	ALA	15.0
3	O	176	SER	15.0
1	A	107	ASP	14.9
1	B	479	TRP	14.9
4	H	176	TYR	14.9
2	C	1052	ASN	14.9
2	D	1031	SER	14.9
4	H	172	SER	14.9
4	H	79	TYR	14.9
1	B	365	SER	14.9
1	B	413	THR	14.9
2	C	1083	ILE	14.9
3	O	12	SER	14.9
4	H	116	THR	14.9
3	L	104	VAL	14.9
1	A	435	TYR	14.9
1	B	250	GLY	14.9
1	B	239	CYS	14.8
4	P	140	CYS	14.8
1	B	427	TRP	14.8
2	C	1014	LEU	14.8
1	B	94	ASN	14.8
3	L	130	ALA	14.8
3	O	84	ALA	14.8
3	L	148	TRP	14.8
1	B	474	ASP	14.8
2	C	1110	GLN	14.8
3	L	24	ARG	14.8

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Mol	Chain	Res	Type	RSRZ
3	O	83	PHE	14.8
4	H	74	SER	14.8
1	B	459	GLY	14.8
4	P	47	TRP	14.8
4	P	170	LEU	14.8
1	A	233	PHE	14.8
1	A	462	ASN	14.8
2	C	1030	ASN	14.8
1	B	457	ASP	14.8
3	L	206	THR	14.8
4	H	107	THR	14.8
1	A	486	TYR	14.8
1	A	422	GLN	14.8
1	B	377	ASN	14.8
1	B	492	GLU	14.8
2	D	1173	ASP	14.8
1	B	112	TRP	14.8
2	C	1043	PHE	14.8
2	C	1068	PRO	14.8
2	D	1009	GLY	14.8
4	P	161	SER	14.7
1	A	241	ASN	14.7
1	B	367	GLY	14.7
4	H	154	TRP	14.7
1	A	498	PRO	14.7
2	C	1145	SER	14.7
4	H	29	PHE	14.7
3	L	112	ALA	14.7
3	L	169	LYS	14.7
2	C	1174	ILE	14.7
4	P	42	GLY	14.7
2	D	1104	SER	14.7
1	B	245	VAL	14.7
1	B	236	THR	14.7
4	P	41	PRO	14.7
3	L	144	ALA	14.7
1	A	259	LEU	14.7
1	B	449	ILE	14.7
3	O	89	GLN	14.7
1	A	387	SER	14.7
1	A	474	ASP	14.7
3	L	73	LEU	14.7

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Mol	Chain	Res	Type	RSRZ
2	D	1070	ILE	14.7
3	O	187	GLU	14.7
3	O	141	PRO	14.6
1	B	299	ALA	14.6
4	P	27	TYR	14.6
4	H	49	GLY	14.6
3	O	38	GLN	14.6
2	D	1067	PHE	14.6
2	C	1038	GLY	14.6
2	C	1082	TYR	14.6
3	L	6	GLN	14.6
3	O	208	SER	14.6
1	A	223	PHE	14.6
1	A	247	CYS	14.6
1	B	66	HIS	14.6
2	D	1145	SER	14.6
3	L	131	SER	14.6
4	H	100(A)	ALA	14.6
3	O	140	TYR	14.6
2	D	1101	THR	14.6
2	C	1131	ARG	14.6
3	L	44	PRO	14.6
1	A	432	LYS	14.6
1	A	61	TYR	14.6
1	A	364	SER	14.6
4	P	112	SER	14.6
2	D	1089	GLN	14.6
2	D	1098	PHE	14.6
2	C	1157	TRP	14.6
1	A	56	SER	14.6
4	H	57	THR	14.6
2	D	1094	GLN	14.6
1	A	214	PRO	14.6
4	P	55	ALA	14.6
1	A	421	LYS	14.5
1	A	38	VAL	14.5
3	O	154	LEU	14.5
1	B	378	CYS	14.5
2	D	1027	HIS	14.5
2	D	1097	VAL	14.5
1	A	111	LEU	14.5
1	A	221	ALA	14.5

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Mol	Chain	Res	Type	RSRZ
1	A	427	TRP	14.5
4	P	97	TRP	14.5
1	A	449	ILE	14.5
3	L	50	ALA	14.5
2	D	1063	ASP	14.5
4	P	177	SER	14.5
1	B	95	MET	14.5
3	O	168	SER	14.5
2	C	1170	PHE	14.4
4	H	75	THR	14.4
4	H	91	TYR	14.4
2	C	1116	LEU	14.4
1	A	497	ALA	14.4
3	L	38	GLN	14.4
2	D	1143	THR	14.4
2	D	1087	GLU	14.4
1	A	215	ILE	14.4
2	D	1114	LEU	14.4
1	B	205	CYS	14.4
1	A	123	THR	14.4
1	B	496	VAL	14.4
3	L	197	THR	14.4
1	B	90	THR	14.4
1	A	473	GLY	14.4
4	H	51	ILE	14.4
4	H	141	LEU	14.4
4	H	63	PHE	14.4
2	C	1019	SER	14.4
2	D	1118	LEU	14.4
2	D	1120	SER	14.4
3	O	96	PHE	14.4
1	A	199	SER	14.4
1	B	294	ILE	14.4
1	B	118	PRO	14.4
1	B	123	THR	14.4
4	H	120	SER	14.4
4	P	37	VAL	14.4
1	A	488	VAL	14.3
3	L	92	ASN	14.3
4	H	142	VAL	14.3
1	A	58	ALA	14.3
1	B	420	ILE	14.3

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Mol	Chain	Res	Type	RSRZ
4	H	33	TYR	14.3
4	H	37	VAL	14.3
2	D	1112	GLN	14.3
3	L	2	ILE	14.3
3	L	171	SER	14.3
4	P	123	PRO	14.3
3	L	175	LEU	14.3
4	H	60	ALA	14.3
4	H	78	GLY	14.3
4	P	136	ALA	14.3
4	H	59	TYR	14.3
1	B	383	PHE	14.3
2	D	1064	GLN	14.3
1	B	339	ASN	14.3
2	C	1013	GLU	14.3
3	L	9	SER	14.3
3	L	159	SER	14.3
4	H	179	SER	14.3
4	H	106	GLY	14.3
1	A	467	ILE	14.3
1	B	238	PRO	14.3
4	P	100(B)	PHE	14.3
2	D	1062	TRP	14.3
3	O	74	THR	14.3
1	B	48	ALA	14.3
4	H	167	PRO	14.2
2	D	1107	HIS	14.2
1	A	253	PRO	14.2
1	B	108	ILE	14.2
4	H	200	HIS	14.2
2	C	1121	PRO	14.2
1	A	455	THR	14.2
1	A	44	VAL	14.2
1	A	73	ALA	14.2
1	A	201	ILE	14.2
4	P	191	THR	14.2
4	P	94	ALA	14.2
1	A	256	SER	14.2
2	D	1095	LEU	14.2
1	A	338	TRP	14.2
2	C	1172	ILE	14.2
3	L	127	SER	14.2

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Mol	Chain	Res	Type	RSRZ
4	H	127	SER	14.2
4	P	166	PHE	14.2
2	C	1000	MET	14.1
3	O	163	VAL	14.1
4	H	164	HIS	14.1
1	B	437	PRO	14.1
4	H	18	VAL	14.1
1	A	264	SER	14.1
2	C	1141	GLY	14.1
4	P	110	SER	14.1
2	C	1027	HIS	14.1
3	L	34	ALA	14.1
4	P	51	ILE	14.1
1	B	297	THR	14.1
2	C	1123	GLY	14.1
2	D	1157	TRP	14.1
3	O	45	LYS	14.1
3	O	67	SER	14.1
4	H	115	SER	14.1
1	A	232	THR	14.1
4	P	152	VAL	14.1
2	D	1011	THR	14.1
3	O	202	SER	14.1
1	A	208	VAL	14.1
1	A	294	ILE	14.1
1	A	389	GLN	14.1
3	O	20	THR	14.1
2	C	1176	VAL	14.0
3	L	193	ALA	14.0
1	A	108	ILE	14.0
1	A	366	GLY	14.0
2	C	1086	VAL	14.0
1	B	61	TYR	14.0
3	O	66	GLY	14.0
4	H	93	ALA	14.0
1	B	376	PHE	14.0
2	D	1164	ASN	14.0
1	B	96	TRP	14.0
4	P	79	TYR	14.0
2	D	1081	THR	14.0
1	B	242	VAL	14.0
2	C	1067	PHE	14.0

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Mol	Chain	Res	Type	RSRZ
4	P	146	PHE	14.0
1	B	217	TYR	14.0
2	C	1023	SER	14.0
3	L	182	SER	14.0
4	H	82(B)	SER	14.0
1	B	213	ILE	14.0
3	O	48	ILE	14.0
4	P	95	ASP	14.0
1	B	435	TYR	14.0
3	L	57	GLY	13.9
1	B	38	VAL	13.9
1	A	88	ASN	13.9
1	A	35	TRP	13.9
3	L	48	ILE	13.9
4	P	35	TYR	13.9
2	D	1177	LEU	13.9
4	P	82(C)	LEU	13.9
4	P	141	LEU	13.9
1	B	43	PRO	13.9
1	B	249	HIS	13.9
4	H	135	THR	13.9
2	C	1053	ASP	13.9
3	O	91	ALA	13.9
4	H	152	VAL	13.9
4	H	25	SER	13.9
4	H	110	SER	13.9
4	P	21	SER	13.9
3	L	35	TRP	13.9
1	B	73	ALA	13.9
1	B	372	VAL	13.9
1	B	454	LEU	13.8
3	L	28	ASP	13.8
2	D	1066	ASN	13.8
2	D	1002	LYS	13.8
2	D	1174	ILE	13.8
4	P	56	ASP	13.8
1	A	274	SER	13.8
1	A	379	GLY	13.8
4	P	116	THR	13.8
1	A	200	VAL	13.8
2	C	1101	THR	13.8
4	P	183	THR	13.8

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Mol	Chain	Res	Type	RSRZ
3	L	56	SER	13.8
1	B	65	VAL	13.8
1	B	226	LEU	13.8
2	D	1038	GLY	13.8
1	B	277	PHE	13.8
3	L	210	ASN	13.8
4	P	24	ALA	13.8
1	B	116	LEU	13.8
2	D	1074	LEU	13.8
1	B	278	THR	13.8
4	H	153	SER	13.8
3	L	76	ASN	13.8
3	O	152	ASN	13.8
4	P	196	CYS	13.8
1	A	336	ALA	13.8
1	A	468	PHE	13.8
1	A	45	TRP	13.7
1	A	420	ILE	13.7
4	P	60	ALA	13.7
2	C	1118	LEU	13.7
1	B	439	ILE	13.7
3	L	12	SER	13.7
1	A	98	ASN	13.7
1	A	458	GLY	13.7
1	B	203	GLN	13.7
2	D	1054	ARG	13.7
1	B	489	VAL	13.7
2	D	1030	ASN	13.7
3	L	8	PRO	13.7
1	A	476	ARG	13.7
2	D	1029	LYS	13.7
1	B	63	THR	13.7
1	A	362	LYS	13.7
1	A	39	TYR	13.7
3	O	2	ILE	13.7
1	A	212	PRO	13.7
1	A	463	ASN	13.7
4	H	122	PHE	13.7
3	O	196	VAL	13.6
2	D	1151	LEU	13.6
1	A	345	ILE	13.6
1	B	350	ARG	13.6

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Mol	Chain	Res	Type	RSRZ
3	L	97	THR	13.6
1	B	453	LEU	13.6
1	B	494	LEU	13.6
3	O	21	ILE	13.6
2	C	1126	PRO	13.6
3	L	150	VAL	13.6
4	P	124	LEU	13.6
4	P	118	GLY	13.6
1	B	60	ALA	13.6
1	A	67	ASN	13.6
4	P	45	LEU	13.6
1	A	220	PRO	13.6
2	D	1106	THR	13.6
3	O	164	THR	13.6
4	P	29	PHE	13.6
4	P	104	GLY	13.6
2	D	1050	LYS	13.6
1	A	359	ILE	13.5
1	A	399	THR	13.5
2	D	1049	SER	13.5
1	A	483	LEU	13.5
3	L	125	LEU	13.5
2	C	1041	GLY	13.5
1	A	490	LYS	13.5
1	B	415	THR	13.5
2	C	1064	GLN	13.5
3	O	34	ALA	13.5
3	L	15	VAL	13.5
2	C	1104	SER	13.5
4	P	205	THR	13.5
1	B	204	ALA	13.5
1	A	456	ARG	13.5
1	A	417	PRO	13.5
1	B	93	PHE	13.5
4	H	68	THR	13.5
1	B	40	TYR	13.5
2	C	1177	LEU	13.5
2	D	1144	LEU	13.5
3	O	133	VAL	13.5
2	C	1016	CYS	13.5
1	B	102	GLU	13.5
1	A	382	PHE	13.5

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Mol	Chain	Res	Type	RSRZ
1	A	395	TRP	13.5
1	B	419	ARG	13.5
2	C	1094	GLN	13.5
1	A	480	ARG	13.4
3	L	18	ARG	13.4
3	O	137	ASN	13.4
1	A	250	GLY	13.4
1	B	37	THR	13.4
1	A	50	THR	13.4
2	C	1144	LEU	13.4
3	L	49	TYR	13.4
1	A	347	SER	13.4
1	B	275	VAL	13.4
4	P	67	VAL	13.4
2	D	1022	LYS	13.4
1	A	62	ASP	13.4
1	A	82	GLN	13.4
1	B	418	CYS	13.4
4	H	61	GLU	13.4
3	O	210	ASN	13.4
1	B	104	MET	13.4
1	A	397	ASN	13.4
1	A	240	THR	13.4
1	A	225	ILE	13.4
1	B	35	TRP	13.4
1	A	339	ASN	13.4
3	O	8	PRO	13.3
3	L	154	LEU	13.3
2	C	1039	ASN	13.3
3	O	192	TYR	13.3
4	H	80	LEU	13.3
4	H	118	GLY	13.3
2	D	1060	SER	13.3
4	H	192	GLN	13.3
1	B	386	ASN	13.3
4	H	54	ASP	13.3
1	A	110	SER	13.3
4	H	145	TYR	13.3
4	P	81	GLU	13.3
3	L	89	GLN	13.3
1	B	468	PHE	13.3
1	A	266	ALA	13.3

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Mol	Chain	Res	Type	RSRZ
4	H	52	ASP	13.3
1	B	272	ILE	13.3
4	H	41	PRO	13.3
1	A	281	ALA	13.3
2	D	1092	GLU	13.3
4	P	155	ASN	13.3
1	A	365	SER	13.3
1	A	433	ALA	13.3
4	P	181	VAL	13.2
1	B	425	ASN	13.2
1	A	283	THR	13.2
4	P	5	VAL	13.2
4	P	108	LEU	13.2
1	B	99	ASP	13.2
4	P	6	GLN	13.2
2	D	1093	VAL	13.2
1	A	386	ASN	13.2
3	L	186	TYR	13.2
1	A	437	PRO	13.2
1	B	89	VAL	13.2
2	C	1026	PHE	13.2
4	H	102	VAL	13.2
4	H	211	VAL	13.2
4	P	202	PRO	13.2
1	A	424	ILE	13.2
1	A	288	LEU	13.2
3	O	136	LEU	13.2
1	A	42	VAL	13.2
2	C	1003	VAL	13.2
1	B	261	LEU	13.1
3	O	143	GLU	13.1
1	A	289	ASN	13.1
1	B	114	GLN	13.1
3	O	110	VAL	13.1
2	D	1126	PRO	13.1
3	O	52	SER	13.1
4	H	5	VAL	13.1
4	P	103	TRP	13.1
2	C	1090	LYS	13.1
1	A	106	GLU	13.1
1	A	430	VAL	13.1
3	L	190	LYS	13.1

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Mol	Chain	Res	Type	RSRZ
2	D	1078	ASP	13.1
3	O	25	ALA	13.1
1	A	280	ASN	13.1
4	P	199	ASN	13.1
1	B	491	ILE	13.1
3	O	113	PRO	13.1
2	C	1128	VAL	13.1
2	D	1012	VAL	13.1
3	O	90	GLN	13.1
4	P	36	TRP	13.1
2	C	1151	LEU	13.0
2	C	1050	LYS	13.0
3	O	189	HIS	13.0
1	A	49	THR	13.0
3	O	193	ALA	13.0
1	B	258	GLN	13.0
4	H	50	LEU	13.0
4	H	146	PHE	13.0
4	P	185	PRO	13.0
2	D	1046	LYS	13.0
4	P	16	ALA	13.0
3	L	26	SER	13.0
3	L	85	THR	13.0
2	C	1173	ASP	13.0
3	O	212	GLY	13.0
1	B	74	CYS	13.0
1	A	244	THR	13.0
1	A	475	MET	13.0
2	C	1098	PHE	13.0
2	D	1056	ASP	13.0
2	C	1106	THR	12.9
2	D	1016	CYS	12.9
4	P	3	GLN	12.9
1	A	292	VAL	12.9
1	B	355	ASN	12.9
1	A	411	SER	12.9
3	O	174	SER	12.9
1	B	389	GLN	12.9
2	D	1032	ASN	12.9
3	L	142	ARG	12.9
3	O	205	VAL	12.9
4	H	55	ALA	12.9

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Mol	Chain	Res	Type	RSRZ
3	O	82	ASP	12.9
3	L	55	GLN	12.9
3	L	155	GLN	12.9
3	O	166	GLN	12.9
4	H	83	ARG	12.9
1	B	98	ASN	12.9
2	C	1096	LEU	12.9
1	B	113	ASP	12.9
3	L	31	THR	12.9
2	D	1034	ILE	12.9
4	P	169	VAL	12.9
1	A	278	THR	12.9
4	P	70	THR	12.9
4	H	123	PRO	12.9
1	B	199	SER	12.9
2	C	1105	ASP	12.9
2	D	1182	ALA	12.9
4	P	68	THR	12.9
4	P	131	THR	12.9
3	L	45	LYS	12.9
1	B	115	SER	12.9
1	B	342	LEU	12.9
4	P	4	LEU	12.9
2	C	1018	ALA	12.9
4	H	213	PRO	12.9
2	D	1163	GLN	12.8
4	H	69	ILE	12.8
1	B	243	SER	12.8
3	O	58	VAL	12.8
4	P	1	GLU	12.8
1	A	493	PRO	12.8
2	C	1137	ASN	12.8
1	A	261	LEU	12.8
3	L	121	SER	12.8
4	H	201	LYS	12.8
1	A	380	GLY	12.8
4	P	163	VAL	12.8
1	A	334	ALA	12.8
3	L	140	TYR	12.8
1	A	109	ILE	12.8
1	A	349	LEU	12.8
4	H	133	GLY	12.8

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Mol	Chain	Res	Type	RSRZ
1	B	36	VAL	12.8
1	B	448	ASN	12.8
1	B	100	MET	12.8
1	B	201	ILE	12.8
3	L	66	GLY	12.8
3	L	117	ILE	12.8
4	H	2	VAL	12.8
2	C	1089	GLN	12.8
4	P	98	GLU	12.8
1	A	489	VAL	12.8
4	P	85	GLU	12.8
1	B	353	PHE	12.8
1	B	284	ILE	12.8
1	B	340	ASN	12.8
1	A	414	ILE	12.7
2	C	1070	ILE	12.7
1	A	87	VAL	12.7
1	A	37	THR	12.7
1	B	391	PHE	12.7
4	H	199	ASN	12.7
4	H	23	LYS	12.7
3	L	105	GLU	12.7
1	A	207	LYS	12.7
2	C	1171	LYS	12.7
3	L	110	VAL	12.7
1	B	124	GLY	12.7
2	D	1025	GLN	12.7
1	B	216	HIS	12.7
1	B	234	ASN	12.7
2	D	1169	GLU	12.7
3	L	109	THR	12.7
2	C	1042	SER	12.7
3	O	23	CYS	12.7
2	C	1138	ILE	12.7
1	A	114	GLN	12.7
2	D	1160	THR	12.7
3	O	206	THR	12.7
1	A	116	LEU	12.7
1	A	390	LEU	12.7
1	B	331	CYS	12.7
1	B	84	VAL	12.7
1	B	266	ALA	12.7

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Mol	Chain	Res	Type	RSRZ
1	B	483	LEU	12.7
4	H	92	CYS	12.7
4	P	197	ASN	12.7
4	P	63	PHE	12.7
3	O	5	THR	12.7
4	H	144	ASP	12.6
1	B	221	ALA	12.6
1	B	265	LEU	12.6
1	B	412	ASP	12.6
1	A	242	VAL	12.6
3	L	108	ARG	12.6
1	B	31	THR	12.6
4	H	183	THR	12.6
1	A	286	VAL	12.6
1	B	53	PHE	12.6
1	B	480	ARG	12.6
2	D	1122	PRO	12.6
3	O	51	ALA	12.6
2	D	1045	THR	12.6
1	A	32	GLU	12.6
1	B	431	GLY	12.6
2	C	1165	GLN	12.6
2	D	1071	ILE	12.6
1	A	83	GLU	12.6
2	C	1065	GLY	12.6
1	B	442	GLN	12.6
2	D	1121	PRO	12.6
4	H	205	THR	12.6
1	A	254	VAL	12.6
1	B	286	VAL	12.6
1	B	344	GLN	12.5
1	A	89	VAL	12.5
1	A	496	VAL	12.5
1	B	280	ASN	12.5
1	B	373	THR	12.5
3	O	109	THR	12.5
1	B	207	LYS	12.5
1	A	383	PHE	12.5
1	A	265	LEU	12.5
1	A	350	ARG	12.5
2	D	1044	LEU	12.5
2	D	1061	LEU	12.5

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Mol	Chain	Res	Type	RSRZ
2	D	1178	ALA	12.5
4	P	148	GLU	12.5
3	O	119	PRO	12.5
4	P	167	PRO	12.5
3	O	201	LEU	12.5
2	C	1015	THR	12.5
4	P	57	THR	12.5
2	D	1171	LYS	12.5
1	A	464	GLU	12.5
2	C	1139	GLN	12.5
2	D	1180	GLN	12.5
3	O	13	ALA	12.5
4	P	9	ALA	12.5
1	B	33	LYS	12.5
4	H	130	SER	12.5
2	D	1096	LEU	12.5
3	O	180	THR	12.5
4	P	22	CYS	12.5
2	C	1092	GLU	12.4
3	O	197	THR	12.4
4	P	173	SER	12.4
1	B	477	ASP	12.4
2	C	1001	LYS	12.4
3	O	92	ASN	12.4
1	A	423	ILE	12.4
4	H	38	ARG	12.4
1	A	434	MET	12.4
4	H	35	TYR	12.4
4	H	4	LEU	12.4
1	B	411	SER	12.4
3	O	56	SER	12.4
2	D	1043	PHE	12.4
1	B	395	TRP	12.4
1	B	422	GLN	12.4
1	B	392	ASN	12.4
4	H	99	LEU	12.4
1	B	86	LEU	12.4
1	A	492	GLU	12.4
2	D	1115	THR	12.4
3	L	4	MET	12.3
4	P	212	GLU	12.3
1	A	481	SER	12.3

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Mol	Chain	Res	Type	RSRZ
2	C	1058	ARG	12.3
3	L	3	GLN	12.3
1	B	117	LYS	12.3
3	O	65	SER	12.3
4	H	97	TRP	12.3
4	P	164	HIS	12.3
1	A	285	ILE	12.3
3	O	194	CYS	12.3
2	C	1132	SER	12.3
4	H	184	VAL	12.3
2	D	1137	ASN	12.3
1	A	372	VAL	12.3
1	B	69	TRP	12.3
4	H	90	TYR	12.3
1	B	293	GLU	12.3
3	L	78	LEU	12.3
3	O	213	GLU	12.3
3	O	29	ILE	12.3
3	L	195	GLU	12.3
4	H	108	LEU	12.2
3	L	65	SER	12.2
1	B	229	ASN	12.2
4	P	143	LYS	12.2
4	H	148	GLU	12.2
3	O	78	LEU	12.2
2	C	1046	LYS	12.2
4	H	58	MET	12.2
4	P	75	THR	12.2
2	C	1109	LEU	12.2
2	D	1014	LEU	12.2
3	O	151	ASP	12.2
1	A	269	GLU	12.2
4	P	100(A)	ALA	12.2
4	P	2	VAL	12.2
4	P	182	VAL	12.2
1	B	424	ILE	12.2
2	C	1034	ILE	12.2
3	L	20	THR	12.2
1	B	279	ASP	12.2
1	A	93	PHE	12.2
4	H	85	GLU	12.2
1	A	297	THR	12.2

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Mol	Chain	Res	Type	RSRZ
2	C	1074	LEU	12.2
1	A	238	PRO	12.2
3	O	186	TYR	12.2
4	P	39	GLN	12.2
3	L	138	ASN	12.2
2	C	1175	VAL	12.2
3	O	32	TRP	12.2
1	A	341	THR	12.2
2	C	1024	ILE	12.1
3	O	159	SER	12.1
3	O	203	SER	12.1
1	B	224	ALA	12.1
4	H	150	VAL	12.1
2	D	1141	GLY	12.1
1	A	270	VAL	12.1
1	B	430	VAL	12.1
3	L	33	LEU	12.1
1	B	262	ASN	12.1
1	B	381	GLU	12.1
3	L	54	LEU	12.1
1	A	410	GLY	12.1
3	O	26	SER	12.1
4	P	99	LEU	12.1
1	B	363	GLN	12.1
1	B	356	ASN	12.1
1	A	277	PHE	12.1
3	O	142	ARG	12.1
4	P	54	ASP	12.1
3	O	57	GLY	12.1
2	C	1115	THR	12.0
3	L	42	LYS	12.0
1	B	465	SER	12.0
2	D	1023	SER	12.0
4	P	12	LYS	12.0
4	H	159	LEU	12.0
1	B	78	ASP	12.0
4	P	65	GLY	12.0
2	D	1139	GLN	12.0
3	L	160	GLN	12.0
1	B	209	SER	12.0
4	H	168	ALA	12.0
1	A	90	THR	12.0

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Mol	Chain	Res	Type	RSRZ
1	A	444	ARG	12.0
1	B	91	GLU	12.0
1	B	462	ASN	12.0
4	P	83	ARG	12.0
2	D	1176	VAL	12.0
1	B	215	ILE	12.0
1	B	52	LEU	12.0
3	L	1	ASP	12.0
4	P	52	ASP	12.0
1	B	51	THR	12.0
1	B	255	VAL	12.0
3	O	155	GLN	12.0
4	H	139	GLY	12.0
4	P	207	VAL	12.0
1	B	291	SER	12.0
3	O	148	TRP	12.0
3	L	157	GLY	11.9
2	D	1134	ARG	11.9
3	O	158	ASN	11.9
1	A	346	ALA	11.9
3	O	184	ALA	11.9
1	A	257	SER	11.9
3	L	135	LEU	11.9
3	O	18	ARG	11.9
1	A	271	VAL	11.9
2	C	1147	SER	11.9
2	C	1108	LEU	11.9
3	O	175	LEU	11.9
1	A	477	ASP	11.9
1	A	469	ARG	11.9
1	B	254	VAL	11.9
4	H	132	SER	11.9
1	A	457	ASP	11.9
1	B	211	GLU	11.9
3	O	126	LYS	11.9
4	P	82(A)	SER	11.9
1	B	341	THR	11.9
4	H	191	THR	11.9
4	P	30	SER	11.9
3	O	173	TYR	11.9
1	A	298	GLY	11.9
4	P	209	LYS	11.9

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Mol	Chain	Res	Type	RSRZ
2	C	1066	ASN	11.9
4	H	67	VAL	11.9
1	B	330	HIS	11.9
1	A	279	ASP	11.9
1	A	342	LEU	11.9
4	P	62	LYS	11.8
2	C	1119	GLU	11.8
2	D	1110	GLN	11.8
3	L	94	PHE	11.8
3	L	63	SER	11.8
2	C	1161	VAL	11.8
2	D	1172	ILE	11.8
4	P	122	PHE	11.8
4	P	213	PRO	11.8
4	H	44	GLY	11.8
4	H	114	ALA	11.8
3	O	71	PHE	11.8
3	O	139	PHE	11.8
4	P	32	PHE	11.8
2	C	1060	SER	11.8
3	L	141	PRO	11.8
1	A	113	ASP	11.8
2	C	1056	ASP	11.8
2	D	1088	ASP	11.8
3	O	68	GLY	11.8
3	L	115	VAL	11.8
1	B	349	LEU	11.8
1	B	421	LYS	11.8
1	B	476	ARG	11.8
4	H	13	LYS	11.8
3	O	120	PRO	11.8
2	C	1033	GLN	11.8
1	A	66	HIS	11.8
4	P	38	ARG	11.8
3	O	47	LEU	11.8
3	O	170	ASP	11.8
4	P	144	ASP	11.8
1	B	499	THR	11.8
4	H	19	LYS	11.7
4	P	125	ALA	11.7
3	L	118	PHE	11.7
1	B	64	GLU	11.7

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Mol	Chain	Res	Type	RSRZ
1	B	473	GLY	11.7
3	L	162	SER	11.7
4	P	48	MET	11.7
4	P	159	LEU	11.7
1	A	470	PRO	11.7
1	B	214	PRO	11.7
1	B	263	GLY	11.7
3	L	211	ARG	11.7
4	P	174	GLY	11.7
2	C	1100	LEU	11.7
1	A	368	ASP	11.7
2	D	1152	GLN	11.7
2	D	1108	LEU	11.7
1	B	440	SER	11.7
2	D	1057	SER	11.7
1	B	58	ALA	11.7
1	B	246	GLN	11.7
1	A	65	VAL	11.6
4	H	202	PRO	11.6
1	A	484	TYR	11.6
1	B	260	LEU	11.6
1	A	202	THR	11.6
2	D	1004	VAL	11.6
2	D	1168	VAL	11.6
4	H	131	THR	11.6
3	O	190	LYS	11.6
4	P	96	PRO	11.6
4	H	143	LYS	11.6
1	B	466	GLU	11.6
4	P	7	SER	11.6
4	P	40	ALA	11.6
1	B	463	ASN	11.6
4	P	82(B)	SER	11.6
2	C	1168	VAL	11.6
1	A	353	PHE	11.6
3	O	172	THR	11.6
4	H	198	VAL	11.6
4	H	101	ASN	11.5
1	A	100	MET	11.5
1	A	454	LEU	11.5
3	O	106	ILE	11.5
3	L	145	LYS	11.5

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Mol	Chain	Res	Type	RSRZ
3	O	146	VAL	11.5
3	O	49	TYR	11.5
3	O	116	PHE	11.5
1	B	62	ASP	11.5
1	A	340	ASN	11.5
1	B	382	PHE	11.5
1	A	251	ILE	11.5
3	L	185	ASP	11.5
1	A	260	LEU	11.5
4	H	7	SER	11.5
4	P	192	GLN	11.5
2	C	1073	ASN	11.5
3	L	61	ARG	11.5
1	A	358	THR	11.4
1	A	415	THR	11.4
4	H	171	GLN	11.4
1	B	256	SER	11.4
2	C	1127	SER	11.4
1	A	255	VAL	11.4
3	O	79	GLN	11.4
4	P	11	VAL	11.4
3	O	93	SER	11.4
4	P	133	GLY	11.4
2	D	1021	LYS	11.4
2	D	1150	GLU	11.4
4	H	56	ASP	11.4
4	P	208	ASP	11.4
1	B	289	ASN	11.4
3	O	94	PHE	11.4
1	B	444	ARG	11.4
4	H	158	ALA	11.4
4	H	64	ARG	11.4
2	C	1150	GLU	11.4
4	P	154	TRP	11.4
1	B	247	CYS	11.4
3	L	153	ALA	11.4
2	C	1140	GLY	11.4
2	C	1025	GLN	11.4
4	H	39	GLN	11.4
3	O	100	GLY	11.4
4	P	127	SER	11.4
3	O	27	GLN	11.3

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Mol	Chain	Res	Type	RSRZ
1	B	41	GLY	11.3
2	C	1035	LYS	11.3
1	B	75	VAL	11.3
4	P	14	PRO	11.3
1	A	377	ASN	11.3
1	A	378	CYS	11.3
3	L	152	ASN	11.3
2	D	1091	GLU	11.3
2	D	1148	GLN	11.3
1	B	446	SER	11.3
1	B	274	SER	11.3
1	B	290	THR	11.3
4	P	194	TYR	11.3
2	C	1072	LYS	11.3
3	L	75	ILE	11.3
1	A	248	THR	11.3
3	O	153	ALA	11.3
1	A	92	ASN	11.3
1	A	252	ARG	11.3
3	L	96	PHE	11.2
1	B	237	GLY	11.2
3	L	64	GLY	11.2
2	D	1059	ARG	11.2
4	H	10	GLU	11.2
2	C	1021	LYS	11.2
1	A	441	GLY	11.2
3	L	205	VAL	11.2
2	C	1169	GLU	11.2
3	O	123	GLU	11.2
3	O	10	SER	11.2
2	D	1036	ILE	11.2
3	O	160	GLN	11.2
1	B	472	GLY	11.2
1	A	376	PHE	11.2
3	O	115	VAL	11.2
1	B	464	GLU	11.2
1	B	347	SER	11.2
1	B	288	LEU	11.2
4	H	14	PRO	11.2
4	H	189	LEU	11.2
1	B	85	VAL	11.2
3	O	11	VAL	11.2

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Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	11.2
1	B	432	LYS	11.2
2	C	1029	LYS	11.2
4	H	206	LYS	11.2
1	B	396	PHE	11.1
1	B	417	PRO	11.1
1	A	409	GLU	11.1
1	A	226	LEU	11.1
2	C	1045	THR	11.1
3	L	196	VAL	11.1
3	O	195	GLU	11.1
2	C	1044	LEU	11.1
3	L	90	GLN	11.1
1	A	391	PHE	11.1
4	P	147	PRO	11.1
1	A	371	ILE	11.1
3	O	121	SER	11.1
4	P	46	GLU	11.1
2	C	1149	LEU	11.1
3	L	143	GLU	11.1
4	H	155	ASN	11.1
1	A	344	GLN	11.1
3	O	6	GLN	11.1
3	O	55	GLN	11.1
1	B	416	LEU	11.1
1	B	467	ILE	11.0
1	B	470	PRO	11.0
1	A	485	LYS	11.0
1	A	234	ASN	11.0
2	D	1135	GLY	11.0
4	P	119	PRO	11.0
1	B	455	THR	11.0
1	A	478	ASN	11.0
1	B	241	ASN	11.0
1	A	78	ASP	11.0
1	B	82	GLN	11.0
2	C	1179	PHE	11.0
4	P	189	LEU	11.0
3	O	122	ASP	11.0
1	B	39	TYR	11.0
2	D	1100	LEU	11.0
4	H	46	GLU	11.0

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Mol	Chain	Res	Type	RSRZ
4	P	201	LYS	11.0
2	C	1047	GLY	11.0
4	H	147	PRO	11.0
1	A	381	GLU	11.0
3	L	184	ALA	11.0
3	O	76	ASN	11.0
4	H	66	ARG	11.0
1	A	291	SER	11.0
1	B	445	CYS	11.0
2	D	1001	LYS	11.0
1	A	211	GLU	11.0
1	A	452	LEU	11.0
1	B	292	VAL	11.0
3	O	183	LYS	10.9
1	A	363	GLN	10.9
1	B	248	THR	10.9
1	A	102	GLU	10.9
2	D	1085	GLU	10.9
1	B	358	THR	10.9
1	B	257	SER	10.9
4	P	66	ARG	10.9
2	C	1017	THR	10.9
3	O	81	GLU	10.9
1	A	282	LYS	10.9
1	B	106	GLU	10.9
2	D	1129	GLN	10.9
2	C	1004	VAL	10.8
2	C	1107	HIS	10.8
1	A	419	ARG	10.8
2	D	1018	ALA	10.8
1	A	450	THR	10.8
4	H	73	THR	10.8
2	D	1179	PHE	10.8
1	A	268	GLU	10.8
4	H	124	LEU	10.8
4	H	214	LYS	10.8
3	L	128	GLY	10.8
1	A	428	GLN	10.8
1	B	380	GLY	10.8
2	D	1024	ILE	10.8
2	D	1147	SER	10.8
2	C	1091	GLU	10.8

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Mol	Chain	Res	Type	RSRZ
2	D	1008	LYS	10.8
1	A	461	SER	10.8
1	A	80	ASN	10.7
1	A	361	PHE	10.7
4	P	162	GLY	10.7
3	L	209	PHE	10.7
1	B	34	LEU	10.7
1	B	487	LYS	10.7
4	P	77	THR	10.7
1	A	224	ALA	10.7
3	O	50	ALA	10.7
2	C	1142	LYS	10.7
3	L	62	PHE	10.7
3	O	161	GLU	10.7
2	D	1005	LEU	10.7
2	C	1135	GLY	10.7
1	B	357	LYS	10.7
4	P	198	VAL	10.7
4	P	190	GLY	10.7
2	C	1057	SER	10.7
3	O	70	ASP	10.7
1	B	361	PHE	10.7
3	O	156	SER	10.7
1	A	482	GLU	10.7
1	B	452	LEU	10.7
4	P	168	ALA	10.6
2	D	1042	SER	10.6
3	L	192	TYR	10.6
1	A	352	GLN	10.6
1	A	117	LYS	10.6
3	L	103	LYS	10.6
2	D	1026	PHE	10.6
3	L	146	VAL	10.6
4	P	128	SER	10.6
1	B	471	GLY	10.6
4	P	105	GLN	10.6
1	B	32	GLU	10.6
1	B	390	LEU	10.6
4	H	8	GLY	10.6
3	O	37	GLN	10.6
1	A	360	ILE	10.6
1	B	42	VAL	10.6

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Mol	Chain	Res	Type	RSRZ
3	L	161	GLU	10.6
4	H	6	GLN	10.5
2	D	1041	GLY	10.5
1	B	233	PHE	10.5
4	P	195	ILE	10.5
3	L	123	GLU	10.5
3	L	199	GLN	10.5
1	B	235	GLY	10.5
2	C	1007	LYS	10.5
4	P	72	ASP	10.5
4	H	104	GLY	10.5
4	P	23	LYS	10.5
1	A	103	GLN	10.5
3	L	151	ASP	10.5
2	C	1075	LYS	10.5
1	B	461	SER	10.5
3	O	117	ILE	10.5
2	C	1178	ALA	10.4
2	D	1058	ARG	10.4
1	B	198	GLY	10.4
1	B	46	LYS	10.4
1	B	88	ASN	10.4
3	L	189	HIS	10.4
2	C	1002	LYS	10.4
4	H	169	VAL	10.4
1	A	243	SER	10.4
3	O	169	LYS	10.4
4	H	12	LYS	10.3
1	A	31	THR	10.3
1	A	351	GLU	10.3
3	O	77	SER	10.3
3	L	133	VAL	10.3
2	C	1088	ASP	10.3
4	H	98	GLU	10.3
3	L	200	GLY	10.3
1	B	387	SER	10.3
1	A	263	GLY	10.3
3	L	16	GLY	10.3
2	C	1164	ASN	10.3
1	A	494	LEU	10.3
3	L	27	GLN	10.3
1	A	124	GLY	10.3

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Mol	Chain	Res	Type	RSRZ
4	P	210	LYS	10.3
1	B	332	ASN	10.2
1	B	428	GLN	10.2
2	D	1033	GLN	10.2
4	H	3	GLN	10.2
4	H	105	GLN	10.2
3	O	108	ARG	10.2
1	A	440	SER	10.2
4	P	171	GLN	10.2
1	B	47	GLU	10.2
3	O	9	SER	10.2
2	D	1090	LYS	10.2
1	A	396	PHE	10.1
1	B	79	PRO	10.1
1	B	57	ASP	10.1
1	A	59	LYS	10.1
1	B	423	ILE	10.1
1	B	231	LYS	10.1
1	B	298	GLY	10.1
2	C	1008	LYS	10.1
3	O	179	LEU	10.1
4	P	64	ARG	10.1
2	D	1124	SER	10.1
1	B	469	ARG	10.1
1	B	282	LYS	10.1
1	A	284	ILE	10.1
2	D	1053	ASP	10.1
3	L	187	GLU	10.1
3	L	207	LYS	10.1
1	A	354	GLY	10.1
1	B	351	GLU	10.1
2	D	1048	PRO	10.1
3	L	165	GLU	10.1
1	A	348	LYS	10.0
3	O	28	ASP	10.0
3	O	198	HIS	10.0
4	P	53	GLU	10.0
4	H	82	LEU	10.0
1	B	121	LYS	10.0
4	P	78	GLY	10.0
2	C	1163	GLN	10.0
4	H	212	GLU	10.0

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Mol	Chain	Res	Type	RSRZ
1	A	453	LEU	10.0
1	B	478	ASN	10.0
4	P	15	GLY	10.0
1	A	416	LEU	10.0
3	L	201	LEU	10.0
2	D	1183	SER	10.0
3	L	213	GLU	10.0
1	A	501	ALA	9.9
2	D	1123	GLY	9.9
1	A	64	GLU	9.9
2	D	1065	GLY	9.9
2	D	1155	GLY	9.9
3	L	212	GLY	9.9
2	C	1071	ILE	9.9
1	B	485	LYS	9.9
2	C	1020	GLN	9.9
2	D	1039	ASN	9.9
3	O	62	PHE	9.9
3	O	149	LYS	9.9
1	B	460	ASN	9.9
4	P	150	VAL	9.9
1	B	287	GLN	9.9
4	H	42	GLY	9.8
4	P	10	GLU	9.8
2	D	1149	LEU	9.8
4	H	173	SER	9.8
1	B	268	GLU	9.8
3	L	126	LYS	9.8
3	O	207	LYS	9.8
3	L	183	LYS	9.8
1	A	367	GLY	9.8
3	L	122	ASP	9.8
1	B	97	LYS	9.8
1	B	362	LYS	9.8
3	O	131	SER	9.8
4	H	113	SER	9.7
1	A	394	THR	9.7
2	C	1022	LYS	9.7
4	P	206	LYS	9.7
3	O	200	GLY	9.7
4	H	190	GLY	9.7
4	H	43	LYS	9.7

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Mol	Chain	Res	Type	RSRZ
1	B	101	VAL	9.7
1	B	371	ILE	9.7
1	A	97	LYS	9.7
2	D	1013	GLU	9.7
2	C	1181	LYS	9.7
3	L	166	GLN	9.7
1	A	273	ARG	9.6
2	D	1131	ARG	9.6
2	C	1085	GLU	9.6
2	D	1035	LYS	9.6
1	B	364	SER	9.6
1	B	273	ARG	9.6
1	B	456	ARG	9.6
2	D	1019	SER	9.6
3	O	171	SER	9.6
4	H	210	LYS	9.6
1	A	34	LEU	9.6
1	A	86	LEU	9.6
4	H	62	LYS	9.6
3	L	129	THR	9.6
3	L	208	SER	9.6
2	D	1105	ASP	9.6
3	O	54	LEU	9.6
3	O	191	LEU	9.6
4	H	117	LYS	9.6
2	D	1167	LYS	9.6
1	A	121	LYS	9.5
2	C	1180	GLN	9.5
1	B	59	LYS	9.5
1	B	498	PRO	9.5
4	P	126	PRO	9.5
4	P	158	ALA	9.5
4	H	53	GLU	9.5
1	B	441	GLY	9.5
1	B	267	GLU	9.5
2	D	1136	LYS	9.4
3	O	3	GLN	9.4
3	O	42	LYS	9.4
1	B	334	ALA	9.4
3	L	124	GLN	9.4
1	A	471	GLY	9.4
1	A	237	GLY	9.4

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Mol	Chain	Res	Type	RSRZ
4	P	193	THR	9.4
3	L	100	GLY	9.4
2	C	1166	LYS	9.4
4	H	1	GLU	9.3
3	O	61	ARG	9.3
4	P	82	LEU	9.3
2	D	1181	LYS	9.3
3	O	188	LYS	9.3
2	D	1165	GLN	9.3
1	A	460	ASN	9.3
2	D	1007	LYS	9.3
4	P	117	LYS	9.3
3	O	162	SER	9.2
1	B	348	LYS	9.2
4	H	26	GLY	9.2
1	A	91	GLU	9.2
4	H	125	ALA	9.2
3	O	211	ARG	9.2
2	C	1059	ARG	9.2
1	B	285	ILE	9.2
1	A	258	GLN	9.1
3	O	199	GLN	9.1
4	H	48	MET	9.1
2	D	1072	LYS	9.1
3	O	185	ASP	9.1
3	O	157	GLY	9.0
1	A	46	LYS	9.0
1	B	227	LYS	9.0
4	H	72	ASP	9.0
1	A	356	ASN	9.0
3	L	147	GLN	9.0
1	A	439	ILE	9.0
4	P	106	GLY	9.0
1	A	500	LYS	9.0
1	B	490	LYS	9.0
3	L	188	LYS	9.0
1	B	232	THR	9.0
2	D	1076	ILE	9.0
1	A	499	THR	9.0
4	P	43	LYS	9.0
1	A	337	LYS	9.0
2	C	1087	GLU	9.0

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Mol	Chain	Res	Type	RSRZ
3	O	105	GLU	9.0
1	A	290	THR	9.0
3	L	149	LYS	8.9
3	O	107	LYS	8.9
1	B	83	GLU	8.9
3	O	63	SER	8.9
4	H	129	LYS	8.9
1	B	370	GLU	8.8
4	P	49	GLY	8.8
3	O	118	PHE	8.8
4	P	132	SER	8.7
4	P	25	SER	8.7
3	O	24	ARG	8.7
1	A	287	GLN	8.7
4	P	204	ASN	8.7
1	B	451	GLY	8.7
1	A	267	GLU	8.6
1	A	343	LYS	8.6
1	B	481	SER	8.6
1	A	442	GLN	8.6
3	L	13	ALA	8.6
1	B	200	VAL	8.6
1	A	329	GLY	8.5
3	O	128	GLY	8.5
1	A	370	GLU	8.5
2	D	1166	LYS	8.5
3	O	103	LYS	8.5
3	O	124	GLN	8.5
1	A	47	GLU	8.5
2	C	1077	GLU	8.5
2	C	1152	GLN	8.5
1	A	472	GLY	8.4
3	O	147	GLN	8.4
1	B	346	ALA	8.4
1	A	466	GLU	8.4
3	O	165	GLU	8.3
3	O	16	GLY	8.3
1	A	487	LYS	8.3
4	P	61	GLU	8.3
2	C	1099	GLY	8.3
2	C	1134	ARG	8.3
1	A	293	GLU	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	33	LYS	8.2
3	O	99	GLY	8.2
2	C	1167	LYS	8.2
3	L	107	LYS	8.1
4	H	65	GLY	8.1
1	B	429	LYS	8.1
1	B	352	GLN	8.1
1	B	343	LYS	8.1
2	D	1077	GLU	8.1
4	H	128	SER	8.1
1	B	335	ARG	8.0
1	B	269	GLU	8.0
4	H	209	LYS	8.0
3	O	33	LEU	7.9
1	B	103	GLN	7.8
2	D	1020	GLN	7.8
3	L	39	LYS	7.8
2	D	1075	LYS	7.8
4	P	13	LYS	7.8
1	A	51	THR	7.8
1	B	56	SER	7.7
1	A	231	LYS	7.7
1	A	101	VAL	7.6
1	B	252	ARG	7.6
1	A	429	LYS	7.5
3	O	39	LYS	7.4
3	O	19	VAL	7.4
1	B	482	GLU	7.4
1	A	227	LYS	7.4
4	P	129	LYS	7.3
1	A	335	ARG	7.3
2	C	1136	LYS	7.0
3	O	145	LYS	7.0
1	A	355	ASN	6.7
3	L	158	ASN	6.7
1	B	337	LYS	6.0
1	A	451	GLY	6.0
2	D	1142	LYS	5.9

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. 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, 95th 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 ²)	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
5	NAG	B	789	14/15	-0.11	1.22	1.40	139,187,198,202	0
5	NAG	A	789	14/15	-0.09	1.16	0.56	86,104,117,128	0
5	NAG	A	776	14/15	-0.22	1.19	0.52	80,95,117,119	0
5	NAG	B	734	14/15	-0.31	1.17	0.50	167,184,193,194	0
5	NAG	A	886	14/15	-0.13	1.29	0.16	70,97,131,139	0
5	NAG	A	897	14/15	-0.03	1.10	0.06	124,150,169,175	0
5	NAG	A	762	14/15	-0.10	1.09	-0.28	70,75,96,97	0
5	NAG	A	734	14/15	0.04	1.10	-0.29	113,130,148,153	0
5	NAG	B	762	14/15	0.01	1.01	-0.37	102,122,145,155	0
6	GOL	B	1	6/6	-0.05	0.87	-0.75	127,132,138,143	0
5	NAG	A	948	14/15	-0.14	1.04	-0.80	143,154,166,166	0
5	NAG	B	776	14/15	0.07	1.04	-1.09	118,135,157,161	0
6	GOL	P	215	6/6	0.26	0.82	-2.38	134,147,156,162	0
5	NAG	B	892	14/15	0.07	1.09	-	166,204,227,236	0
5	NAG	B	795	14/15	-0.14	1.04	-	169,190,203,209	0
5	NAG	A	892	14/15	-0.01	1.13	-	117,148,182,193	0
5	NAG	A	588	14/15	0.07	1.09	-	99,141,159,174	0
5	NAG	B	886	14/15	-0.20	1.05	-	105,122,143,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	B	948	14/15	-0.20	1.11	-	147,169,175,179	0
5	NAG	A	741	14/15	-0.02	1.01	-	141,160,164,166	0
5	NAG	B	588	14/15	-0.13	0.86	-	119,161,167,169	0

6.5 Other polymers [i](#)

There are no such residues in this entry.