



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:52 PM UTC

PDB ID : 3JWD / pdb_00003jwd
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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

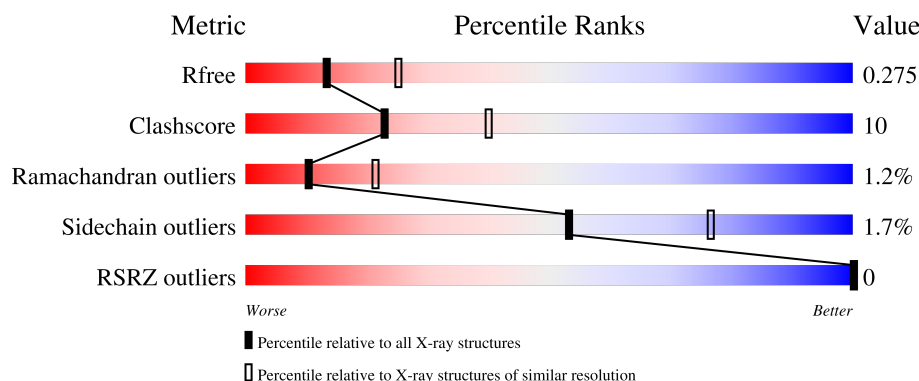
1 Overall quality at a glance

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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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 ≥ 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	 76% 23% .
3	O	213	 82% 18%
4	H	220	 77% 23%
4	P	220	 71% 28% .

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	-	-	-
5	NAG	A	948	X	-	-	-
5	NAG	B	588	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
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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



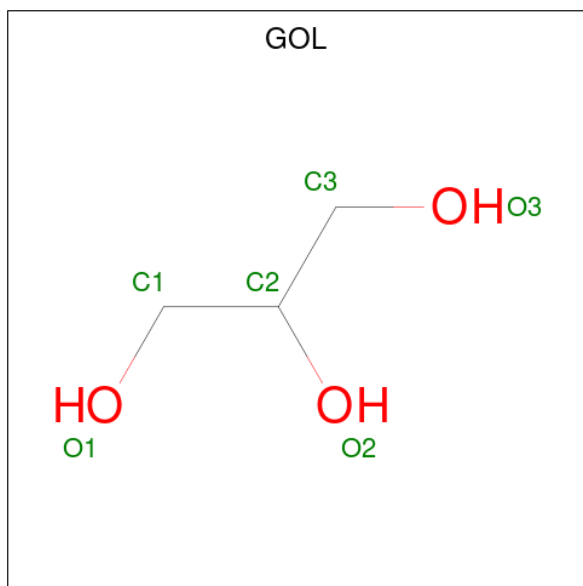
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1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

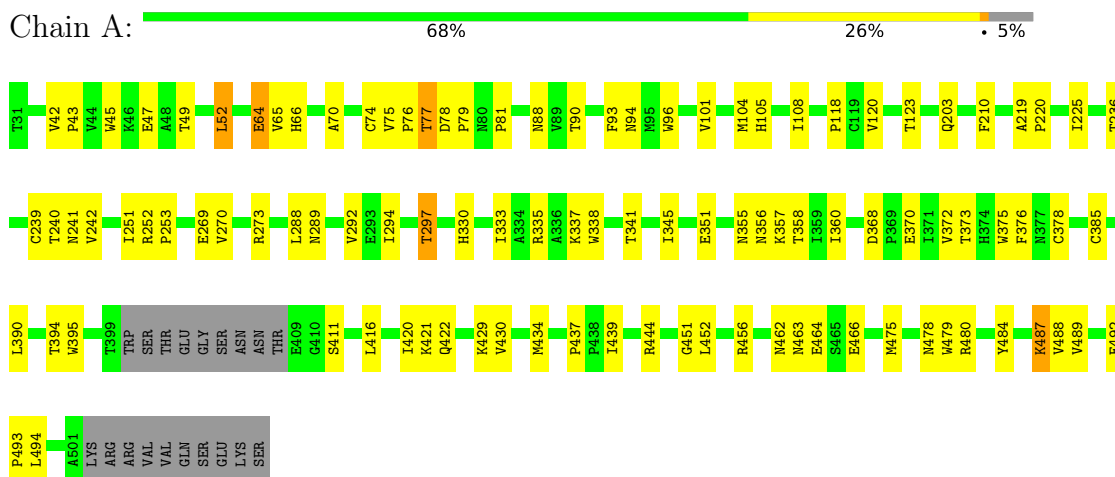
- Molecule 7 is water.

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

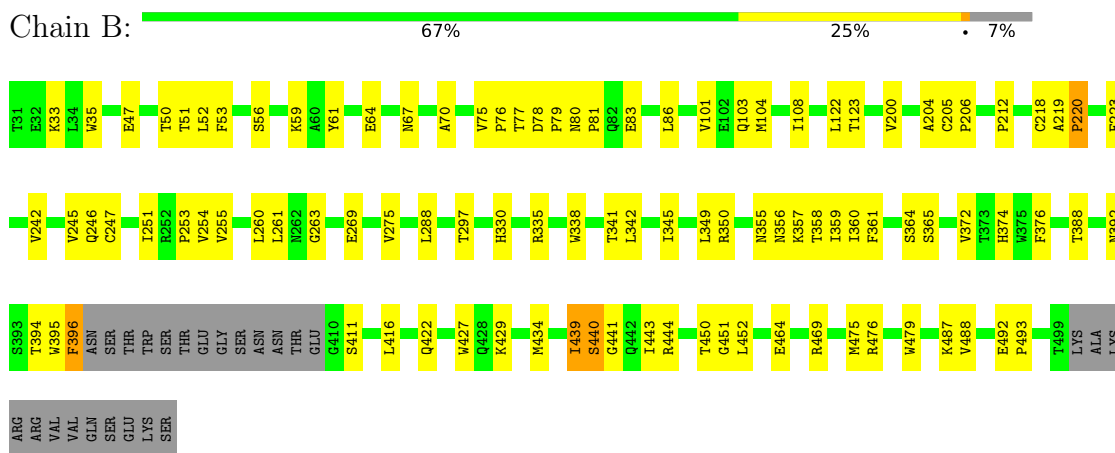
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

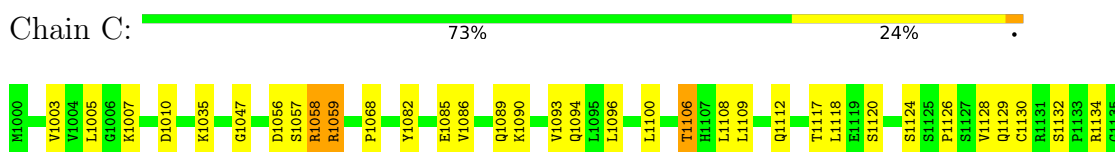
• Molecule 1: HIV-1 GP120 ENVELOPE GLYCOPROTEIN



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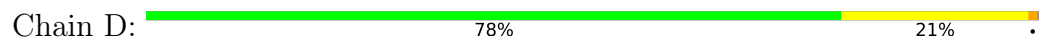


• Molecule 2: T-cell surface glycoprotein CD4

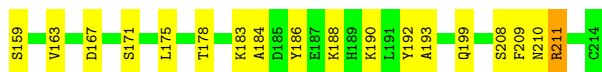




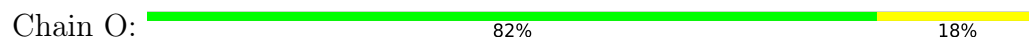
- Molecule 2: T-cell surface glycoprotein CD4



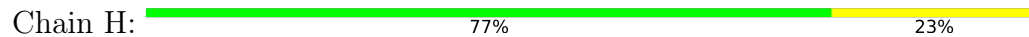
- Molecule 3: FAB 48D LIGHT CHAIN



- Molecule 3: FAB 48D LIGHT CHAIN

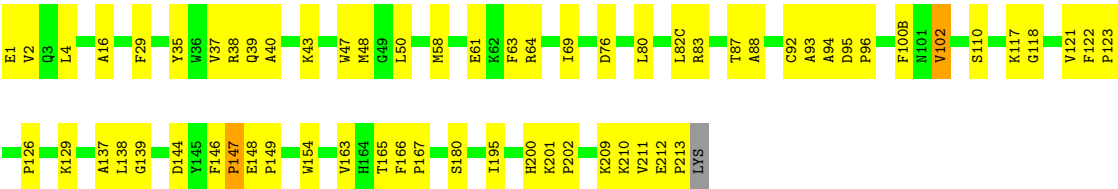


- Molecule 4: FAB 48D HEAVY CHAIN



- 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, 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 0.197 , 0.275	Depositor DCC
R_{free} test set	6030 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	-10.7	Xtriage
Anisotropy	-7.799	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 80.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/2865	0.72	0/3900
1	B	0.26	0/2821	0.70	0/3841
2	C	0.28	0/1452	0.75	2/1955 (0.1%)
2	D	0.25	0/1444	0.67	0/1945
3	L	0.27	0/1659	0.71	2/2252 (0.1%)
3	O	0.27	0/1659	0.72	1/2252 (0.0%)
4	H	0.28	0/1695	0.71	2/2311 (0.1%)
4	P	0.26	0/1685	0.69	0/2300
All	All	0.27	0/15280	0.71	7/20756 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1120	SER	CA-C-N	6.97	124.75	119.66
2	C	1120	SER	C-N-CA	6.97	124.75	119.66
3	L	43	ALA	CA-C-N	5.39	125.34	119.78
3	L	43	ALA	C-N-CA	5.39	125.34	119.78
4	H	125	ALA	CA-C-N	5.30	125.22	119.76
4	H	125	ALA	C-N-CA	5.30	125.22	119.76
3	O	30	SER	CB-CA-C	-5.09	110.69	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2800	0	2724	72	0
1	B	2756	0	2683	71	0
2	C	1432	0	1460	35	0
2	D	1424	0	1451	23	0
3	L	1635	0	1582	29	0
3	O	1624	0	1574	21	0
4	H	1654	0	1613	30	0
4	P	1644	0	1600	40	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	2	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	313	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 (313) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:451:GLY:C	1:A:452:LEU:HD12	2.29	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
1:A:434:MET:HE2	3:L:93:SER:HA	1.86	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
2:C:1089:GLN:C	2:C:1090:LYS:HD2	2.32	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
1:A:104:MET:HE1	1:A:251:ILE:CG2	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:451:GLY:C	1:B:452:LEU:HD12	2.34	0.51
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:104:MET:HE1	1:A:251:ILE:HG22	1.93	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:D:1089:GLN:C	2:D:1090:LYS:HD2	2.37	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
4:P:129:LYS:HD3	4:P:129:LYS:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:H:50:LEU:HD12	4:H:50:LEU:C	2.40	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:263:GLY:C	1:B:450:THR:HG21	2.40	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
3:O:4:MET:HE1	3:O:33:LEU:HD21	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:78:ASP:HB2	1:B:79:PRO:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:O:174:SER:C	4:P:166:PHE:HE2	2.26	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
4:P:82(C):LEU:C	4:P:83:ARG:HG3	2.44	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
2:D:1056:ASP:CG	2:D:1057:SER:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:ASP:CG	1:A:81:PRO:HG3	2.45	0.42
1:A:292:VAL:HG13	1:A:337:LYS:HE3	2.00	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:A:479:TRP:NE1	7:A:589:HOH:O	2.53	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
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:104:MET:HE1	1:B:251:ILE:HG21	2.02	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
1:B:204:ALA:C	1:B:206:PRO:HD3	2.46	0.41
3:O:112:ALA:HA	3:O:113:PRO:HD3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:122:PHE:HA	4:P:123:PRO:HD3	1.82	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
4:P:39:GLN:C	4:P:88:ALA:HB1	2.46	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
2:C:1108:LEU:O	2:C:1109:LEU:HB2	2.20	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
2:D:1066:ASN:C	2:D:1068:PRO:HD3	2.46	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%)	9	17
1	B	350/379 (92%)	314 (90%)	31 (9%)	5 (1%)	9	17
2	C	182/184 (99%)	168 (92%)	13 (7%)	1 (0%)	24	44
2	D	181/184 (98%)	159 (88%)	22 (12%)	0	100	100
3	L	211/213 (99%)	194 (92%)	14 (7%)	3 (1%)	9	17
3	O	210/213 (99%)	181 (86%)	26 (12%)	3 (1%)	9	17
4	H	218/220 (99%)	193 (88%)	22 (10%)	3 (1%)	9	17
4	P	217/220 (99%)	194 (89%)	20 (9%)	3 (1%)	9	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1925/1992 (97%)	1714 (89%)	188 (10%)	23 (1%)	10	21

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
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%)	307 (98%)	8 (2%)	42	68
1	B	310/333 (93%)	307 (99%)	3 (1%)	68	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	166/166 (100%)	160 (96%)	6 (4%)	31	56
2	D	165/166 (99%)	162 (98%)	3 (2%)	51	75
3	L	184/184 (100%)	180 (98%)	4 (2%)	45	70
3	O	184/184 (100%)	184 (100%)	0	100	100
4	H	185/185 (100%)	182 (98%)	3 (2%)	55	78
4	P	184/185 (100%)	183 (100%)	1 (0%)	81	91
All	All	1693/1736 (98%)	1665 (98%)	28 (2%)	53	76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	52	LEU
1	A	64	GLU
1	A	77	THR
1	A	120	VAL
1	A	242	VAL
1	A	297	THR
1	A	488	VAL
2	C	1010	ASP
2	C	1058	ARG
2	C	1059	ARG
2	C	1106	THR
2	C	1166	LYS
2	C	1177	LEU
3	L	105	GLU
3	L	122	ASP
3	L	199	GLN
3	L	211	ARG
4	H	150	VAL
4	H	151	THR
4	H	211	VAL
1	B	275	VAL
1	B	396	PHE
1	B	488	VAL
2	D	1015	THR
2	D	1106	THR
2	D	1168	VAL
4	P	102	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	ASN
1	A	344	GLN
2	C	1107	HIS
1	B	229	ASN
1	B	344	GLN
1	B	389	GLN
2	D	1107	HIS
2	D	1163	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	8,10,10	1.11	0	6,12,12	0.76	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	OXT-C-CA-N
3	L	214	YCM	CE-CD-SG-CB
3	L	214	YCM	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	886	1	14,14,15	0.50	0	17,19,21	0.78	1 (5%)
5	NAG	A	588	1	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
5	NAG	B	886	1	14,14,15	0.49	0	17,19,21	0.89	1 (5%)
5	NAG	B	892	1	14,14,15	0.53	0	17,19,21	0.66	0
5	NAG	A	762	1	14,14,15	0.52	0	17,19,21	0.84	1 (5%)
5	NAG	B	776	1	14,14,15	0.49	0	17,19,21	0.80	1 (5%)
5	NAG	B	588	1	14,14,15	0.50	0	17,19,21	0.74	1 (5%)
5	NAG	A	892	1	14,14,15	0.61	0	17,19,21	1.37	2 (11%)
5	NAG	A	734	1	14,14,15	0.53	0	17,19,21	0.79	0
5	NAG	A	776	1	14,14,15	0.48	0	17,19,21	0.84	1 (5%)
6	GOL	B	1	-	5,5,5	0.40	0	5,5,5	0.29	0
5	NAG	B	762	1	14,14,15	0.52	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	948	1	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
5	NAG	A	741	1	14,14,15	0.47	0	17,19,21	0.90	1 (5%)
5	NAG	A	789	1	14,14,15	0.57	0	17,19,21	0.87	1 (5%)
5	NAG	A	897	1	14,14,15	0.55	0	17,19,21	0.75	0
5	NAG	B	734	1	14,14,15	0.50	0	17,19,21	0.73	0
6	GOL	P	215	-	5,5,5	0.40	0	5,5,5	0.27	0
5	NAG	B	795	1	14,14,15	0.46	0	17,19,21	0.80	1 (5%)
5	NAG	B	789	1	14,14,15	0.51	0	17,19,21	0.88	1 (5%)
5	NAG	B	948	1	14,14,15	0.51	0	17,19,21	0.72	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	886	1	-	4/6/23/26	0/1/1/1
5	NAG	A	588	1	-	2/6/23/26	0/1/1/1
5	NAG	B	886	1	-	2/6/23/26	0/1/1/1
5	NAG	B	892	1	-	4/6/23/26	0/1/1/1
5	NAG	A	762	1	-	2/6/23/26	0/1/1/1
5	NAG	B	776	1	-	0/6/23/26	0/1/1/1
5	NAG	B	588	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	A	892	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	A	776	1	-	2/6/23/26	0/1/1/1
6	GOL	B	1	-	-	0/4/4/4	-
5	NAG	B	762	1	-	3/6/23/26	0/1/1/1
5	NAG	A	948	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	A	741	1	-	2/6/23/26	0/1/1/1
5	NAG	A	789	1	-	2/6/23/26	0/1/1/1
5	NAG	A	897	1	-	3/6/23/26	0/1/1/1
5	NAG	B	734	1	-	3/6/23/26	0/1/1/1
6	GOL	P	215	-	-	2/4/4/4	-
5	NAG	B	795	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	948	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	892	NAG	C1-O5-C5	3.81	117.29	112.19
5	A	892	NAG	O5-C1-C2	3.41	116.56	111.29
5	A	588	NAG	C1-O5-C5	3.11	116.35	112.19
5	B	886	NAG	C1-O5-C5	2.94	116.12	112.19
5	A	741	NAG	C1-O5-C5	2.86	116.02	112.19
5	B	762	NAG	C1-O5-C5	2.54	115.59	112.19
5	A	776	NAG	C1-O5-C5	2.41	115.42	112.19
5	A	948	NAG	O5-C1-C2	2.31	114.87	111.29
5	A	886	NAG	C1-O5-C5	2.26	115.22	112.19
5	B	795	NAG	C1-O5-C5	2.26	115.21	112.19
5	A	762	NAG	C1-O5-C5	2.22	115.16	112.19
5	B	776	NAG	C1-O5-C5	2.22	115.16	112.19
5	B	588	NAG	C1-O5-C5	2.20	115.13	112.19
5	B	789	NAG	C1-O5-C5	2.14	115.06	112.19
5	A	789	NAG	O5-C1-C2	2.03	114.44	111.29

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 (47) 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	C1-C2-N2-C7
5	A	734	NAG	C8-C7-N2-C2
5	A	734	NAG	O7-C7-N2-C2
5	A	741	NAG	O7-C7-N2-C2
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

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Mol	Chain	Res	Type	Atoms
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	A	886	NAG	O5-C5-C6-O6
5	B	948	NAG	O7-C7-N2-C2
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	B	762	NAG	O7-C7-N2-C2
5	A	886	NAG	C4-C5-C6-O6
6	P	215	GOL	O1-C1-C2-O2
5	B	762	NAG	O5-C5-C6-O6
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
5	A	948	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
5	B	762	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-2.16	0 100 100	45, 78, 151, 254	0
1	B	354/379 (93%)	-2.23	0 100 100	66, 113, 190, 233	0
2	C	184/184 (100%)	-2.20	0 100 100	56, 83, 125, 144	0
2	D	183/184 (99%)	-2.28	0 100 100	74, 127, 165, 188	0
3	L	212/213 (99%)	-2.22	0 100 100	59, 101, 179, 240	0
3	O	212/213 (99%)	-2.27	0 100 100	91, 147, 189, 220	0
4	H	220/220 (100%)	-2.20	0 100 100	70, 121, 179, 251	0
4	P	219/220 (99%)	-2.22	0 100 100	66, 121, 195, 243	0
All	All	1944/1992 (97%)	-2.22	0 100 100	45, 110, 180, 254	0

There are no RSRZ outliers to report.

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, 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	B-factors(Å ²)	Q<0.9
3	YCM	L	214	11/11	-0.43	0.00	180,198,236,238	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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, 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	B-factors(Å ²)	Q<0.9
5	NAG	A	741	14/15	-0.94	0.01	141,160,164,166	0
5	NAG	B	948	14/15	-0.94	0.01	147,169,175,179	0
5	NAG	A	948	14/15	-0.93	0.01	143,154,166,166	0
6	GOL	B	1	6/6	-0.93	0.01	127,132,138,143	0
5	NAG	B	588	14/15	-0.90	0.00	119,161,167,169	0
6	GOL	P	215	6/6	-0.90	0.01	134,147,156,162	0
5	NAG	B	734	14/15	-0.88	0.01	167,184,193,194	0
5	NAG	B	776	14/15	-0.88	0.01	118,135,157,161	0
5	NAG	B	795	14/15	-0.88	0.00	169,190,203,209	0
5	NAG	A	734	14/15	-0.87	0.01	113,130,148,153	0
5	NAG	A	892	14/15	-0.87	0.01	117,148,182,193	0
5	NAG	B	789	14/15	-0.86	0.00	139,187,198,202	0
5	NAG	A	897	14/15	-0.85	0.01	124,150,169,175	0
5	NAG	A	789	14/15	-0.84	0.01	86,104,117,128	0
5	NAG	B	892	14/15	-0.80	0.00	166,204,227,236	0
5	NAG	A	776	14/15	-0.79	0.01	80,95,117,119	0
5	NAG	A	588	14/15	-0.78	0.01	99,141,159,174	0
5	NAG	A	762	14/15	-0.77	0.01	70,75,96,97	0
5	NAG	B	886	14/15	-0.77	0.01	105,122,143,147	0
5	NAG	B	762	14/15	-0.75	0.01	102,122,145,155	0
5	NAG	A	886	14/15	-0.73	0.01	70,97,131,139	0

6.5 Other polymers

There are no such residues in this entry.