Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:25 AM GMT

PDB ID	:	3IDY
Title	:	Crystal structure of HIV-gp120 core in complex with CD4-binding site antibody b13, space group C2221
Authors	:	Chen, L.; Kwon, Y.D.; Zhou, T.; Wu, X.; O'Dell, S.; Cavacini, L.; Hessell, A.J.; Pancera, M.; Tang, M.; Xu, L.; Yang, Z.Y.; Zhang, M.Y.; Arthos, J.; Burton, D.R.; Dimitrov, D.S.; Nabel, G.J.; Posner, M.; Sodroski, J.; Wyatt, R.; Mascola, J.R.; Kwong, P.D.
Deposited on	:	2009-07-22
Resolution	:	3.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

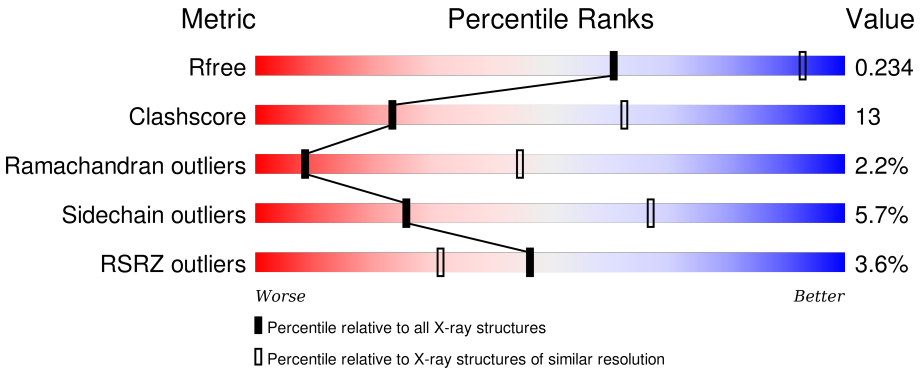
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 <=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	317	2% 68% 25%
1	G	317	3% 68% 24%
2	B	231	9% 65% 32%
2	H	231	3% 67% 31%
3	C	215	3% 72% 25%

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Mol	Chain	Length	Quality of chain
3	L	215	3% 73% 24%

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
4	NAG	A	730	-	-	-	X
4	NAG	A	839	-	-	-	X
4	NAG	A	856	-	-	-	X
4	NAG	G	588	X	-	-	-
4	NAG	G	856	-	-	-	X
4	NAG	G	948	-	-	-	X
4	NAG	G	963	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12038 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 HxBc2 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	306	Total	C	N	O	S	0	0	0
			2367	1483	412	448	24			
1	A	303	Total	C	N	O	S	0	0	0
			2354	1476	409	445	24			

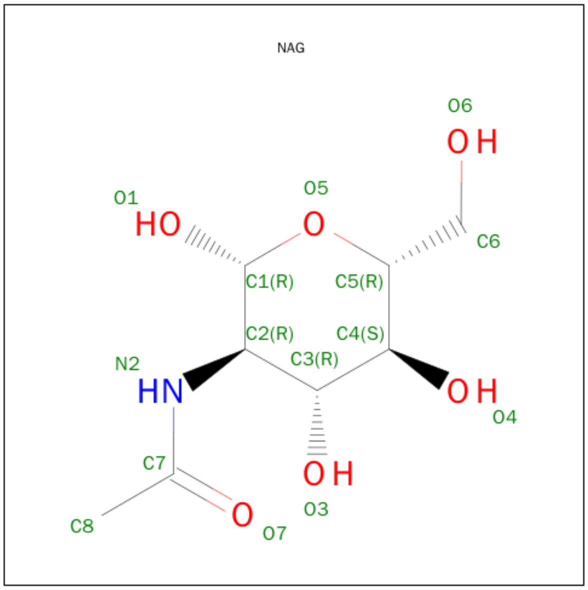
- Molecule 2 is a protein called Fab b13 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	229	Total	C	N	O	S	0	0	0
			1730	1092	297	334	7			
2	B	229	Total	C	N	O	S	0	0	0
			1730	1092	297	334	7			

- Molecule 3 is a protein called Fab b13 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1654	1028	284	337	5			
3	C	214	Total	C	N	O	S	0	0	0
			1654	1028	284	337	5			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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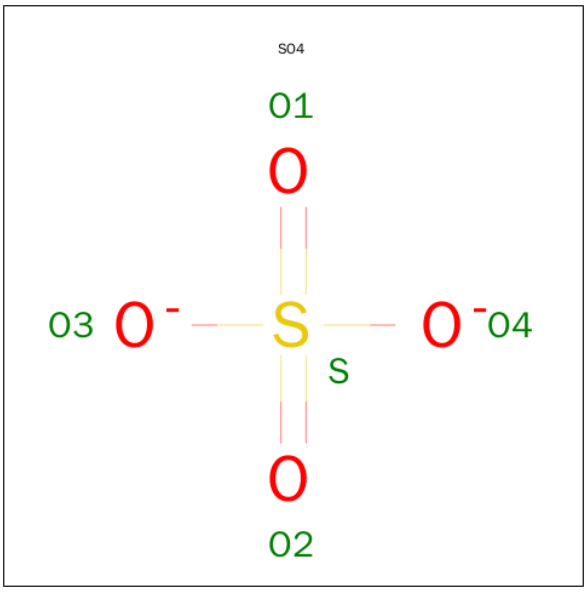
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

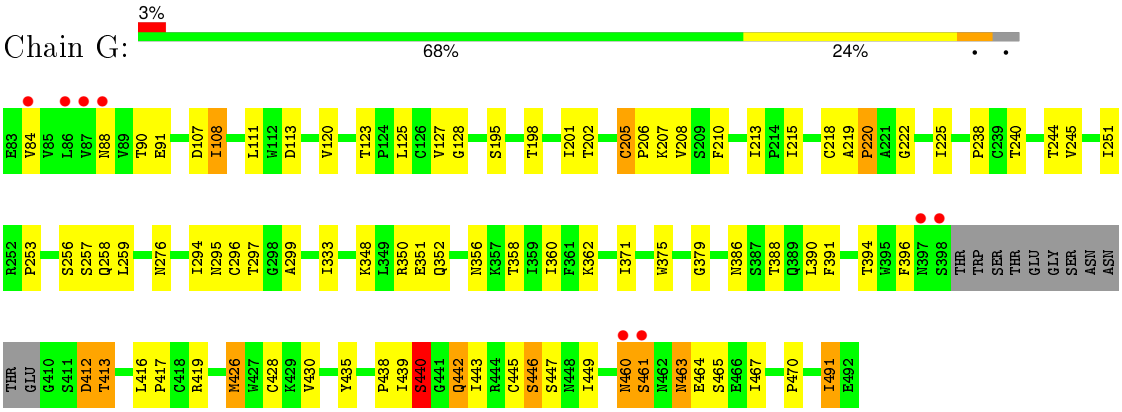
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	30	Total O 30 30	0	0
6	H	12	Total O 12 12	0	0
6	L	12	Total O 12 12	0	0
6	A	41	Total O 41 41	0	0
6	B	30	Total O 30 30	0	0
6	C	27	Total O 27 27	0	0

3 Residue-property plots (i)

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

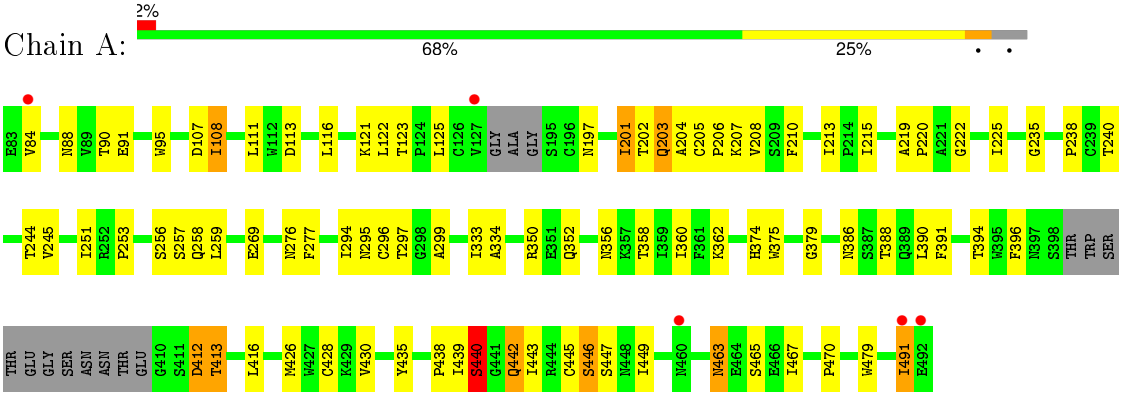
- Molecule 1: HIV-1 HxBc2 gp120 core

Chain G:



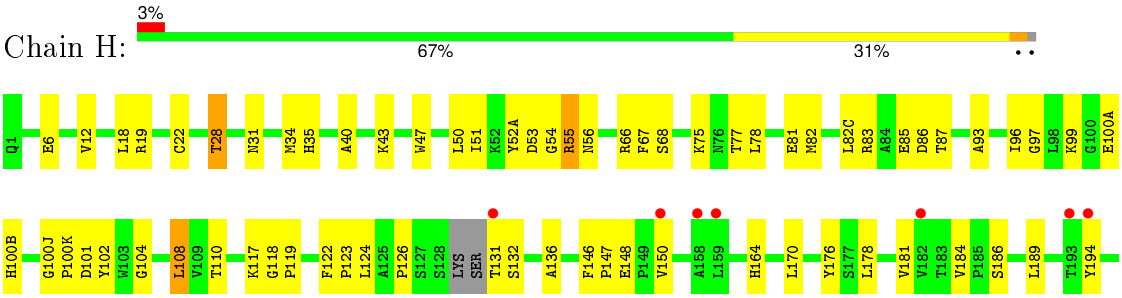
- Molecule 1: HIV-1 HxBc2 gp120 core

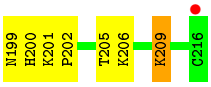
Chain A:



- Molecule 2: Fab b13 heavy chain

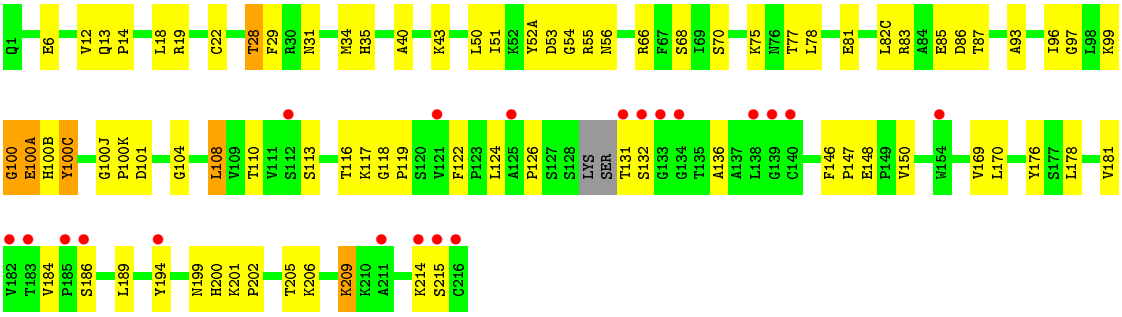
Chain H:





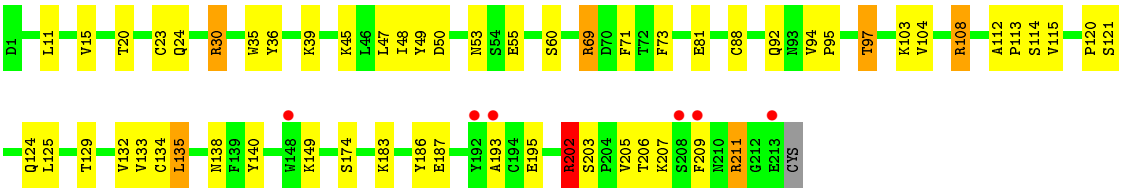
• Molecule 2: Fab b13 heavy chain

Chain B:



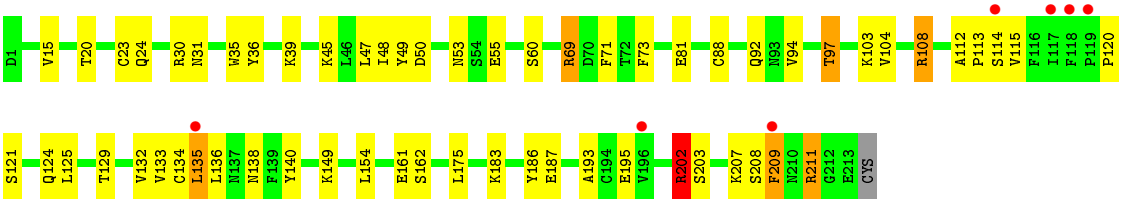
• Molecule 3: Fab b13 light chain

Chain L:



• Molecule 3: Fab b13 light chain

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	106.17Å 204.32Å 216.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.20 – 3.20 43.20 – 2.76	Depositor EDS
% Data completeness (in resolution range)	47.1 (43.20-3.20) 61.9 (43.20-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.237 0.194 , 0.234	Depositor DCC
R_{free} test set	1782 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	92.9	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 98.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 37678 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12038	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0/2401	0.45	0/3254
1	G	0.27	0/2415	0.45	0/3274
2	B	0.27	0/1771	0.44	0/2407
2	H	0.29	0/1771	0.43	0/2407
3	C	0.23	0/1688	0.43	0/2291
3	L	0.24	0/1688	0.43	0/2291
All	All	0.27	0/11734	0.44	0/15924

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

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	2354	0	2285	62	0
1	G	2367	0	2298	63	0
2	B	1730	0	1696	68	0
2	H	1730	0	1696	59	0
3	C	1654	0	1602	35	0
3	L	1654	0	1602	40	0
4	A	196	0	181	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	196	0	182	7	0
5	G	5	0	0	1	0
6	A	41	0	0	2	0
6	B	30	0	0	9	0
6	C	27	0	0	3	0
6	G	30	0	0	2	0
6	H	12	0	0	0	0
6	L	12	0	0	0	0
All	All	12038	0	11542	314	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 13.

All (314) 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)
2:H:100(A):GLU:HG2	3:L:53:ASN:ND2	1.85	0.92
2:H:100(A):GLU:HG2	3:L:53:ASN:HD21	1.35	0.90
1:G:461:SER:CA	4:G:963:NAG:H82	2.03	0.89
1:G:388:THR:HG21	4:G:886:NAG:H5	1.54	0.88
1:G:463:ASN:HD22	1:G:464:GLU:H	1.30	0.80
1:A:121:LYS:HE2	1:A:204:ALA:HB3	1.63	0.80
1:G:461:SER:HA	4:G:963:NAG:H82	1.63	0.79
1:A:269:GLU:HB3	4:A:789:NAG:H61	1.63	0.79
1:G:461:SER:CB	4:G:963:NAG:H82	2.13	0.77
1:A:439:ILE:H	1:A:439:ILE:HD12	1.52	0.75
1:A:113:ASP:HB2	1:A:213:ILE:HD11	1.69	0.74
2:B:118:GLY:HA2	6:B:220:HOH:O	1.89	0.73
1:G:296:CYS:H	1:G:446:SER:HB3	1.54	0.73
1:A:296:CYS:H	1:A:446:SER:HB3	1.55	0.72
2:B:119:PRO:HD3	6:B:220:HOH:O	1.90	0.71
1:G:439:ILE:H	1:G:439:ILE:HD12	1.55	0.71
1:G:113:ASP:HB2	1:G:213:ILE:HD11	1.72	0.70
2:H:209:LYS:HE3	2:H:209:LYS:HA	1.73	0.70
1:G:438:PRO:HB2	1:G:443:ILE:HG13	1.73	0.69
1:G:296:CYS:H	1:G:446:SER:CB	2.06	0.69
1:A:296:CYS:H	1:A:446:SER:CB	2.05	0.69
1:G:219:ALA:HB2	1:G:225:ILE:HG13	1.75	0.69
1:A:438:PRO:HB2	1:A:443:ILE:HG13	1.72	0.69
1:G:90:THR:HG22	1:G:240:THR:HA	1.73	0.69
1:A:90:THR:HG22	1:A:240:THR:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.74	0.68
1:G:463:ASN:HD22	1:G:464:GLU:N	1.92	0.68
2:B:209:LYS:HE3	2:B:209:LYS:HA	1.75	0.67
2:H:87:THR:HG23	2:H:110:THR:HA	1.76	0.67
2:B:87:THR:HG23	2:B:110:THR:HA	1.77	0.66
2:H:100(A):GLU:CG	3:L:53:ASN:HD21	2.08	0.65
1:A:295:ASN:HA	1:A:446:SER:HB2	1.78	0.65
1:G:391:PHE:CG	1:G:470:PRO:HG3	2.31	0.65
1:A:391:PHE:CG	1:A:470:PRO:HG3	2.32	0.65
1:G:295:ASN:HA	1:G:446:SER:HB2	1.77	0.64
1:A:439:ILE:HD12	1:A:439:ILE:N	2.12	0.64
2:H:96:ILE:HG13	2:H:100(J):GLY:O	1.97	0.64
1:A:334:ALA:N	4:A:795:NAG:H81	2.12	0.64
1:G:348:LYS:HE3	6:G:496:HOH:O	1.97	0.64
1:G:362:LYS:HD2	1:G:467:ILE:HD13	1.78	0.64
3:C:92:GLN:HG3	3:C:92:GLN:O	1.97	0.64
2:H:68:SER:HB3	2:H:81:GLU:HG2	1.80	0.64
2:H:18:LEU:HD23	2:H:19:ARG:N	2.13	0.63
1:A:362:LYS:HD2	1:A:467:ILE:HD13	1.80	0.63
1:G:439:ILE:HD12	1:G:439:ILE:N	2.13	0.63
2:B:100(K):PRO:HD2	3:C:36:TYR:OH	1.98	0.63
2:B:18:LEU:HD23	2:B:19:ARG:N	2.14	0.63
2:B:96:ILE:HG13	2:B:100(J):GLY:O	2.00	0.62
3:L:30:ARG:HH11	3:L:30:ARG:HB3	1.64	0.62
3:C:88:CYS:O	3:C:97:THR:HB	2.00	0.62
2:B:68:SER:HB3	2:B:81:GLU:HG2	1.81	0.61
2:B:199:ASN:HD21	2:B:206:LYS:HE2	1.65	0.61
1:A:439:ILE:HD13	1:A:442:GLN:NE2	2.15	0.61
3:C:161:GLU:HB2	6:C:231:HOH:O	2.00	0.61
1:A:391:PHE:CD1	1:A:470:PRO:HG3	2.36	0.61
3:C:120:PRO:HD3	3:C:132:VAL:HG22	1.82	0.60
1:G:463:ASN:ND2	1:G:464:GLU:H	1.99	0.60
1:G:391:PHE:CD1	1:G:470:PRO:HG3	2.36	0.60
1:G:440:SER:C	1:G:442:GLN:N	2.53	0.60
1:G:439:ILE:HD13	1:G:442:GLN:NE2	2.17	0.60
3:L:202:ARG:HD2	3:L:203:SER:N	2.17	0.60
2:H:199:ASN:HD21	2:H:206:LYS:HE2	1.67	0.59
3:L:88:CYS:O	3:L:97:THR:HB	2.02	0.59
1:G:440:SER:C	1:G:442:GLN:H	2.06	0.59
1:A:374:HIS:HA	6:A:31:HOH:O	2.01	0.59
3:C:202:ARG:HD2	3:C:203:SER:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:MET:HB3	2:B:78:LEU:HD22	1.84	0.59
3:L:92:GLN:O	3:L:92:GLN:HG3	2.01	0.59
1:G:259:LEU:HD13	1:G:449:ILE:HD13	1.84	0.59
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.84	0.59
1:A:388:THR:HG21	4:A:886:NAG:H5	1.84	0.58
2:H:181:VAL:HG21	3:L:135:LEU:HD11	1.83	0.58
1:G:360:ILE:HB	1:G:467:ILE:HG12	1.85	0.58
1:G:205:CYS:N	1:G:206:PRO:HD3	2.18	0.58
1:A:360:ILE:HB	1:A:467:ILE:HG12	1.86	0.58
3:L:202:ARG:HD2	3:L:203:SER:H	1.68	0.58
3:C:202:ARG:HD2	3:C:203:SER:H	1.69	0.58
1:A:440:SER:C	1:A:442:GLN:N	2.55	0.58
2:B:150:VAL:HG23	2:B:178:LEU:HD21	1.85	0.57
2:H:100(K):PRO:HD2	3:L:36:TYR:OH	2.04	0.57
3:L:125:LEU:O	3:L:183:LYS:HD2	2.05	0.56
1:A:259:LEU:HD13	1:A:449:ILE:HD13	1.87	0.56
3:C:125:LEU:O	3:C:183:LYS:HD2	2.05	0.56
2:H:108:LEU:HD11	2:H:148:GLU:HB2	1.87	0.56
1:A:440:SER:C	1:A:442:GLN:H	2.08	0.56
2:H:136:ALA:HB3	2:H:189:LEU:HD11	1.88	0.56
1:G:127:VAL:HG13	1:G:128:GLY:H	1.71	0.55
2:B:99:LYS:C	2:B:100(A):GLU:H	2.07	0.55
2:B:136:ALA:HB3	2:B:189:LEU:HD11	1.87	0.55
1:A:210:PHE:CD2	1:A:442:GLN:HG3	2.42	0.55
3:C:24:GLN:HA	3:C:69:ARG:O	2.07	0.55
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.88	0.55
2:B:6:GLU:OE2	2:B:104:GLY:HA3	2.06	0.55
1:A:334:ALA:H	4:A:795:NAG:H81	1.70	0.55
2:H:150:VAL:HG23	2:H:178:LEU:HD21	1.87	0.55
2:H:122:PHE:CD2	3:L:124:GLN:HB2	2.40	0.55
1:A:350:ARG:HD3	1:A:396:PHE:CE2	2.41	0.55
1:G:426:MET:HA	1:G:426:MET:HE3	1.87	0.55
1:G:440:SER:H	1:G:442:GLN:HB2	1.72	0.55
2:B:181:VAL:HG21	3:C:135:LEU:HD11	1.89	0.55
2:B:108:LEU:HD11	2:B:148:GLU:HB2	1.87	0.55
2:H:6:GLU:OE2	2:H:104:GLY:HA3	2.08	0.54
1:A:440:SER:H	1:A:442:GLN:HB2	1.71	0.54
2:B:99:LYS:O	2:B:100(A):GLU:N	2.37	0.54
1:G:350:ARG:HD3	1:G:396:PHE:CE2	2.41	0.54
2:H:200:HIS:HE1	2:H:202:PRO:HB2	1.72	0.54
2:B:51:ILE:HD11	2:B:54:GLY:HA2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:CYS:N	1:A:206:PRO:HD3	2.23	0.54
2:B:184:VAL:HG11	2:B:194:TYR:CE1	2.43	0.54
1:A:84:VAL:HG23	1:A:244:THR:HB	1.89	0.53
3:L:108:ARG:HD2	3:L:140:TYR:CG	2.43	0.53
2:H:122:PHE:HB3	3:L:121:SER:OG	2.08	0.53
2:B:83:ARG:HD2	2:B:85:GLU:OE2	2.09	0.53
3:C:133:VAL:HG12	3:C:134:CYS:H	1.73	0.53
2:H:96:ILE:HG12	2:H:101:ASP:HB3	1.91	0.52
1:G:205:CYS:H	1:G:206:PRO:HD3	1.74	0.52
2:B:200:HIS:HE1	2:B:202:PRO:HB2	1.73	0.52
1:G:84:VAL:HG23	1:G:244:THR:HB	1.90	0.52
2:B:122:PHE:HB3	3:C:121:SER:OG	2.10	0.52
3:C:108:ARG:HD2	3:C:140:TYR:CG	2.44	0.52
2:H:184:VAL:HG11	2:H:194:TYR:CE1	2.43	0.52
3:L:133:VAL:HG12	3:L:134:CYS:H	1.74	0.52
2:H:51:ILE:HD11	2:H:54:GLY:HA2	1.92	0.52
1:G:362:LYS:HD3	5:G:1003:SO4:O1	2.10	0.52
3:C:39:LYS:HE2	3:C:81:GLU:O	2.10	0.52
3:L:24:GLN:HA	3:L:69:ARG:O	2.09	0.52
1:A:447:SER:HB3	4:A:762:NAG:HN2	1.75	0.52
2:H:83:ARG:HD2	2:H:85:GLU:OE2	2.09	0.52
1:G:210:PHE:CD2	1:G:442:GLN:HG3	2.44	0.51
2:B:96:ILE:HG12	2:B:101:ASP:HB3	1.91	0.51
2:B:100(A):GLU:HG2	2:B:100(C):TYR:HB3	1.93	0.51
2:B:77:THR:N	6:B:229:HOH:O	2.43	0.51
3:L:39:LYS:HE2	3:L:81:GLU:O	2.11	0.51
3:C:175:LEU:HG	6:C:231:HOH:O	2.11	0.50
2:B:119:PRO:HD2	2:B:205:THR:HG21	1.93	0.50
2:H:28:THR:HG21	2:H:31:ASN:ND2	2.27	0.50
2:H:68:SER:HB3	2:H:81:GLU:CG	2.42	0.50
3:L:108:ARG:HD2	3:L:140:TYR:CB	2.42	0.50
1:G:412:ASP:OD1	1:G:413:THR:HG22	2.12	0.50
3:C:23:CYS:HB2	3:C:35:TRP:CH2	2.46	0.50
3:L:30:ARG:HB3	3:L:30:ARG:NH1	2.27	0.50
2:B:100:GLY:O	2:B:100(B):HIS:N	2.43	0.50
1:A:269:GLU:CB	4:A:789:NAG:H61	2.37	0.50
1:G:206:PRO:O	1:G:207:LYS:C	2.50	0.50
2:H:123:PRO:HD2	3:L:121:SER:CB	2.42	0.50
1:G:491:ILE:O	1:G:491:ILE:HD13	2.12	0.50
1:A:334:ALA:H	4:A:795:NAG:C8	2.25	0.49
1:A:201:ILE:HD13	1:A:201:ILE:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:SER:HB2	6:B:223:HOH:O	2.13	0.49
2:H:100(A):GLU:CG	3:L:53:ASN:ND2	2.68	0.49
2:B:136:ALA:CB	2:B:189:LEU:HD11	2.43	0.49
2:B:170:LEU:HD13	2:B:176:TYR:CE1	2.46	0.49
2:H:200:HIS:CE1	2:H:202:PRO:HB2	2.48	0.49
2:B:108:LEU:CD1	2:B:148:GLU:HB2	2.43	0.49
3:C:108:ARG:HD2	3:C:140:TYR:CB	2.43	0.49
2:B:68:SER:HB3	2:B:81:GLU:CG	2.43	0.49
1:A:107:ASP:O	1:A:108:ILE:HB	2.13	0.49
2:H:47:TRP:CZ3	3:L:95:PRO:HB3	2.48	0.49
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.94	0.49
1:G:428:CYS:HB3	1:G:435:TYR:HB3	1.95	0.49
2:H:108:LEU:CD1	2:H:148:GLU:HB2	2.42	0.48
1:G:127:VAL:HG12	1:G:195:SER:O	2.13	0.48
3:L:47:LEU:C	3:L:48:ILE:HD12	2.32	0.48
2:H:170:LEU:HD13	2:H:176:TYR:CE1	2.47	0.48
3:C:49:TYR:O	3:C:53:ASN:HB2	2.13	0.48
2:H:93:ALA:HB1	2:H:100(K):PRO:HB3	1.96	0.48
2:B:28:THR:HG21	2:B:31:ASN:ND2	2.29	0.48
1:A:412:ASP:OD1	1:A:413:THR:HG22	2.13	0.48
2:B:93:ALA:HB1	2:B:100(K):PRO:HB3	1.96	0.48
2:H:136:ALA:CB	2:H:189:LEU:HD11	2.44	0.48
3:C:47:LEU:C	3:C:48:ILE:HD12	2.33	0.48
1:G:218:CYS:N	6:G:500:HOH:O	2.42	0.48
1:A:206:PRO:O	1:A:207:LYS:C	2.52	0.48
1:A:439:ILE:H	1:A:439:ILE:CD1	2.24	0.47
2:B:100:GLY:C	2:B:100(B):HIS:H	2.16	0.47
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.95	0.47
1:G:91:GLU:O	1:G:238:PRO:HA	2.14	0.47
3:C:115:VAL:HG13	3:C:207:LYS:HE3	1.96	0.47
3:L:49:TYR:O	3:L:53:ASN:HB2	2.14	0.47
1:A:428:CYS:HB3	1:A:435:TYR:HB3	1.97	0.47
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.96	0.47
1:A:251:ILE:O	1:A:253:PRO:HD3	2.14	0.47
1:G:386:ASN:O	1:G:416:LEU:HD22	2.15	0.47
1:G:352:GLN:O	1:G:352:GLN:HG3	2.15	0.47
1:A:386:ASN:O	1:A:416:LEU:HD22	2.14	0.47
1:G:107:ASP:O	1:G:108:ILE:HB	2.15	0.46
3:L:115:VAL:HG13	3:L:207:LYS:HE3	1.97	0.46
1:A:91:GLU:O	1:A:238:PRO:HA	2.14	0.46
2:B:200:HIS:CE1	2:B:202:PRO:HB2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:124:GLN:HG2	3:L:129:THR:O	2.16	0.46
1:A:352:GLN:O	1:A:352:GLN:HG3	2.16	0.46
3:C:124:GLN:HG2	3:C:129:THR:O	2.15	0.46
1:G:447:SER:HB3	4:G:762:NAG:N2	2.30	0.46
1:A:358:THR:HB	1:A:465:SER:HB3	1.98	0.46
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.50	0.46
2:H:99:LYS:H	2:H:100(B):HIS:CD2	2.34	0.46
2:H:12:VAL:HG11	2:H:82(C):LEU:HD13	1.98	0.46
2:H:201:LYS:N	2:H:202:PRO:CD	2.79	0.46
1:A:204:ALA:C	1:A:206:PRO:HD3	2.36	0.46
1:A:445:CYS:O	1:A:446:SER:CB	2.64	0.45
1:A:197:ASN:HB2	6:A:494:HOH:O	2.15	0.45
1:A:491:ILE:HD13	1:A:491:ILE:O	2.15	0.45
1:G:445:CYS:O	1:G:446:SER:CB	2.64	0.45
1:G:208:VAL:O	1:G:208:VAL:HG13	2.16	0.45
2:H:178:LEU:C	2:H:178:LEU:HD12	2.37	0.45
2:B:116:THR:HB	6:B:230:HOH:O	2.17	0.45
1:A:360:ILE:HG12	1:A:394:THR:HG23	1.99	0.45
2:B:201:LYS:N	2:B:202:PRO:CD	2.80	0.45
2:B:169:VAL:HG22	3:C:162:SER:HB2	1.99	0.45
1:A:294:ILE:O	1:A:294:ILE:HG23	2.17	0.45
1:G:251:ILE:O	1:G:253:PRO:HD3	2.17	0.45
3:L:112:ALA:HA	3:L:113:PRO:HD3	1.71	0.45
3:C:103:LYS:HB2	3:C:103:LYS:NZ	2.33	0.44
1:A:208:VAL:HG13	1:A:208:VAL:O	2.17	0.44
1:G:294:ILE:O	1:G:294:ILE:HG23	2.17	0.44
2:H:101:ASP:OD2	2:H:102:TYR:N	2.47	0.44
2:B:35:HIS:CE1	2:B:50:LEU:HD13	2.53	0.44
2:B:12:VAL:HG11	2:B:82(C):LEU:HD13	1.99	0.44
1:G:358:THR:HB	1:G:465:SER:HB3	1.99	0.44
1:A:296:CYS:H	1:A:446:SER:HB2	1.81	0.44
2:B:150:VAL:HG12	2:B:200:HIS:HB2	1.99	0.44
2:B:66:ARG:HG2	6:B:225:HOH:O	2.18	0.44
3:C:120:PRO:HG2	3:C:186:TYR:CE1	2.53	0.43
2:H:199:ASN:ND2	2:H:206:LYS:HE2	2.33	0.43
2:H:186:SER:HA	2:H:189:LEU:HG	1.99	0.43
2:B:199:ASN:ND2	2:B:206:LYS:HE2	2.32	0.43
2:B:186:SER:HA	2:B:189:LEU:HG	1.99	0.43
2:B:75:LYS:O	2:B:77:THR:HG23	2.17	0.43
2:H:83:ARG:HB2	2:H:85:GLU:HG2	2.00	0.43
3:C:187:GLU:HA	3:C:211:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:149:LYS:HB2	3:L:193:ALA:HB3	2.01	0.43
1:A:222:GLY:O	1:A:491:ILE:HG22	2.18	0.43
2:H:52(A):TYR:CG	2:H:53:ASP:N	2.87	0.43
1:G:333:ILE:HD12	1:G:390:LEU:HD21	2.01	0.43
1:G:222:GLY:O	1:G:491:ILE:HG22	2.19	0.43
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.99	0.43
2:B:83:ARG:HB2	2:B:85:GLU:HG2	2.00	0.43
3:L:23:CYS:HB3	3:L:71:PHE:HB2	2.01	0.43
2:B:202:PRO:HG2	6:B:231:HOH:O	2.17	0.43
2:B:29:PHE:CE2	6:B:229:HOH:O	2.57	0.43
3:C:23:CYS:HB3	3:C:71:PHE:HB2	2.00	0.43
3:L:187:GLU:HA	3:L:211:ARG:HH22	1.84	0.43
3:L:11:LEU:HD12	3:L:11:LEU:O	2.19	0.43
2:H:150:VAL:HG12	2:H:200:HIS:HB2	2.01	0.43
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.78	0.43
1:G:460:ASN:ND2	4:G:963:NAG:H83	2.34	0.42
3:C:35:TRP:CD2	3:C:73:PHE:HB2	2.54	0.42
2:B:52(A):TYR:CG	2:B:53:ASP:N	2.87	0.42
4:A:588:NAG:O7	4:A:588:NAG:C3	2.67	0.42
1:G:256:SER:HA	1:G:375:TRP:O	2.18	0.42
3:C:149:LYS:HB2	3:C:193:ALA:HB3	2.01	0.42
1:A:439:ILE:HD13	1:A:442:GLN:HE21	1.85	0.42
2:H:146:PHE:HA	2:H:147:PRO:HA	1.86	0.42
2:B:117:LYS:HD3	2:B:118:GLY:N	2.35	0.42
3:L:120:PRO:HG2	3:L:186:TYR:CE1	2.54	0.42
2:H:75:LYS:O	2:H:77:THR:HG23	2.19	0.42
2:B:178:LEU:C	2:B:178:LEU:HD12	2.40	0.42
2:B:66:ARG:NH2	2:B:86:ASP:OD2	2.52	0.42
2:B:131:THR:HG22	2:B:132:SER:N	2.34	0.42
2:B:22:CYS:HB3	2:B:78:LEU:HB3	2.00	0.42
2:H:85:GLU:HG2	2:H:85:GLU:H	1.68	0.42
2:H:35:HIS:CE1	2:H:50:LEU:HD13	2.55	0.42
1:A:333:ILE:HD12	1:A:390:LEU:HD21	2.00	0.42
1:G:447:SER:HB3	4:G:762:NAG:HN2	1.84	0.42
2:B:50:LEU:HD12	2:B:51:ILE:H	1.84	0.42
3:L:149:LYS:HE3	3:L:195:GLU:OE1	2.20	0.42
3:L:103:LYS:HB2	3:L:103:LYS:NZ	2.34	0.42
2:B:117:LYS:HD3	2:B:118:GLY:O	2.20	0.42
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.91	0.42
1:G:360:ILE:HG12	1:G:394:THR:HG23	2.01	0.42
3:L:35:TRP:CD2	3:L:73:PHE:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:HIS:CD2	3:L:174:SER:HG	2.37	0.42
1:G:219:ALA:HA	1:G:220:PRO:HD3	1.91	0.42
2:B:100(J):GLY:HA2	2:B:100(K):PRO:HD3	1.89	0.42
2:H:122:PHE:HA	2:H:123:PRO:HD3	1.82	0.42
1:G:386:ASN:HB3	1:G:417:PRO:HD2	2.02	0.42
4:A:588:NAG:H3	4:A:588:NAG:O7	2.20	0.42
2:H:55:ARG:HE	2:H:55:ARG:HB3	1.68	0.41
3:C:112:ALA:HA	3:C:113:PRO:HD3	1.72	0.41
2:H:117:LYS:HD3	2:H:118:GLY:O	2.20	0.41
1:A:297:THR:HG23	1:A:299:ALA:HB3	2.01	0.41
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.52	0.41
2:B:70:SER:O	2:B:78:LEU:HD12	2.20	0.41
1:A:277:PHE:HE1	4:A:734:NAG:H81	1.84	0.41
1:A:203:GLN:HG2	1:A:203:GLN:O	2.20	0.41
1:A:257:SER:O	1:A:258:GLN:HB2	2.20	0.41
2:B:85:GLU:HG2	2:B:85:GLU:H	1.68	0.41
3:C:133:VAL:HG12	3:C:134:CYS:N	2.35	0.41
2:B:214:LYS:HB3	2:B:215:SER:H	1.58	0.41
1:A:256:SER:HA	1:A:375:TRP:O	2.21	0.41
1:G:351:GLU:HG2	1:G:351:GLU:O	2.21	0.41
2:H:131:THR:HG22	2:H:132:SER:N	2.34	0.41
1:A:108:ILE:HG21	1:A:479:TRP:CH2	2.56	0.41
2:B:56:ASN:N	2:B:56:ASN:OD1	2.53	0.41
3:C:30:ARG:HB3	3:C:31:ASN:H	1.49	0.41
3:C:208:SER:O	3:C:209:PHE:HB3	2.21	0.41
2:B:13:GLN:HA	2:B:14:PRO:HD3	1.95	0.41
1:G:257:SER:O	1:G:258:GLN:HB2	2.21	0.41
3:L:133:VAL:HG12	3:L:134:CYS:N	2.35	0.41
1:G:125:LEU:HD23	1:G:125:LEU:HA	1.78	0.41
1:A:95:TRP:CD1	1:A:235:GLY:HA3	2.56	0.41
3:C:135:LEU:HD23	3:C:136:LEU:N	2.35	0.41
2:H:118:GLY:HA2	2:H:119:PRO:HD3	1.85	0.41
2:B:100(B):HIS:HA	6:B:241:HOH:O	2.20	0.40
2:H:67:PHE:CE1	2:H:82:MET:HB3	2.57	0.40
3:C:149:LYS:HE3	3:C:195:GLU:OE1	2.21	0.40
2:B:100(C):TYR:C	2:B:100(C):TYR:CD1	2.94	0.40
1:G:297:THR:HG23	1:G:299:ALA:HB3	2.02	0.40
2:H:56:ASN:N	2:H:56:ASN:OD1	2.54	0.40
2:B:14:PRO:HA	2:B:82(C):LEU:O	2.22	0.40
3:C:154:LEU:HG	6:C:240:HOH:O	2.20	0.40
3:L:205:VAL:HG12	3:L:206:THR:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:ILE:HD12	1:G:371:ILE:O	2.21	0.40
2:B:146:PHE:HA	2:B:147:PRO:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	297/317 (94%)	258 (87%)	32 (11%)	7 (2%)	7 43
1	G	302/317 (95%)	260 (86%)	33 (11%)	9 (3%)	5 35
2	B	225/231 (97%)	183 (81%)	35 (16%)	7 (3%)	5 34
2	H	225/231 (97%)	189 (84%)	32 (14%)	4 (2%)	11 51
3	C	212/215 (99%)	185 (87%)	24 (11%)	3 (1%)	14 57
3	L	212/215 (99%)	183 (86%)	26 (12%)	3 (1%)	14 57
All	All	1473/1526 (96%)	1258 (85%)	182 (12%)	33 (2%)	8 45

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	440	SER
1	A	440	SER
2	B	100(A)	GLU
1	G	379	GLY
2	H	55	ARG
2	H	97	GLY
3	L	202	ARG
1	A	379	GLY
1	A	463	ASN
2	B	55	ARG

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Mol	Chain	Res	Type
2	B	97	GLY
2	B	100(C)	TYR
3	C	202	ARG
1	G	111	LEU
2	H	28	THR
2	H	126	PRO
3	L	209	PHE
1	A	111	LEU
2	B	28	THR
2	B	126	PRO
3	C	209	PHE
1	G	276	ASN
1	G	446	SER
3	L	138	ASN
1	A	446	SER
3	C	138	ASN
1	G	108	ILE
1	A	108	ILE
1	A	276	ASN
2	B	100	GLY
1	G	460	ASN
1	G	205	CYS
1	G	220	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	271/281 (96%)	253 (93%)	18 (7%)	21 61
1	G	271/281 (96%)	252 (93%)	19 (7%)	19 58
2	B	189/191 (99%)	186 (98%)	3 (2%)	70 91
2	H	189/191 (99%)	186 (98%)	3 (2%)	70 91
3	C	189/190 (100%)	174 (92%)	15 (8%)	15 53
3	L	189/190 (100%)	173 (92%)	16 (8%)	13 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1298/1324 (98%)	1224 (94%)	74 (6%)	25 67

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	88	ASN
1	G	120	VAL
1	G	123	THR
1	G	198	THR
1	G	201	ILE
1	G	202	THR
1	G	215	ILE
1	G	245	VAL
1	G	356	ASN
1	G	412	ASP
1	G	413	THR
1	G	419	ARG
1	G	426	MET
1	G	430	VAL
1	G	440	SER
1	G	442	GLN
1	G	461	SER
1	G	463	ASN
1	G	491	ILE
2	H	108	LEU
2	H	124	LEU
2	H	209	LYS
3	L	15	VAL
3	L	20	THR
3	L	30	ARG
3	L	45	LYS
3	L	50	ASP
3	L	55	GLU
3	L	60	SER
3	L	69	ARG
3	L	94	VAL
3	L	97	THR
3	L	104	VAL
3	L	108	ARG
3	L	114	SER
3	L	135	LEU
3	L	202	ARG

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Mol	Chain	Res	Type
3	L	211	ARG
1	A	88	ASN
1	A	122	LEU
1	A	123	THR
1	A	125	LEU
1	A	201	ILE
1	A	202	THR
1	A	203	GLN
1	A	215	ILE
1	A	245	VAL
1	A	356	ASN
1	A	412	ASP
1	A	413	THR
1	A	426	MET
1	A	430	VAL
1	A	440	SER
1	A	442	GLN
1	A	463	ASN
1	A	491	ILE
2	B	108	LEU
2	B	124	LEU
2	B	209	LYS
3	C	15	VAL
3	C	20	THR
3	C	45	LYS
3	C	50	ASP
3	C	55	GLU
3	C	60	SER
3	C	69	ARG
3	C	94	VAL
3	C	97	THR
3	C	104	VAL
3	C	108	ARG
3	C	114	SER
3	C	135	LEU
3	C	202	ARG
3	C	211	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

29 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	$\#\|Z\| > 2$
4	NAG	A	588	1	14,14,15	0.57	0	15,19,21	1.40	1 (6%)
4	NAG	A	730	1	14,14,15	0.51	0	15,19,21	0.73	0
4	NAG	A	734	1	14,14,15	0.45	0	15,19,21	0.98	1 (6%)
4	NAG	A	741	1	14,14,15	0.56	0	15,19,21	0.73	0
4	NAG	A	762	1	14,14,15	0.52	0	15,19,21	1.03	1 (6%)
4	NAG	A	776	1	14,14,15	1.29	1 (7%)	15,19,21	1.39	1 (6%)
4	NAG	A	789	1	14,14,15	0.49	0	15,19,21	0.82	0
4	NAG	A	795	1	14,14,15	0.51	0	15,19,21	0.70	0
4	NAG	A	839	1	14,14,15	0.52	0	15,19,21	0.78	0
4	NAG	A	856	1	14,14,15	0.54	0	15,19,21	1.38	1 (6%)
4	NAG	A	886	1	14,14,15	0.60	0	15,19,21	0.59	0
4	NAG	A	892	1	14,14,15	0.61	0	15,19,21	1.00	1 (6%)
4	NAG	A	948	1	14,14,15	0.47	0	15,19,21	1.31	3 (20%)
4	NAG	A	963	1	14,14,15	0.56	0	15,19,21	0.93	1 (6%)
5	SO4	G	1003	-	4,4,4	0.22	0	6,6,6	0.11	0
4	NAG	G	588	1	14,14,15	0.51	0	15,19,21	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	G	730	1	14,14,15	0.44	0	15,19,21	0.93	1 (6%)
4	NAG	G	734	1	14,14,15	0.59	0	15,19,21	0.76	0
4	NAG	G	741	1	14,14,15	0.41	0	15,19,21	1.04	1 (6%)
4	NAG	G	762	1	14,14,15	0.59	0	15,19,21	1.23	1 (6%)
4	NAG	G	776	1	14,14,15	0.44	0	15,19,21	1.08	1 (6%)
4	NAG	G	789	1	14,14,15	0.44	0	15,19,21	0.87	1 (6%)
4	NAG	G	795	1	14,14,15	0.48	0	15,19,21	0.67	0
4	NAG	G	839	1	14,14,15	0.53	0	15,19,21	0.73	0
4	NAG	G	856	1	14,14,15	0.55	0	15,19,21	1.12	1 (6%)
4	NAG	G	886	1	14,14,15	0.62	0	15,19,21	1.09	1 (6%)
4	NAG	G	892	1	14,14,15	0.55	0	15,19,21	0.87	0
4	NAG	G	948	1	14,14,15	0.39	0	15,19,21	2.31	3 (20%)
4	NAG	G	963	1	14,14,15	0.49	0	15,19,21	0.85	1 (6%)

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
4	NAG	A	588	1	-	0/6/23/26	0/1/1/1
4	NAG	A	730	1	-	0/6/23/26	0/1/1/1
4	NAG	A	734	1	-	0/6/23/26	0/1/1/1
4	NAG	A	741	1	-	0/6/23/26	0/1/1/1
4	NAG	A	762	1	-	0/6/23/26	0/1/1/1
4	NAG	A	776	1	-	0/6/23/26	0/1/1/1
4	NAG	A	789	1	-	0/6/23/26	0/1/1/1
4	NAG	A	795	1	-	0/6/23/26	0/1/1/1
4	NAG	A	839	1	-	0/6/23/26	0/1/1/1
4	NAG	A	856	1	-	0/6/23/26	0/1/1/1
4	NAG	A	886	1	-	0/6/23/26	0/1/1/1
4	NAG	A	892	1	-	0/6/23/26	0/1/1/1
4	NAG	A	948	1	-	0/6/23/26	0/1/1/1
4	NAG	A	963	1	-	0/6/23/26	0/1/1/1
5	SO4	G	1003	-	-	0/0/0/0	0/0/0/0
4	NAG	G	588	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	G	730	1	-	0/6/23/26	0/1/1/1
4	NAG	G	734	1	-	0/6/23/26	0/1/1/1
4	NAG	G	741	1	-	0/6/23/26	0/1/1/1
4	NAG	G	762	1	-	0/6/23/26	0/1/1/1
4	NAG	G	776	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	789	1	-	0/6/23/26	0/1/1/1
4	NAG	G	795	1	-	0/6/23/26	0/1/1/1
4	NAG	G	839	1	-	0/6/23/26	0/1/1/1
4	NAG	G	856	1	-	1/6/23/26	0/1/1/1
4	NAG	G	886	1	-	0/6/23/26	0/1/1/1
4	NAG	G	892	1	-	0/6/23/26	0/1/1/1
4	NAG	G	948	1	-	0/6/23/26	0/1/1/1
4	NAG	G	963	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	776	NAG	C8-C7	-4.41	1.41	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	948	NAG	C4-C3-C2	-4.03	104.96	111.23
4	A	776	NAG	C2-N2-C7	-4.02	117.88	123.04
4	G	948	NAG	C2-N2-C7	-2.48	119.85	123.04
4	A	948	NAG	C2-N2-C7	-2.43	119.92	123.04
4	A	762	NAG	C2-N2-C7	-2.41	119.95	123.04
4	A	948	NAG	C4-C3-C2	-2.28	107.68	111.23
4	G	789	NAG	C2-N2-C7	-2.03	120.43	123.04
4	G	963	NAG	C1-O5-C5	2.24	115.09	112.25
4	G	588	NAG	C1-O5-C5	2.31	115.19	112.25
4	G	886	NAG	C4-C3-C2	2.63	115.33	111.23
4	A	963	NAG	C1-O5-C5	2.65	115.61	112.25
4	A	892	NAG	C4-C3-C2	2.68	115.40	111.23
4	G	776	NAG	C1-O5-C5	2.76	115.75	112.25
4	G	730	NAG	C1-O5-C5	2.82	115.83	112.25
4	A	734	NAG	C1-O5-C5	2.84	115.86	112.25
4	G	741	NAG	C1-O5-C5	3.11	116.19	112.25
4	A	948	NAG	C1-O5-C5	3.56	116.76	112.25
4	G	856	NAG	C1-O5-C5	3.60	116.82	112.25
4	G	762	NAG	C1-O5-C5	3.82	117.09	112.25
4	A	588	NAG	C2-N2-C7	3.84	127.97	123.04
4	A	856	NAG	C1-O5-C5	4.43	117.86	112.25
4	G	948	NAG	C1-O5-C5	7.34	121.56	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	588	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	856	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	588	NAG	2	0
4	A	734	NAG	1	0
4	A	762	NAG	1	0
4	A	789	NAG	2	0
4	A	795	NAG	3	0
4	A	886	NAG	1	0
5	G	1003	SO4	1	0
4	G	762	NAG	2	0
4	G	886	NAG	1	0
4	G	963	NAG	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	303/317 (95%)	-0.18	5 (1%) 73 60	95, 125, 199, 271	0
1	G	306/317 (96%)	-0.22	8 (2%) 59 45	92, 125, 205, 271	0
2	B	229/231 (99%)	0.12	20 (8%) 13 7	100, 167, 237, 289	0
2	H	229/231 (99%)	-0.07	8 (3%) 48 32	91, 165, 234, 288	0
3	C	214/215 (99%)	-0.13	7 (3%) 50 35	104, 151, 234, 303	0
3	L	214/215 (99%)	-0.12	6 (2%) 56 42	93, 145, 232, 262	0
All	All	1495/1526 (97%)	-0.11	54 (3%) 46 31	91, 142, 231, 303	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	87	VAL	6.7
2	B	139	GLY	6.5
1	A	492	GLU	6.4
2	B	216	CYS	5.8
2	B	138	LEU	5.7
2	B	183	THR	4.7
2	B	131	THR	4.5
3	C	196	VAL	4.0
2	B	182	VAL	3.6
2	B	215	SER	3.5
2	H	216	CYS	3.5
2	H	158	ALA	3.4
1	G	88	ASN	3.4
1	G	397	ASN	3.4
2	H	194	TYR	3.4
1	G	460	ASN	3.4
2	B	140	CYS	3.2
2	B	154	TRP	3.2
1	G	398	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	209	PHE	3.2
1	A	84	VAL	3.1
3	C	135	LEU	3.1
2	B	125	ALA	3.1
1	A	491	ILE	3.0
3	L	209	PHE	2.9
2	H	182	VAL	2.8
2	B	134	GLY	2.8
1	G	84	VAL	2.8
2	H	193	THR	2.8
1	G	461	SER	2.8
3	L	192	TYR	2.7
1	G	86	LEU	2.6
1	A	460	ASN	2.6
2	B	186	SER	2.6
2	B	121	VAL	2.6
3	L	148	TRP	2.6
2	B	112	SER	2.6
3	L	208	SER	2.6
3	C	118	PHE	2.6
1	A	127	VAL	2.5
2	B	133	GLY	2.5
2	B	214	LYS	2.5
2	H	131	THR	2.4
2	B	132	SER	2.4
2	B	185	PRO	2.3
3	C	114	SER	2.3
2	B	211	ALA	2.3
2	H	159	LEU	2.3
3	C	117	ILE	2.3
3	L	213	GLU	2.2
2	B	194	TYR	2.2
2	H	150	VAL	2.1
3	L	193	ALA	2.1
3	C	119	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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
4	NAG	G	856	14/15	-0.08	1.43	9.16	184,252,279,292	0
4	NAG	A	856	14/15	0.04	0.60	5.00	170,250,287,291	0
4	NAG	A	730	14/15	0.57	0.32	3.88	180,212,233,238	0
4	NAG	A	839	14/15	0.76	0.55	3.81	131,213,220,222	0
4	NAG	G	948	14/15	0.86	0.26	2.04	86,148,198,201	0
4	NAG	G	734	14/15	0.89	0.20	1.56	158,195,210,225	0
4	NAG	G	963	14/15	0.81	0.48	1.21	211,229,239,241	0
4	NAG	G	741	14/15	0.84	0.21	0.80	146,204,232,238	0
4	NAG	G	839	14/15	0.87	0.27	0.76	153,188,211,216	0
4	NAG	G	795	14/15	0.93	0.20	0.68	124,161,166,195	0
4	NAG	A	762	14/15	0.95	0.26	0.52	77,94,125,144	0
4	NAG	A	948	14/15	0.92	0.22	0.20	117,140,165,165	0
4	NAG	A	886	14/15	0.93	0.19	-0.15	113,154,172,179	0
4	NAG	A	795	14/15	0.93	0.18	-0.27	120,152,170,189	0
4	NAG	G	886	14/15	0.94	0.15	-0.53	109,142,159,171	0
4	NAG	G	789	14/15	0.93	0.19	-0.63	108,146,178,179	0
4	NAG	G	762	14/15	0.96	0.17	-1.01	76,96,128,130	0
4	NAG	A	789	14/15	0.95	0.15	-1.78	112,128,141,152	0
4	NAG	A	588	14/15	0.73	0.43	-	143,206,225,236	0
4	NAG	A	741	14/15	0.85	0.22	-	113,213,241,245	0
4	NAG	G	776	14/15	0.92	0.18	-	151,175,183,195	0
4	NAG	G	892	14/15	0.90	0.14	-	118,177,197,209	0
4	NAG	G	588	14/15	0.42	0.79	-	187,247,265,266	0
4	NAG	G	730	14/15	0.78	0.22	-	158,229,236,237	0
4	NAG	A	892	14/15	0.89	0.30	-	132,192,205,212	0
4	NAG	A	963	14/15	0.63	0.73	-	170,225,242,246	0
4	NAG	A	734	14/15	0.86	0.17	-	165,188,209,216	0
5	SO4	G	1003	5/5	0.90	0.15	-	162,173,190,220	0
4	NAG	A	776	14/15	0.84	0.26	-	133,183,194,197	0

6.5 Other polymers (i)

There are no such residues in this entry.