Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID	:	3LZF
Title	:	Crystal Structure of Fab 2D1 in Complex with the 1918 Influenza Virus Hemagglutinin
Authors	:	Ekiert, D.C.; Wilson, I.A.
Deposited on	:	2010-03-01
Resolution	:	2.80 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:

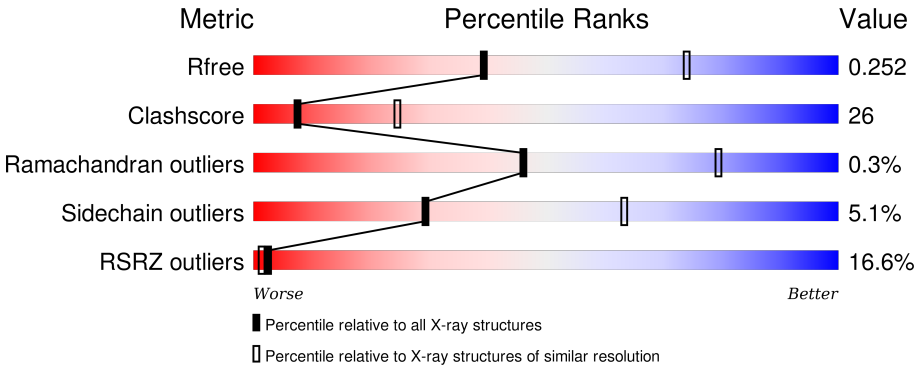
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	331	3% 67% 28%
2	B	179	21% 65% 28%
3	H	230	17% 53% 38% 6%
4	L	217	30% 66% 30%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7207 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 Hemagglutinin, HA1 Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2506	1580	430	485	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q9WFX3
A	8	ASP	-	EXPRESSION TAG	UNP Q9WFX3
A	9	PRO	-	EXPRESSION TAG	UNP Q9WFX3
A	10	GLY	-	EXPRESSION TAG	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin, HA2 Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1391	868	239	278	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	EXPRESSION TAG	UNP Q9WFX3
B	178	GLY	-	EXPRESSION TAG	UNP Q9WFX3
B	179	ARG	-	EXPRESSION TAG	UNP Q9WFX3

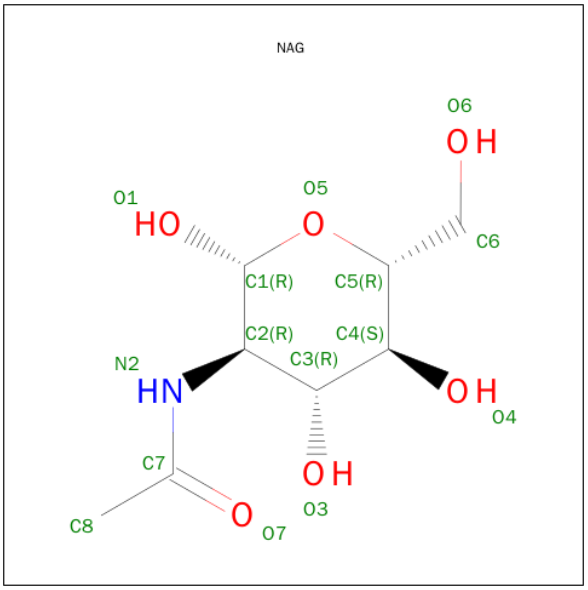
- Molecule 3 is a protein called 2D1 Fab, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1623	1030	264	322	7			

- Molecule 4 is a protein called 2D1 Fab, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1567	982	260	321	4			

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



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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

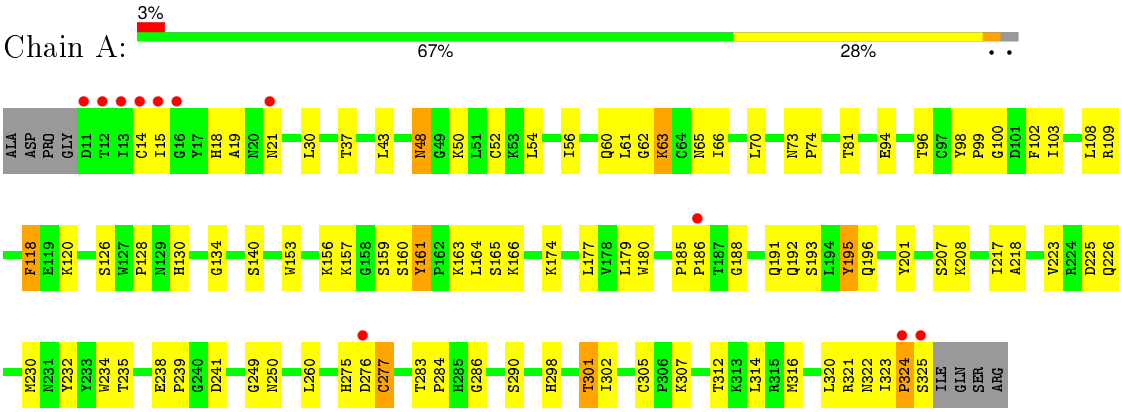
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	4	Total	C	N	O	0	0
			50	28	2	20		

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.

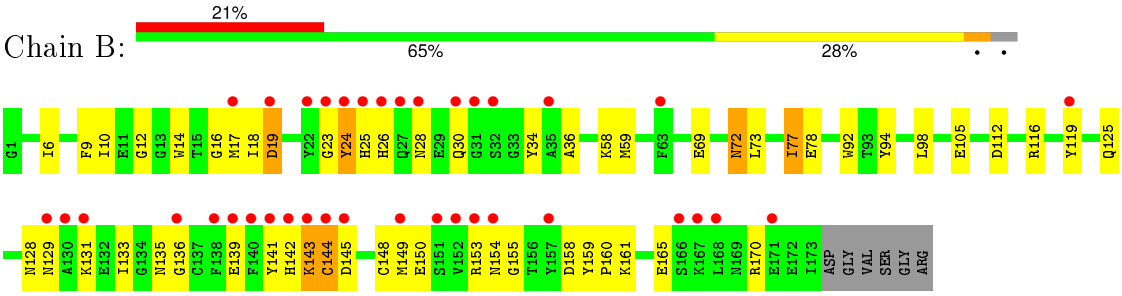
- Molecule 1: Hemagglutinin, HA1 Subunit

Chain A:



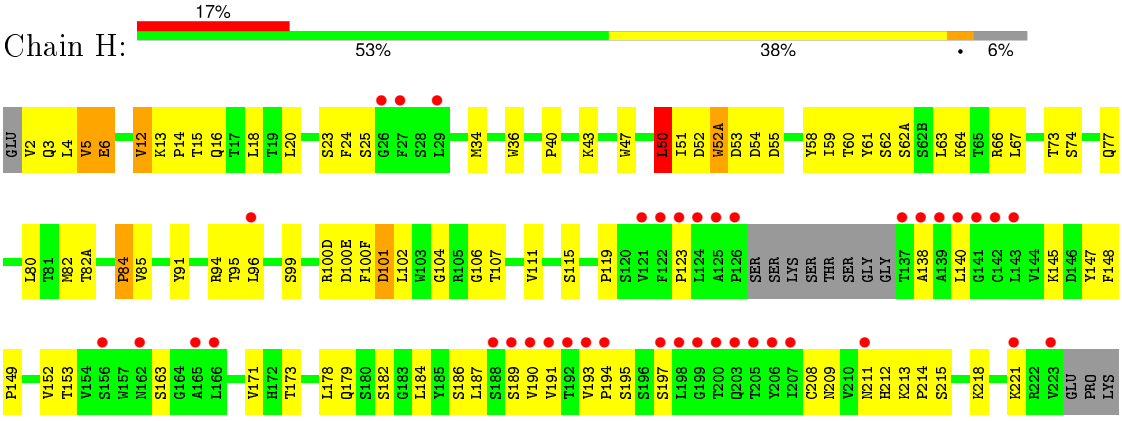
- Molecule 2: Hemagglutinin, HA2 Subunit

Chain B:



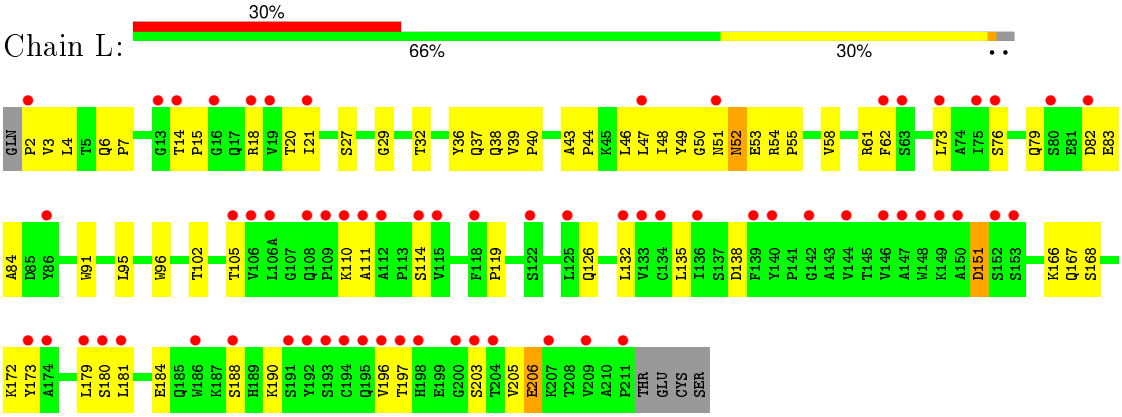
- Molecule 3: 2D1 Fab, Heavy Chain

Chain H:



SER
CYS

- Molecule 4: 2D1 Fab, Light Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.75Å 161.75Å 143.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.69 – 2.80 49.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.69-2.80) 98.1 (49.67-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.230 , 0.259 0.226 , 0.252	Depositor DCC
R_{free} test set	2596 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 96.7	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 52718 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7207	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.90	2/2570 (0.1%)	0.93	2/3501 (0.1%)
2	B	0.69	1/1418 (0.1%)	0.74	0/1909
3	H	0.74	1/1660 (0.1%)	0.96	4/2274 (0.2%)
4	L	0.62	2/1608 (0.1%)	0.72	1/2199 (0.0%)
All	All	0.76	6/7256 (0.1%)	0.86	7/9883 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	CYS	CB-SG	-9.33	1.66	1.82
1	A	120	LYS	CE-NZ	6.36	1.65	1.49
4	L	91	TRP	CB-CG	-5.49	1.40	1.50
3	H	101	ASP	CB-CG	-5.32	1.40	1.51
2	B	78	GLU	CB-CG	-5.30	1.42	1.52
4	L	96	TRP	CB-CG	-5.19	1.41	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	101	ASP	CB-CG-OD1	-10.04	109.26	118.30
1	A	120	LYS	CD-CE-NZ	7.23	128.34	111.70
3	H	101	ASP	CB-CG-OD2	5.87	123.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	12	VAL	CB-CA-C	-5.35	101.23	111.40
3	H	50	LEU	CB-CG-CD2	5.31	120.03	111.00
4	L	95	LEU	CA-CB-CG	-5.08	103.61	115.30
1	A	174	LYS	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	ASP	Peptide

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	2506	0	2427	91	0
2	B	1391	0	1302	87	0
3	H	1623	0	1601	122	0
4	L	1567	0	1511	70	0
5	A	14	0	13	1	0
6	A	56	0	50	0	0
7	A	50	0	43	1	0
All	All	7207	0	6947	360	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 26.

All (360) 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:B:26:HIS:HB2	2:B:149:MET:CE	1.66	1.24
3:H:6:GLU:OE1	3:H:106:GLY:HA2	1.41	1.17
2:B:133:ILE:HD12	2:B:139:GLU:HB2	1.18	1.15
2:B:30:GLN:HE22	2:B:145:ASP:HB2	1.07	1.11
2:B:26:HIS:CB	2:B:149:MET:CE	2.29	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:96:LEU:HB3	3:H:100(D):ARG:HG3	1.32	1.10
3:H:123:PRO:HG3	3:H:221:LYS:HE3	1.30	1.09
2:B:26:HIS:CB	2:B:149:MET:HE2	1.82	1.09
4:L:151:ASP:CB	4:L:190:LYS:HE3	1.82	1.08
4:L:151:ASP:HB3	4:L:190:LYS:CE	1.84	1.08
4:L:39:VAL:HG13	4:L:40:PRO:HD2	1.31	1.07
3:H:96:LEU:HB3	3:H:100(D):ARG:CG	1.85	1.07
2:B:24:TYR:CE1	2:B:153:ARG:HG2	1.89	1.07
3:H:96:LEU:HB3	3:H:100(D):ARG:CB	1.88	1.04
2:B:141:TYR:HE1	2:B:170:ARG:CD	1.74	1.00
2:B:141:TYR:HE1	2:B:170:ARG:HD3	1.20	0.99
2:B:142:HIS:HD2	2:B:143:LYS:O	1.46	0.99
2:B:141:TYR:CE1	2:B:170:ARG:CG	2.47	0.98
3:H:34:MET:O	3:H:52(A):TRP:HB2	1.64	0.97
4:L:151:ASP:OD1	4:L:190:LYS:HG2	1.64	0.97
3:H:54:ASP:O	3:H:55:ASP:HB2	1.65	0.97
2:B:141:TYR:CE1	2:B:170:ARG:HG3	2.00	0.95
2:B:25:HIS:HD2	2:B:34:TYR:CE2	1.84	0.95
2:B:158:ASP:OD1	2:B:160:PRO:HD2	1.65	0.95
1:A:301:THR:HG23	1:A:305:CYS:SG	2.07	0.94
2:B:133:ILE:HD12	2:B:139:GLU:CB	1.95	0.94
3:H:4:LEU:HD21	3:H:24:PHE:CE1	2.02	0.94
4:L:51:ASN:O	4:L:52:ASN:CG	2.06	0.94
1:A:50:LYS:HD3	1:A:275:HIS:ND1	1.83	0.94
1:A:128:PRO:O	1:A:157:LYS:NZ	2.01	0.92
1:A:323:ILE:HG22	1:A:323:ILE:O	1.70	0.92
1:A:50:LYS:CD	1:A:275:HIS:ND1	2.33	0.91
2:B:26:HIS:HB2	2:B:149:MET:HE2	0.94	0.91
2:B:141:TYR:CE1	2:B:170:ARG:HD3	2.05	0.91
3:H:52(A):TRP:O	3:H:52(A):TRP:HE3	1.54	0.91
1:A:157:LYS:HE2	3:H:54:ASP:OD2	1.70	0.90
4:L:6:GLN:HE21	4:L:102:THR:HG23	1.38	0.89
2:B:141:TYR:CD1	2:B:170:ARG:HB2	2.07	0.89
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.55	0.89
2:B:30:GLN:NE2	2:B:145:ASP:HB2	1.87	0.89
4:L:39:VAL:CG1	4:L:40:PRO:HD2	2.03	0.88
3:H:4:LEU:CD2	3:H:24:PHE:CE1	2.57	0.87
3:H:171:VAL:HG22	3:H:191:VAL:HG22	1.55	0.87
3:H:96:LEU:HB3	3:H:100(D):ARG:HB2	1.55	0.86
4:L:151:ASP:HB3	4:L:190:LYS:HE3	0.91	0.86
4:L:50:GLY:O	4:L:51:ASN:HB2	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:6:GLN:NE2	4:L:102:THR:HG23	1.91	0.84
3:H:52(A):TRP:HH2	3:H:73:THR:HA	1.43	0.84
2:B:133:ILE:CG2	2:B:133:ILE:O	2.25	0.83
3:H:14:PRO:O	3:H:15:THR:OG1	1.96	0.82
2:B:158:ASP:OD2	2:B:161:LYS:HB2	1.79	0.82
3:H:6:GLU:OE1	3:H:106:GLY:CA	2.27	0.82
3:H:123:PRO:HG3	3:H:221:LYS:CE	2.09	0.82
2:B:28:ASN:ND2	2:B:149:MET:CG	2.44	0.81
4:L:48:ILE:HG23	4:L:52:ASN:HA	1.62	0.81
2:B:142:HIS:CD2	2:B:143:LYS:O	2.34	0.81
4:L:14:THR:HG23	4:L:15:PRO:HD2	1.62	0.79
1:A:283:THR:CG2	1:A:284:PRO:HD2	2.12	0.79
2:B:24:TYR:CD1	2:B:153:ARG:HG2	2.16	0.79
3:H:60:THR:HG21	3:H:63:LEU:HD11	1.62	0.79
4:L:37:GLN:HB2	4:L:47:LEU:CD1	2.11	0.79
4:L:7:PRO:O	4:L:102:THR:HG22	1.83	0.79
2:B:25:HIS:CD2	2:B:34:TYR:CE2	2.71	0.78
1:A:156:LYS:HD3	1:A:196:GLN:HG2	1.64	0.77
3:H:3:GLN:HG2	3:H:4:LEU:N	1.99	0.77
3:H:96:LEU:CB	3:H:100(D):ARG:HB2	2.15	0.76
1:A:320:LEU:HD12	1:A:320:LEU:C	2.07	0.76
2:B:133:ILE:HG22	2:B:133:ILE:O	1.86	0.75
3:H:96:LEU:CB	3:H:100(D):ARG:HG3	2.16	0.75
2:B:28:ASN:HD21	2:B:149:MET:CG	1.98	0.75
3:H:59:ILE:HG22	3:H:64:LYS:HD2	1.68	0.74
3:H:6:GLU:OE1	3:H:91:TYR:HA	1.87	0.74
2:B:141:TYR:CE1	2:B:170:ARG:CD	2.62	0.73
3:H:63:LEU:HD13	3:H:67:LEU:HD11	1.70	0.73
3:H:3:GLN:HB3	3:H:25:SER:OG	1.89	0.73
2:B:150:GLU:O	2:B:154:ASN:HB2	1.90	0.72
3:H:4:LEU:CD2	3:H:24:PHE:CZ	2.73	0.72
2:B:26:HIS:HB3	2:B:149:MET:CE	2.18	0.71
2:B:128:ASN:HB3	2:B:170:ARG:NH1	2.05	0.71
2:B:141:TYR:CE1	2:B:170:ARG:HB2	2.25	0.71
3:H:52(A):TRP:CH2	3:H:73:THR:HA	2.25	0.71
4:L:48:ILE:CG2	4:L:52:ASN:H	2.03	0.71
2:B:19:ASP:HB2	2:B:36:ALA:CB	2.20	0.70
4:L:52:ASN:OD1	4:L:52:ASN:C	2.28	0.70
1:A:283:THR:HG22	1:A:284:PRO:HD2	1.73	0.70
2:B:131:LYS:HE3	2:B:133:ILE:CG1	2.23	0.69
1:A:50:LYS:HD3	1:A:275:HIS:CE1	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ASN:HD21	2:B:149:MET:HG2	1.56	0.69
2:B:24:TYR:CE1	2:B:153:ARG:CG	2.71	0.69
4:L:14:THR:CG2	4:L:15:PRO:HD2	2.21	0.69
1:A:50:LYS:HD2	1:A:275:HIS:ND1	2.09	0.68
2:B:141:TYR:CZ	2:B:170:ARG:HG3	2.29	0.67
2:B:28:ASN:ND2	2:B:149:MET:HG2	2.08	0.67
2:B:19:ASP:HB2	2:B:36:ALA:HB3	1.74	0.67
3:H:52:ASP:HB3	3:H:54:ASP:HB3	1.76	0.67
3:H:94:ARG:O	3:H:101:ASP:N	2.26	0.66
1:A:52:CYS:HG	1:A:277:CYS:CB	2.09	0.66
2:B:9:PHE:O	2:B:135:ASN:HA	1.95	0.66
2:B:26:HIS:CB	2:B:149:MET:HE3	2.23	0.65
1:A:48:ASN:HB3	1:A:50:LYS:H	1.62	0.65
4:L:38:GLN:O	4:L:84:ALA:HB1	1.96	0.65
1:A:283:THR:HG22	1:A:284:PRO:CD	2.26	0.65
2:B:30:GLN:HE22	2:B:145:ASP:CB	1.98	0.64
3:H:123:PRO:CG	3:H:221:LYS:HE3	2.16	0.64
2:B:141:TYR:CE1	2:B:170:ARG:CB	2.79	0.64
4:L:51:ASN:O	4:L:52:ASN:CB	2.45	0.64
3:H:213:LYS:N	3:H:214:PRO:CD	2.60	0.64
1:A:54:LEU:HD21	1:A:302:ILE:HG22	1.78	0.64
3:H:3:GLN:HG2	3:H:4:LEU:H	1.62	0.63
4:L:3:VAL:HG12	4:L:4:LEU:N	2.12	0.63
2:B:131:LYS:HE3	2:B:133:ILE:HD11	1.81	0.63
4:L:51:ASN:O	4:L:52:ASN:ND2	2.31	0.63
2:B:59:MET:HE3	2:B:59:MET:HA	1.81	0.63
1:A:48:ASN:ND2	1:A:50:LYS:HB2	2.13	0.63
1:A:60:GLN:HE21	1:A:62:GLY:H	1.46	0.62
3:H:4:LEU:HD21	3:H:24:PHE:CZ	2.34	0.62
4:L:55:PRO:HD2	4:L:58:VAL:HG21	1.82	0.62
3:H:47:TRP:HZ2	3:H:50:LEU:HB3	1.65	0.61
1:A:283:THR:HG23	1:A:284:PRO:HD2	1.81	0.61
3:H:194:PRO:HG2	3:H:197:SER:OG	1.99	0.61
3:H:3:GLN:NE2	3:H:5:VAL:HG22	2.14	0.61
4:L:21:ILE:CG2	4:L:102:THR:HG21	2.30	0.61
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.36	0.61
3:H:96:LEU:CA	3:H:100(D):ARG:HB2	2.31	0.60
3:H:190:VAL:HG12	3:H:191:VAL:N	2.16	0.60
3:H:193:VAL:HB	3:H:194:PRO:HD2	1.84	0.60
2:B:133:ILE:HD11	2:B:139:GLU:OE1	2.01	0.60
3:H:4:LEU:HD22	3:H:24:PHE:CZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:48:ILE:HG23	4:L:52:ASN:CA	2.31	0.59
4:L:48:ILE:CG2	4:L:52:ASN:HA	2.31	0.59
3:H:13:LYS:O	3:H:16:GLN:HG3	2.02	0.59
2:B:159:TYR:N	2:B:160:PRO:CD	2.66	0.59
3:H:67:LEU:HD21	3:H:82:MET:CE	2.33	0.59
1:A:164:LEU:C	1:A:164:LEU:HD12	2.22	0.58
2:B:129:ASN:ND2	2:B:159:TYR:CD2	2.72	0.58
2:B:24:TYR:CZ	2:B:153:ARG:HG2	2.36	0.58
3:H:54:ASP:O	3:H:55:ASP:CB	2.43	0.58
3:H:59:ILE:CG2	3:H:64:LYS:HD2	2.34	0.58
3:H:187:LEU:C	3:H:187:LEU:HD12	2.24	0.58
1:A:96:THR:HG23	1:A:232:TYR:CE1	2.39	0.58
1:A:283:THR:CG2	1:A:298:HIS:HB3	2.34	0.57
3:H:67:LEU:HD21	3:H:82:MET:HE2	1.85	0.57
7:A:601:NAG:H62	7:A:602:NAG:C1	2.35	0.57
2:B:131:LYS:CE	2:B:133:ILE:HD11	2.35	0.57
1:A:283:THR:HG22	1:A:284:PRO:N	2.19	0.57
1:A:52:CYS:HG	1:A:277:CYS:HB3	1.69	0.57
1:A:98:TYR:CD2	1:A:230:MET:HB2	2.40	0.57
4:L:196:VAL:HG22	4:L:205:VAL:HG13	1.87	0.57
4:L:46:LEU:HG	4:L:55:PRO:HG3	1.86	0.56
3:H:34:MET:O	3:H:52(A):TRP:CB	2.48	0.56
3:H:52:ASP:OD2	3:H:54:ASP:HB2	2.06	0.56
3:H:18:LEU:HD21	3:H:20:LEU:CG	2.35	0.56
4:L:48:ILE:CG2	4:L:52:ASN:N	2.68	0.56
3:H:18:LEU:HD21	3:H:20:LEU:HG	1.87	0.56
3:H:3:GLN:HE22	3:H:5:VAL:HG22	1.70	0.56
1:A:283:THR:HG23	1:A:298:HIS:HB3	1.88	0.56
1:A:156:LYS:HD3	1:A:196:GLN:CG	2.34	0.56
3:H:36:TRP:CG	3:H:80:LEU:HD22	2.41	0.56
1:A:157:LYS:CE	3:H:54:ASP:OD2	2.50	0.55
4:L:48:ILE:HD12	4:L:52:ASN:HA	1.88	0.55
3:H:163:SER:HA	3:H:209:ASN:OD1	2.06	0.55
1:A:61:LEU:HD11	1:A:66:ILE:HD13	1.88	0.55
4:L:138:ASP:HA	4:L:172:LYS:HB3	1.87	0.55
3:H:60:THR:HG23	3:H:60:THR:O	2.06	0.55
3:H:18:LEU:HD21	3:H:20:LEU:HD11	1.89	0.55
1:A:48:ASN:ND2	1:A:52:CYS:SG	2.79	0.55
3:H:147:TYR:CE1	3:H:152:VAL:HG23	2.42	0.55
1:A:320:LEU:CD1	1:A:321:ARG:O	2.54	0.55
2:B:94:TYR:CZ	2:B:98:LEU:HD22	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:184:GLU:O	4:L:188:SER:HB2	2.07	0.55
3:H:60:THR:O	3:H:64:LYS:HD3	2.06	0.54
1:A:323:ILE:O	1:A:323:ILE:CG2	2.44	0.54
1:A:195:TYR:CE2	1:A:250:ASN:N	2.65	0.54
2:B:133:ILE:HG23	2:B:133:ILE:O	2.07	0.54
4:L:3:VAL:CG1	4:L:4:LEU:N	2.71	0.54
4:L:126:GLN:O	4:L:126:GLN:NE2	2.40	0.54
2:B:131:LYS:HE3	2:B:133:ILE:CD1	2.37	0.54
1:A:43:LEU:HB2	1:A:314:LEU:HB2	1.88	0.54
4:L:20:THR:HA	4:L:73:LEU:O	2.07	0.54
4:L:83:GLU:HG3	4:L:105:THR:HA	1.89	0.54
1:A:188:GLY:HA2	1:A:217:ILE:HD13	1.90	0.53
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.90	0.53
2:B:72:ASN:C	2:B:72:ASN:HD22	2.11	0.53
3:H:2:VAL:HG11	3:H:94:ARG:NH1	2.23	0.53
1:A:65:ASN:C	1:A:65:ASN:OD1	2.47	0.53
3:H:96:LEU:H	3:H:100(D):ARG:HB2	1.74	0.52
2:B:142:HIS:HB2	2:B:165:GLU:OE2	2.08	0.52
3:H:100(F):PHE:HB2	4:L:36:TYR:CE1	2.44	0.52
2:B:17:MET:SD	2:B:23:GLY:HA3	2.50	0.52
3:H:171:VAL:HG22	3:H:191:VAL:CG2	2.34	0.52
1:A:283:THR:CG2	1:A:298:HIS:CB	2.87	0.52
2:B:142:HIS:HB2	2:B:165:GLU:CD	2.30	0.52
2:B:14:TRP:CH2	2:B:25:HIS:HB2	2.45	0.51
2:B:19:ASP:HB2	2:B:36:ALA:HB2	1.91	0.51
3:H:34:MET:SD	3:H:94:ARG:CD	2.99	0.51
1:A:14:CYS:O	2:B:24:TYR:HA	2.09	0.51
4:L:6:GLN:HB3	4:L:7:PRO:HD2	1.92	0.51
4:L:166:LYS:HE2	4:L:173:TYR:OH	2.10	0.51
1:A:283:THR:CG2	1:A:284:PRO:CD	2.84	0.51
1:A:283:THR:HG21	1:A:298:HIS:CB	2.40	0.51
3:H:6:GLU:OE2	3:H:104:GLY:HA3	2.11	0.51
4:L:197:THR:HA	4:L:203:SER:O	2.10	0.51
2:B:24:TYR:CD1	2:B:153:ARG:CG	2.90	0.51
3:H:152:VAL:HG12	3:H:153:THR:N	2.24	0.51
1:A:159:SER:O	1:A:159:SER:OG	2.22	0.51
3:H:96:LEU:N	3:H:100(D):ARG:HB2	2.26	0.50
4:L:54:ARG:HD3	4:L:62:PHE:O	2.11	0.50
3:H:60:THR:CG2	3:H:63:LEU:HD11	2.37	0.50
1:A:99:PRO:HG3	1:A:223:VAL:O	2.12	0.50
2:B:158:ASP:CG	2:B:161:LYS:HB2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.94	0.50
1:A:160:SER:HA	3:H:99:SER:OG	2.12	0.50
3:H:2:VAL:HG12	3:H:102:LEU:HD21	1.94	0.50
2:B:25:HIS:HD2	2:B:34:TYR:HE2	1.48	0.50
1:A:320:LEU:HD12	1:A:321:ARG:O	2.11	0.50
1:A:324:PRO:O	1:A:325:SER:C	2.50	0.50
2:B:16:GLY:O	2:B:18:ILE:HG23	2.11	0.50
4:L:49:TYR:CE1	4:L:53:GLU:HB2	2.47	0.49
3:H:190:VAL:CG1	3:H:191:VAL:N	2.75	0.49
1:A:30:LEU:HD12	2:B:105:GLU:OE2	2.11	0.49
2:B:24:TYR:CD1	2:B:153:ARG:CD	2.95	0.49
3:H:60:THR:HG21	3:H:63:LEU:CD1	2.38	0.49
1:A:56:ILE:N	1:A:56:ILE:HD12	2.28	0.49
3:H:149:PRO:O	3:H:212:HIS:HE1	1.95	0.49
2:B:28:ASN:ND2	2:B:149:MET:HG3	2.26	0.49
4:L:32:THR:HG22	4:L:51:ASN:ND2	2.27	0.49
1:A:18:HIS:CG	1:A:19:ALA:N	2.81	0.49
2:B:145:ASP:O	2:B:148:CYS:HB3	2.13	0.49
3:H:94:ARG:NH2	3:H:101:ASP:OD2	2.42	0.49
4:L:6:GLN:HE21	4:L:102:THR:CG2	2.19	0.49
1:A:126:SER:HB3	1:A:166:LYS:HE3	1.94	0.49
1:A:60:GLN:NE2	1:A:62:GLY:H	2.09	0.48
3:H:18:LEU:CD2	3:H:20:LEU:HG	2.43	0.48
1:A:320:LEU:C	1:A:320:LEU:CD1	2.80	0.48
3:H:12:VAL:CG1	3:H:16:GLN:HB2	2.43	0.48
3:H:140:LEU:HD12	3:H:140:LEU:C	2.33	0.48
2:B:72:ASN:HD22	2:B:73:LEU:N	2.12	0.48
1:A:307:LYS:HE3	2:B:92:TRP:CD1	2.48	0.48
4:L:6:GLN:HB3	4:L:102:THR:CG2	2.44	0.48
1:A:130:HIS:NE2	1:A:164:LEU:HB3	2.29	0.48
1:A:283:THR:HG21	1:A:298:HIS:HB2	1.95	0.48
1:A:180:TRP:HZ3	1:A:235:THR:HG22	1.78	0.47
3:H:40:PRO:HB2	3:H:43:LYS:CG	2.44	0.47
4:L:49:TYR:CD1	4:L:53:GLU:O	2.67	0.47
1:A:323:ILE:HG21	2:B:12:GLY:HA2	1.96	0.47
3:H:18:LEU:HD21	3:H:20:LEU:CD1	2.43	0.47
3:H:61:TYR:CE2	4:L:2:PRO:HG2	2.50	0.47
3:H:95:THR:HA	3:H:100(D):ARG:O	2.14	0.47
3:H:73:THR:HG23	3:H:74:SER:N	2.29	0.47
1:A:103:ILE:N	1:A:103:ILE:HD12	2.29	0.47
3:H:34:MET:HA	3:H:95:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:18:ARG:HG2	4:L:76:SER:HA	1.96	0.47
1:A:15:ILE:HD12	1:A:15:ILE:N	2.30	0.47
1:A:179:LEU:N	1:A:179:LEU:HD12	2.30	0.47
4:L:184:GLU:N	4:L:184:GLU:OE1	2.45	0.47
3:H:145:LYS:HA	3:H:186:SER:OG	2.15	0.47
1:A:156:LYS:HE2	1:A:193:SER:O	2.15	0.47
1:A:322:ASN:O	1:A:324:PRO:HD3	2.15	0.46
3:H:212:HIS:HD2	3:H:215:SER:OG	1.97	0.46
4:L:119:PRO:HA	4:L:132:LEU:HD23	1.96	0.46
3:H:23:SER:OG	3:H:77:GLN:HG2	2.15	0.46
1:A:238:GLU:O	1:A:239:PRO:C	2.54	0.46
2:B:133:ILE:CD1	2:B:139:GLU:CD	2.84	0.46
3:H:63:LEU:C	3:H:63:LEU:HD12	2.36	0.46
3:H:13:LYS:HB2	3:H:16:GLN:HG3	1.98	0.46
1:A:161:TYR:HD2	1:A:161:TYR:O	1.99	0.46
3:H:60:THR:C	3:H:62:SER:H	2.19	0.46
4:L:54:ARG:HB3	4:L:58:VAL:HB	1.97	0.46
3:H:50:LEU:HD23	3:H:50:LEU:C	2.36	0.46
1:A:301:THR:CG2	1:A:305:CYS:SG	2.94	0.46
4:L:167:GLN:HG2	4:L:168:SER:N	2.30	0.46
3:H:34:MET:CG	3:H:52(A):TRP:HD1	2.28	0.46
4:L:52:ASN:OD1	4:L:53:GLU:N	2.49	0.46
1:A:320:LEU:HD12	1:A:321:ARG:N	2.30	0.46
2:B:141:TYR:HE1	2:B:170:ARG:CG	1.98	0.46
1:A:164:LEU:O	1:A:164:LEU:HD12	2.16	0.46
1:A:109:ARG:HE	2:B:69:GLU:CD	2.19	0.46
3:H:50:LEU:HD22	3:H:58:TYR:HD2	1.81	0.45
4:L:179:LEU:HD21	4:L:181:LEU:HD21	1.98	0.45
2:B:73:LEU:HA	2:B:73:LEU:HD23	1.75	0.45
2:B:6:ILE:HG13	2:B:112:ASP:HA	1.98	0.45
2:B:125:GLN:HE22	2:B:155:GLY:C	2.19	0.45
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.51	0.45
3:H:52(A):TRP:HH2	3:H:73:THR:CA	2.21	0.45
1:A:118:PHE:C	1:A:118:PHE:HD1	2.20	0.45
3:H:148:PHE:HB2	3:H:184:LEU:HD23	1.99	0.45
4:L:61:ARG:HD2	4:L:76:SER:O	2.17	0.45
2:B:133:ILE:CD1	2:B:139:GLU:OE1	2.63	0.44
3:H:60:THR:CG2	3:H:63:LEU:CD1	2.94	0.44
3:H:13:LYS:H	3:H:16:GLN:HE21	1.65	0.44
3:H:6:GLU:HG2	3:H:6:GLU:H	1.30	0.44
2:B:131:LYS:HE3	2:B:133:ILE:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ASP:H	2:B:148:CYS:HB3	1.83	0.44
1:A:37:THR:HG23	1:A:320:LEU:O	2.17	0.44
1:A:207:SER:HB2	1:A:241:ASP:OD1	2.17	0.44
4:L:39:VAL:CG1	4:L:40:PRO:CD	2.86	0.44
1:A:108:LEU:HB2	1:A:234:TRP:CE2	2.53	0.44
3:H:34:MET:HB2	3:H:95:THR:O	2.17	0.43
4:L:55:PRO:HD2	4:L:58:VAL:CG2	2.48	0.43
1:A:195:TYR:CD2	1:A:250:ASN:N	2.68	0.43
1:A:118:PHE:C	1:A:118:PHE:CD1	2.91	0.43
3:H:190:VAL:HG21	4:L:135:LEU:HD12	1.99	0.43
3:H:152:VAL:CG1	3:H:153:THR:N	2.80	0.43
2:B:131:LYS:HG3	2:B:133:ILE:HG13	2.00	0.43
1:A:283:THR:HB	1:A:286:GLY:O	2.18	0.43
1:A:225:ASP:O	1:A:226:GLN:NE2	2.50	0.43
1:A:163:LYS:HE3	1:A:201:TYR:OH	2.17	0.43
3:H:179:GLN:C	3:H:182:SER:N	2.71	0.43
3:H:173:THR:HA	3:H:189:SER:HA	2.01	0.43
3:H:63:LEU:HD13	3:H:67:LEU:CD1	2.45	0.43
1:A:100:GLY:HA3	1:A:230:MET:O	2.19	0.43
4:L:48:ILE:HG22	4:L:52:ASN:H	1.80	0.42
4:L:18:ARG:CG	4:L:76:SER:HA	2.49	0.42
4:L:14:THR:CG2	4:L:15:PRO:CD	2.95	0.42
1:A:177:LEU:HG	1:A:179:LEU:HD11	2.01	0.42
4:L:43:ALA:HA	4:L:44:PRO:HD3	1.93	0.42
1:A:185:PRO:HG2	1:A:191:GLN:NE2	2.35	0.42
3:H:34:MET:SD	3:H:94:ARG:HD3	2.59	0.42
4:L:166:LYS:HE2	4:L:173:TYR:CZ	2.54	0.42
1:A:18:HIS:CG	1:A:19:ALA:H	2.37	0.42
4:L:48:ILE:HG23	4:L:52:ASN:N	2.34	0.42
1:A:177:LEU:HB2	1:A:260:LEU:HD11	2.01	0.42
3:H:148:PHE:HB2	3:H:184:LEU:CD2	2.49	0.42
3:H:96:LEU:CB	3:H:100(D):ARG:CB	2.72	0.42
3:H:193:VAL:CB	3:H:194:PRO:HD2	2.47	0.42
1:A:186:PRO:HA	1:A:218:ALA:O	2.20	0.42
3:H:14:PRO:C	3:H:15:THR:HG1	2.09	0.42
2:B:59:MET:CE	2:B:59:MET:HA	2.49	0.42
3:H:138:ALA:N	3:H:193:VAL:O	2.51	0.42
1:A:70:LEU:HD12	1:A:108:LEU:HD21	2.02	0.42
1:A:301:THR:HG21	1:A:305:CYS:HB2	2.02	0.41
3:H:61:TYR:CD1	3:H:61:TYR:N	2.88	0.41
4:L:37:GLN:HB2	4:L:47:LEU:HD12	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:66:ARG:HD2	3:H:82(A):THR:O	2.20	0.41
4:L:79:GLN:O	4:L:82:ASP:HB2	2.21	0.41
3:H:152:VAL:HG13	3:H:211:ASN:O	2.19	0.41
2:B:28:ASN:OD1	2:B:144:CYS:O	2.39	0.41
3:H:84:PRO:HA	3:H:111:VAL:HB	2.02	0.41
4:L:52:ASN:OD1	4:L:53:GLU:OE2	2.37	0.41
4:L:110:LYS:HG2	4:L:111:ALA:N	2.35	0.41
2:B:142:HIS:NE2	2:B:144:CYS:HB2	2.36	0.41
3:H:13:LYS:H	3:H:16:GLN:NE2	2.18	0.41
3:H:40:PRO:HB2	3:H:43:LYS:HB2	2.03	0.41
2:B:77:ILE:HD13	2:B:77:ILE:HG21	1.63	0.41
1:A:320:LEU:HD12	1:A:321:ARG:C	2.41	0.41
4:L:27:SER:HA	4:L:29:GLY:HA3	2.03	0.41
3:H:50:LEU:HD23	3:H:51:ILE:N	2.36	0.40
3:H:145:LYS:HG3	3:H:186:SER:OG	2.21	0.40
2:B:58:LYS:HA	2:B:58:LYS:HD3	1.82	0.40
3:H:60:THR:CG2	3:H:60:THR:O	2.69	0.40
3:H:60:THR:CG2	3:H:62:SER:HB3	2.51	0.40
1:A:63:LYS:O	1:A:63:LYS:HG2	2.21	0.40
3:H:60:THR:C	3:H:62:SER:N	2.74	0.40
3:H:12:VAL:O	3:H:111:VAL:HA	2.22	0.40
1:A:21:ASN:ND2	5:A:401:NAG:C7	2.83	0.40
3:H:52(A):TRP:O	3:H:52(A):TRP:CE3	2.47	0.40
4:L:205:VAL:HG22	4:L:206:GLU:N	2.35	0.40
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.57	0.40
1:A:316:MET:HB2	1:A:316:MET:HE3	1.91	0.40
1:A:73:ASN:HA	1:A:74:PRO:HD3	1.93	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	321/331 (97%)	292 (91%)	27 (8%)	2 (1%)	30 65
2	B	171/179 (96%)	159 (93%)	12 (7%)	0	100 100
3	H	212/230 (92%)	199 (94%)	13 (6%)	0	100 100
4	L	210/217 (97%)	193 (92%)	16 (8%)	1 (0%)	34 69
All	All	914/957 (96%)	843 (92%)	68 (7%)	3 (0%)	46 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
4	L	52	ASN
1	A	324	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	279/285 (98%)	265 (95%)	14 (5%)	30 64
2	B	147/152 (97%)	140 (95%)	7 (5%)	31 66
3	H	188/204 (92%)	173 (92%)	15 (8%)	15 40
4	L	176/181 (97%)	172 (98%)	4 (2%)	58 88
All	All	790/822 (96%)	750 (95%)	40 (5%)	29 63

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	81	THR
1	A	94	GLU
1	A	102	PHE
1	A	118	PHE
1	A	140	SER
1	A	161	TYR
1	A	165	SER

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Mol	Chain	Res	Type
1	A	192	GLN
1	A	195	TYR
1	A	208	LYS
1	A	290	SER
1	A	301	THR
1	A	312	THR
2	B	19	ASP
2	B	24	TYR
2	B	72	ASN
2	B	77	ILE
2	B	116	ARG
2	B	143	LYS
2	B	144	CYS
3	H	5	VAL
3	H	6	GLU
3	H	50	LEU
3	H	52(A)	TRP
3	H	53	ASP
3	H	62(A)	SER
3	H	84	PRO
3	H	85	VAL
3	H	100(E)	ASP
3	H	107	THR
3	H	115	SER
3	H	178	LEU
3	H	195	SER
3	H	208	CYS
3	H	218	LYS
4	L	114	SER
4	L	151	ASP
4	L	180	SER
4	L	206	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	48	ASN
1	A	60	GLN
1	A	92	ASN
1	A	192	GLN
2	B	25	HIS

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Mol	Chain	Res	Type
2	B	28	ASN
2	B	30	GLN
2	B	42	GLN
2	B	72	ASN
2	B	125	GLN
2	B	135	ASN
2	B	142	HIS
3	H	3	GLN
3	H	16	GLN
3	H	211	ASN
3	H	212	HIS
4	L	189	HIS

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

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	501	1,6	14,14,15	0.48	0	15,19,21	1.40	4 (26%)
6	NAG	A	502	6	14,14,15	0.63	0	15,19,21	1.47	1 (6%)
7	NAG	A	601	1,7	14,14,15	0.91	1 (7%)	15,19,21	1.57	3 (20%)
7	NAG	A	602	7	14,14,15	0.60	0	15,19,21	2.15	2 (13%)
7	BMA	A	603	7	11,11,12	0.69	0	14,15,17	1.64	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	A	604	7	11,11,12	0.59	0	14,15,17	1.36	1 (7%)
6	NAG	A	701	1,6	14,14,15	0.60	0	15,19,21	1.49	2 (13%)
6	NAG	A	702	6	14,14,15	0.72	1 (7%)	15,19,21	1.28	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	501	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	502	6	-	0/6/23/26	0/1/1/1
7	NAG	A	601	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	602	7	-	0/6/23/26	0/1/1/1
7	BMA	A	603	7	-	0/2/19/22	0/1/1/1
7	MAN	A	604	7	-	0/2/19/22	0/1/1/1
6	NAG	A	701	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	702	6	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	601	NAG	O5-C1	-2.23	1.40	1.43
6	A	702	NAG	C1-C2	2.21	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	702	NAG	C1-O5-C5	-3.31	108.05	112.25
7	A	601	NAG	O6-C6-C5	-3.08	101.16	111.33
7	A	602	NAG	C2-N2-C7	-2.74	119.52	123.04
7	A	601	NAG	O3-C3-C4	-2.61	104.46	110.34
7	A	604	MAN	C1-C2-C3	-2.52	106.56	109.54
6	A	501	NAG	C2-N2-C7	-2.47	119.87	123.04
7	A	603	BMA	C1-O5-C5	-2.12	109.56	112.25
6	A	701	NAG	C6-C5-C4	-2.12	107.79	113.02
6	A	501	NAG	O5-C5-C6	2.12	111.93	107.35
6	A	702	NAG	O5-C5-C6	2.29	112.30	107.35
6	A	501	NAG	C4-C3-C2	2.74	115.48	111.23
7	A	601	NAG	C1-O5-C5	2.75	115.73	112.25
6	A	501	NAG	C3-C4-C5	2.79	115.06	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	502	NAG	O5-C5-C6	3.38	114.66	107.35
6	A	701	NAG	C3-C4-C5	3.92	117.03	110.20
7	A	603	BMA	O5-C5-C6	4.19	116.42	107.35
7	A	602	NAG	C1-O5-C5	6.26	120.19	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	NAG	1	0
7	A	602	NAG	1	0

5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\| > 2$
5	NAG	A	401	1	14,14,15	0.61	0	15,19,21	1.64	3 (20%)

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	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	401	NAG	C4-C3-C2	-3.47	105.83	111.23
5	A	401	NAG	O3-C3-C2	2.21	113.49	109.11
5	A	401	NAG	C1-O5-C5	3.08	116.16	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	323/331 (97%)	0.61	11 (3%) 49 36	68, 80, 91, 101	0
2	B	173/179 (96%)	1.27	37 (21%) 1 1	68, 82, 92, 105	0
3	H	216/230 (93%)	1.12	39 (18%) 2 1	71, 82, 95, 108	1 (0%)
4	L	212/217 (97%)	1.63	66 (31%) 1 0	71, 83, 90, 97	0
All	All	924/957 (96%)	1.08	153 (16%) 2 1	68, 81, 92, 108	1 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	138	ALA	9.2
4	L	194	CYS	9.1
3	H	198	LEU	8.1
4	L	186	TRP	8.0
3	H	139	ALA	7.7
2	B	138	PHE	7.4
4	L	13	GLY	7.3
2	B	140	PHE	7.1
2	B	157	TYR	6.9
4	L	150	ALA	6.7
3	H	206	TYR	6.6
1	A	12	THR	6.5
4	L	192	TYR	6.4
4	L	191	SER	6.4
3	H	141	GLY	6.4
2	B	143	LYS	6.2
4	L	106(A)	LEU	5.9
3	H	192	THR	5.8
3	H	205	THR	5.4
4	L	21	ILE	5.4
3	H	126	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
4	L	122	SER	5.3
3	H	199	GLY	5.3
2	B	27	GLN	5.2
2	B	144	CYS	5.1
3	H	140	LEU	5.1
4	L	193	SER	5.1
3	H	221	LYS	5.0
4	L	108	GLN	5.0
4	L	153	SER	4.9
4	L	148	TRP	4.8
3	H	193	VAL	4.7
3	H	189	SER	4.7
3	H	123	PRO	4.7
4	L	111	ALA	4.7
4	L	198	HIS	4.6
2	B	142	HIS	4.5
2	B	168	LEU	4.5
4	L	109	PRO	4.5
2	B	152	VAL	4.4
2	B	23	GLY	4.4
3	H	137	THR	4.4
2	B	141	TYR	4.3
3	H	203	GLN	4.3
2	B	35	ALA	4.3
1	A	15	ILE	4.3
4	L	133	VAL	4.3
1	A	325	SER	4.1
2	B	139	GLU	4.1
4	L	147	ALA	4.1
4	L	105	THR	4.1
2	B	28	ASN	4.1
2	B	22	TYR	4.0
4	L	75	ILE	4.0
4	L	181	LEU	3.9
3	H	200	THR	3.9
3	H	190	VAL	3.9
4	L	76	SER	3.9
2	B	25	HIS	3.8
4	L	16	GLY	3.8
4	L	132	LEU	3.7
1	A	13	ILE	3.7
4	L	152	SER	3.7

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Mol	Chain	Res	Type	RSRZ
4	L	196	VAL	3.6
4	L	18	ARG	3.6
3	H	122	PHE	3.6
1	A	11	ASP	3.6
1	A	324	PRO	3.6
4	L	19	VAL	3.5
2	B	136	GLY	3.5
3	H	125	ALA	3.5
2	B	149	MET	3.5
3	H	207	ILE	3.4
3	H	142	CYS	3.4
4	L	209	VAL	3.4
4	L	106	VAL	3.3
4	L	149	LYS	3.3
3	H	26	GLY	3.3
4	L	173	TYR	3.2
4	L	134	CYS	3.2
4	L	180	SER	3.2
4	L	73	LEU	3.2
3	H	188	SER	3.1
4	L	118	PHE	3.1
4	L	203	SER	3.1
2	B	171	GLU	3.0
4	L	139	PHE	3.0
4	L	62	PHE	2.9
4	L	142	GLY	2.9
4	L	110	LYS	2.9
4	L	211	PRO	2.9
2	B	26	HIS	2.9
2	B	145	ASP	2.9
4	L	80	SER	2.9
1	A	21	ASN	2.9
3	H	124	LEU	2.8
4	L	140	TYR	2.8
4	L	144	VAL	2.8
3	H	96	LEU	2.8
4	L	204	THR	2.8
3	H	121	VAL	2.8
4	L	82	ASP	2.8
2	B	153	ARG	2.7
3	H	27	PHE	2.7
3	H	197	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	129	ASN	2.7
4	L	197	THR	2.7
1	A	14	CYS	2.7
4	L	86	TYR	2.7
2	B	24	TYR	2.6
4	L	188	SER	2.6
4	L	179	LEU	2.6
2	B	63	PHE	2.6
2	B	30	GLN	2.5
2	B	154	ASN	2.5
2	B	167	LYS	2.5
4	L	174	ALA	2.5
3	H	191	VAL	2.5
4	L	114	SER	2.5
2	B	32	SER	2.5
4	L	112	ALA	2.5
4	L	195	GLN	2.4
3	H	156	SER	2.4
3	H	165	ALA	2.4
1	A	16	GLY	2.4
2	B	17	MET	2.4
4	L	125	LEU	2.4
3	H	166	LEU	2.4
2	B	151	SER	2.4
2	B	119	TYR	2.3
2	B	130	ALA	2.3
4	L	63	SER	2.3
4	L	146	VAL	2.2
3	H	162	ASN	2.2
4	L	115	VAL	2.2
3	H	194	PRO	2.2
3	H	143	LEU	2.2
4	L	14	THR	2.2
2	B	19	ASP	2.1
3	H	223	VAL	2.1
4	L	207	LYS	2.1
3	H	29	LEU	2.1
4	L	51	ASN	2.1
3	H	211	ASN	2.1
2	B	131	LYS	2.1
4	L	200	GLY	2.1
2	B	166	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	276	ASP	2.1
4	L	136	ILE	2.1
4	L	2	PRO	2.0
2	B	31	GLY	2.0
1	A	186	PRO	2.0
4	L	47	LEU	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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
7	NAG	A	601	14/15	0.94	0.24	1.29	70,79,83,89	0
7	NAG	A	602	14/15	0.93	0.25	-	93,96,102,109	0
6	NAG	A	701	14/15	0.70	0.52	-	119,128,130,135	0
7	MAN	A	604	11/12	0.86	0.43	-	128,129,131,131	0
6	NAG	A	502	14/15	0.53	0.54	-	145,147,148,149	0
6	NAG	A	702	14/15	0.73	0.52	-	138,140,141,141	0
6	NAG	A	501	14/15	0.83	0.29	-	122,129,134,140	0
7	BMA	A	603	11/12	0.84	0.31	-	114,116,120,123	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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
5	NAG	A	401	14/15	0.64	0.41	-	119,127,132,133	0

6.5 Other polymers (i)

There are no such residues in this entry.