



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:23 PM 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 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/ValidationPDFNotes.html>

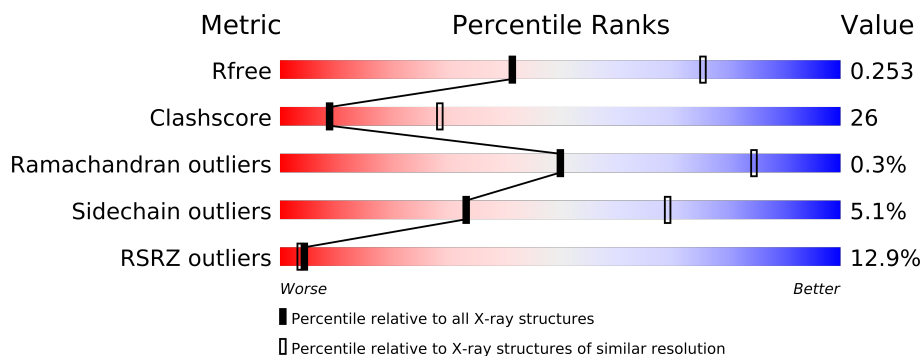
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	331	
2	B	179	
3	H	230	
4	L	217	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7207 atoms, of which 0 are hydrogen and 0 are deuterium.

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

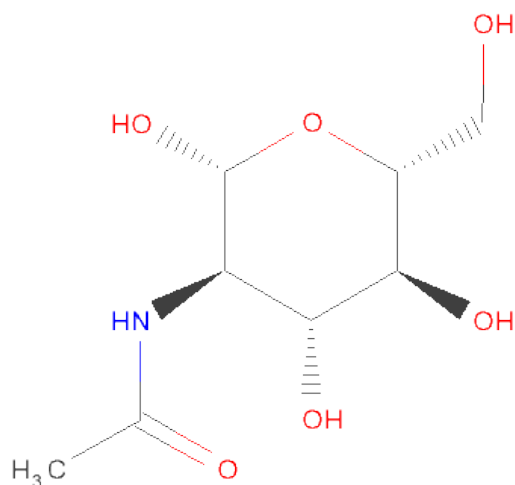
- Molecule 3 is a protein called 2D1 Fab, Heavy Chain.

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		

There are 8 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
A	7	ALA	-	EXPRESSION TAG	UNP Q9WFX3
A	8	ASP	-	EXPRESSION TAG	UNP Q9WFX3

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

- 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		

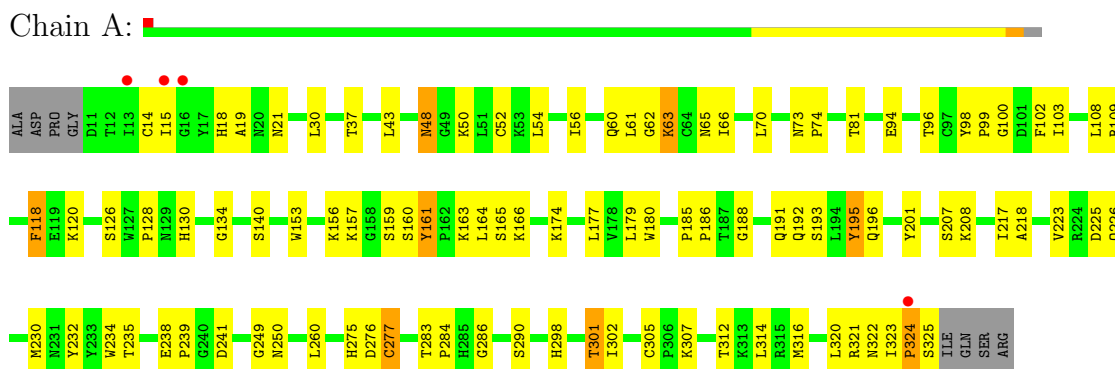
There are 4 discrepancies between the modelled and reference sequences:

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

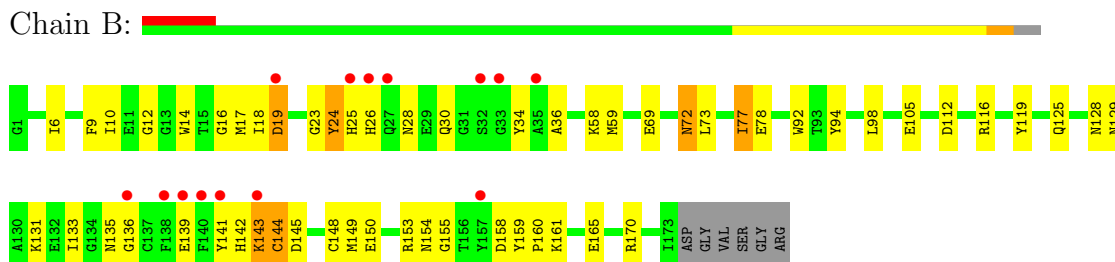
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

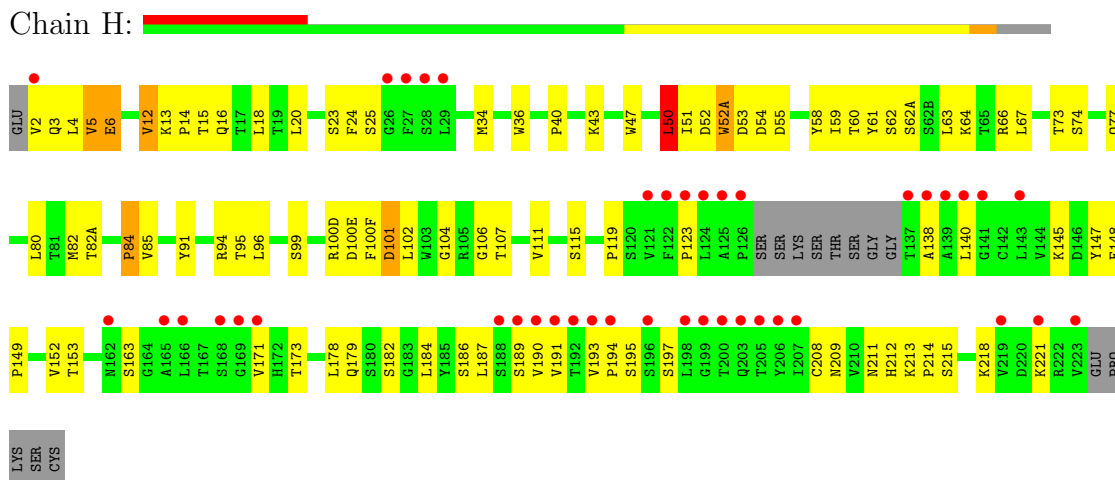
• Molecule 1: Hemagglutinin, HA1 Subunit



• Molecule 2: Hemagglutinin, HA2 Subunit

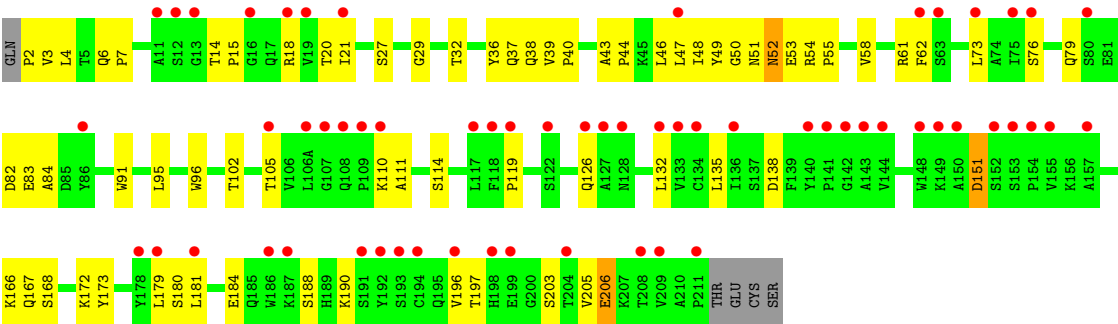


• Molecule 3: 2D1 Fab, Heavy Chain



● Molecule 4: 2D1 Fab, Light Chain

Chain L: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.230 , 0.259 0.223 , 0.253	Depositor DCC
R_{free} test set	2593 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 86.3	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 52718 reflections	Xtriage
F_o, F_c correlation	0.89	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.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (360) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
3:H:96:LEU:HB3	3:H:100(D):ARG:HG3	1.32	1.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	321/331 (97%)	292 (91%)	27 (8%)	2 (1%)	33	72
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%)	38	76
All	All	914/957 (96%)	843 (92%)	68 (7%)	3 (0%)	50	84

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 ⓘ

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%)	34	70
2	B	147/152 (97%)	140 (95%)	7 (5%)	35	72
3	H	188/204 (92%)	173 (92%)	15 (8%)	17	44
4	L	176/181 (97%)	172 (98%)	4 (2%)	63	92
All	All	790/822 (96%)	750 (95%)	40 (5%)	33	69

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
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

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Mol	Chain	Res	Type
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
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 chains 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	12,14,15	0.64	0	15,19,21	1.68	2 (13%)
6	NAG	A	502	6	12,14,15	0.69	0	15,19,21	2.46	2 (13%)
7	NAG	A	601	1,7	12,14,15	0.85	1 (8%)	15,19,21	1.50	3 (20%)
7	NAG	A	602	7	12,14,15	0.79	1 (8%)	15,19,21	1.65	5 (33%)
7	BMA	A	603	7	10,11,12	0.78	0	11,15,17	3.01	2 (18%)
7	MAN	A	604	7	10,11,12	0.62	0	11,15,17	1.76	1 (9%)
6	NAG	A	701	1,6	12,14,15	0.72	0	15,19,21	1.74	4 (26%)
6	NAG	A	702	6	12,14,15	0.60	0	15,19,21	1.64	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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-C5	-2.26	1.41	1.45
7	A	602	NAG	O5-C5	-2.22	1.41	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	603	BMA	O5-C5-C6	9.00	116.42	106.98
6	A	502	NAG	O5-C5-C6	7.32	114.66	106.98
6	A	702	NAG	O5-C5-C6	5.07	112.30	106.98
6	A	501	NAG	O5-C5-C6	4.71	111.93	106.98
7	A	604	MAN	O5-C5-C6	4.46	111.66	106.98
6	A	502	NAG	O5-C5-C4	-4.40	105.07	110.65
6	A	701	NAG	C3-C4-C5	3.83	117.03	110.20
7	A	602	NAG	C3-C2-N2	-3.06	107.10	111.76
6	A	701	NAG	O5-C5-C6	3.05	110.18	106.98
7	A	601	NAG	O6-C6-C5	-2.96	101.16	111.36
6	A	701	NAG	O5-C5-C4	2.78	114.17	110.65
6	A	501	NAG	C3-C4-C5	2.72	115.06	110.20
7	A	601	NAG	O3-C3-C4	-2.63	104.46	110.35
7	A	603	BMA	O5-C5-C4	-2.60	107.36	110.65
7	A	601	NAG	O5-C5-C4	2.52	113.85	110.65
7	A	602	NAG	O5-C5-C6	-2.43	104.43	106.98
6	A	702	NAG	C3-C2-N2	-2.24	108.36	111.76
6	A	701	NAG	C6-C5-C4	-2.16	107.79	113.00
7	A	602	NAG	C2-N2-C7	-2.12	119.52	123.09
7	A	602	NAG	O5-C5-C4	2.12	113.34	110.65
7	A	602	NAG	C6-C5-C4	-2.02	108.13	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

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	12,14,15	0.58	0	15,19,21	1.43	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(°)	Ideal(°)
5	A	401	NAG	O5-C5-C6	3.14	110.28	106.98
5	A	401	NAG	C4-C3-C2	-2.24	105.83	111.32
5	A	401	NAG	O3-C3-C2	2.10	113.49	109.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	323/331 (97%)	0.17	4 (1%) 75 76	68, 80, 91, 101	0
2	B	173/179 (96%)	0.66	14 (8%) 12 10	68, 82, 92, 105	0
3	H	216/230 (93%)	1.06	41 (18%) 2 2	71, 82, 95, 108	1 (0%)
4	L	212/217 (97%)	1.44	61 (28%) 1 1	71, 83, 90, 97	0
All	All	924/957 (96%)	0.76	120 (12%) 4 3	68, 81, 92, 108	1 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	138	ALA	7.5
3	H	198	LEU	6.3
4	L	186	TRP	6.1
3	H	139	ALA	5.8
2	B	143	LYS	5.7
2	B	138	PHE	5.6
3	H	192	THR	5.3
4	L	153	SER	5.2
4	L	19	VAL	5.0
4	L	106(A)	LEU	4.9
4	L	13	GLY	4.9
4	L	142	GLY	4.8
4	L	109	PRO	4.8
3	H	126	PRO	4.8
3	H	193	VAL	4.6
2	B	35	ALA	4.6
3	H	190	VAL	4.5
4	L	122	SER	4.4
4	L	18	ARG	4.3
4	L	133	VAL	4.3
2	B	140	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
3	H	191	VAL	4.2
3	H	200	THR	4.2
4	L	144	VAL	4.2
4	L	154	PRO	4.2
4	L	132	LEU	4.1
2	B	157	TYR	4.1
4	L	155	VAL	4.1
3	H	221	LYS	4.1
4	L	152	SER	4.1
4	L	191	SER	4.1
4	L	75	ILE	4.0
3	H	137	THR	4.0
3	H	206	TYR	4.0
4	L	192	TYR	4.0
4	L	194	CYS	3.9
4	L	12	SER	3.8
3	H	125	ALA	3.8
3	H	196	SER	3.8
3	H	189	SER	3.8
4	L	148	TRP	3.7
2	B	141	TYR	3.6
3	H	29	LEU	3.6
4	L	198	HIS	3.6
3	H	162	ASN	3.6
4	L	21	ILE	3.6
3	H	205	THR	3.5
3	H	140	LEU	3.5
3	H	141	GLY	3.5
4	L	157	ALA	3.5
3	H	199	GLY	3.5
4	L	196	VAL	3.4
3	H	27	PHE	3.4
4	L	105	THR	3.3
4	L	150	ALA	3.3
4	L	211	PRO	3.2
4	L	178	TYR	3.2
3	H	122	PHE	3.1
3	H	194	PRO	3.1
3	H	165	ALA	3.1
4	L	181	LEU	3.0
4	L	126	GLN	3.0
1	A	16	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	139	GLU	3.0
1	A	13	ILE	3.0
3	H	188	SER	2.9
3	H	124	LEU	2.9
4	L	11	ALA	2.9
2	B	26	HIS	2.9
3	H	123	PRO	2.9
4	L	128	ASN	2.9
1	A	15	ILE	2.9
3	H	166	LEU	2.8
3	H	207	ILE	2.8
4	L	107	GLY	2.8
4	L	134	CYS	2.8
2	B	25	HIS	2.8
4	L	16	GLY	2.8
4	L	108	GLN	2.8
4	L	149	LYS	2.7
3	H	2	VAL	2.7
4	L	127	ALA	2.6
3	H	223	VAL	2.6
4	L	193	SER	2.6
4	L	119	PRO	2.6
4	L	118	PHE	2.6
3	H	168	SER	2.5
4	L	47	LEU	2.5
3	H	169	GLY	2.5
4	L	76	SER	2.5
4	L	110	LYS	2.5
4	L	141	PRO	2.4
3	H	26	GLY	2.4
4	L	62	PHE	2.4
4	L	86	TYR	2.4
3	H	203	GLN	2.4
2	B	32	SER	2.4
3	H	28	SER	2.3
4	L	73	LEU	2.3
4	L	187	LYS	2.3
4	L	140	TYR	2.3
2	B	33	GLY	2.3
4	L	117	LEU	2.3
4	L	179	LEU	2.2
2	B	19	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	L	63	SER	2.2
3	H	121	VAL	2.2
4	L	209	VAL	2.2
4	L	136	ILE	2.1
3	H	143	LEU	2.1
3	H	171	VAL	2.1
4	L	80	SER	2.1
2	B	136	GLY	2.1
4	L	199	GLU	2.1
1	A	324	PRO	2.0
3	H	219	VAL	2.0
4	L	204	THR	2.0
2	B	27	GLN	2.0
4	L	208	THR	2.0
4	L	143	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	BMA	A	603	11/12	0.14	-	114,116,120,123	0
7	NAG	A	602	14/15	0.17	-	93,96,102,109	0
6	NAG	A	701	14/15	0.26	-	119,128,130,135	0
7	MAN	A	604	11/12	0.27	-	128,129,131,131	0
6	NAG	A	502	14/15	0.28	-	145,147,148,149	0
6	NAG	A	702	14/15	0.39	-	138,140,141,141	0
6	NAG	A	501	14/15	0.18	-	122,129,134,140	0
7	NAG	A	601	14/15	0.16	-	70,79,83,89	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	401	14/15	0.36	-	119,127,132,133	0

6.5 Other polymers

There are no such residues in this entry.