



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:01 am GMT

PDB ID : 4MHJ
Title : Crystal structure of Fab H5M9 in complex with influenza virus hemagglutinin from A/goose/Guangdong/1/96 (H5N1)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2013-08-29
Resolution : 6.98 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:

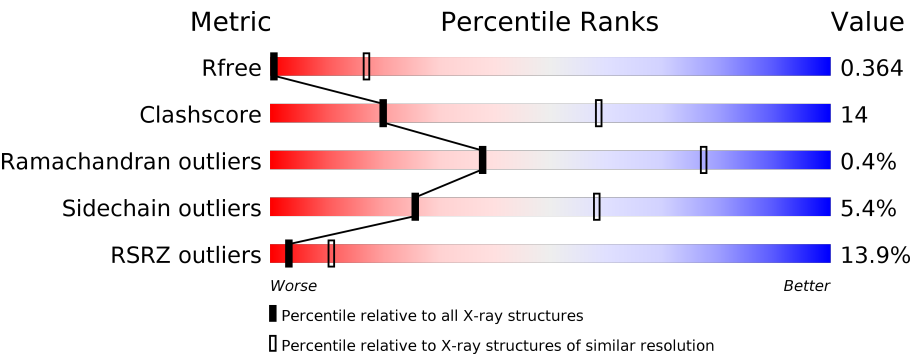
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

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 6.98 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}	100719	1100 (10.00-3.70)
Clashscore	112137	1035 (10.00-3.80)
Ramachandran outliers	110173	1003 (10.00-3.76)
Sidechain outliers	110143	1098 (10.00-3.70)
RSRZ outliers	101464	1003 (10.00-3.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	<div><div>9%</div><div><div></div><div>73%</div><div>22%</div><div>• •</div></div></div>
1	C	334	<div><div>13%</div><div><div></div><div>73%</div><div>22%</div><div>• •</div></div></div>
1	G	334	<div><div>11%</div><div><div></div><div>72%</div><div>23%</div><div>• •</div></div></div>
1	M	334	<div><div>10%</div><div><div></div><div>75%</div><div>20%</div><div>• •</div></div></div>
1	O	334	<div><div>14%</div><div><div></div><div>72%</div><div>22%</div><div>• 5%</div></div></div>
1	S	334	<div><div>11%</div><div><div></div><div>74%</div><div>22%</div><div>• •</div></div></div>

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Mol	Chain	Length	Quality of chain
2	B	182	
2	D	182	
2	I	182	
2	N	182	
2	P	182	
2	U	182	
3	E	218	
3	J	218	
3	L	218	
3	Q	218	
3	V	218	
3	X	218	
4	F	222	
4	H	222	
4	K	222	
4	R	222	
4	T	222	
4	W	222	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	2001	-	-	-	X
5	NAG	O	2001	-	-	-	X
6	NAG	C	2001	-	-	-	X
8	NAG	M	2001	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 43995 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2542	1603	440	484	15			
1	C	321	Total	C	N	O	S	0	0	0
			2533	1598	438	482	15			
1	G	321	Total	C	N	O	S	0	0	0
			2530	1594	439	482	15			
1	M	322	Total	C	N	O	S	0	0	0
			2542	1603	440	484	15			
1	O	318	Total	C	N	O	S	0	0	0
			2514	1587	435	477	15			
1	S	322	Total	C	N	O	S	0	0	0
			2542	1603	440	484	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
A	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
A	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
A	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
C	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
C	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
C	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
C	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
G	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
G	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
G	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
G	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
M	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
M	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
M	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
M	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
O	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6

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Chain	Residue	Modelled	Actual	Comment	Reference
O	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
O	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
O	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
S	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
S	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
S	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
S	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1393	866	239	280	8			
2	D	172	Total	C	N	O	S	0	0	0
			1393	866	239	280	8			
2	N	169	Total	C	N	O	S	0	0	0
			1363	846	233	276	8			
2	P	172	Total	C	N	O	S	0	0	0
			1393	866	239	280	8			
2	I	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	U	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
B	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
B	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
B	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
B	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
B	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
B	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
D	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
D	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
D	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
D	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
D	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
D	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
D	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
N	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6

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Chain	Residue	Modelled	Actual	Comment	Reference
N	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
N	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
N	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
N	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
N	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
N	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
P	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
P	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
P	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
P	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
P	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
P	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
P	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
I	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
I	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
I	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
I	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
I	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
I	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
I	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
U	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
U	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
U	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
U	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
U	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
U	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
U	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6

- Molecule 3 is a protein called H5M9 antibody, light chain (kappa).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1666	1032	289	339	6			
3	E	216	Total	C	N	O	S	0	0	0
			1672	1035	290	341	6			
3	J	211	Total	C	N	O	S	0	0	0
			1634	1015	280	333	6			
3	X	216	Total	C	N	O	S	0	0	0
			1672	1035	290	341	6			
3	Q	215	Total	C	N	O	S	0	0	0
			1665	1031	289	339	6			
3	V	214	Total	C	N	O	S	0	0	0
			1655	1026	285	338	6			

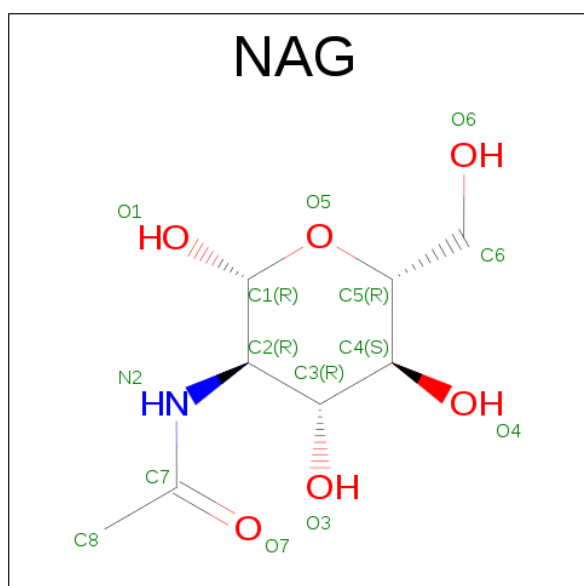
- Molecule 4 is a protein called H5M9 antibody, heavy chain (IgG1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	221	Total	C	N	O	S	0	0	0
			1675	1059	276	331	9			
4	F	221	Total	C	N	O	S	0	0	0
			1675	1059	276	331	9			
4	K	221	Total	C	N	O	S	0	0	0
			1674	1057	276	332	9			
4	T	220	Total	C	N	O	S	0	0	0
			1666	1054	274	329	9			
4	R	221	Total	C	N	O	S	0	0	0
			1675	1059	276	331	9			
4	W	221	Total	C	N	O	S	0	0	0
			1675	1059	276	331	9			

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	S	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	2	Total	C	N	O	0	0
			28	16	2	10		
8	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	G	3	Total	C	N	O	0	0
			39	22	2	15		

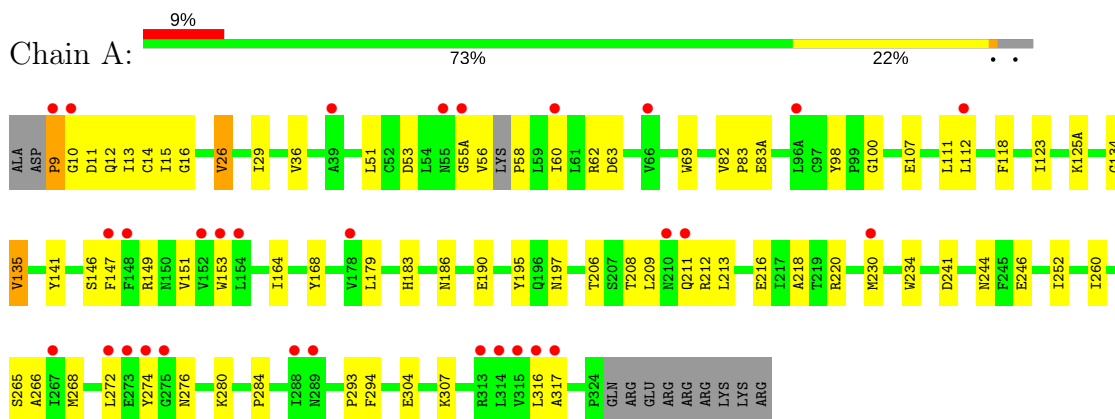
- Molecule 10 is a polymer of unknown type called SUGAR (4-MER).

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

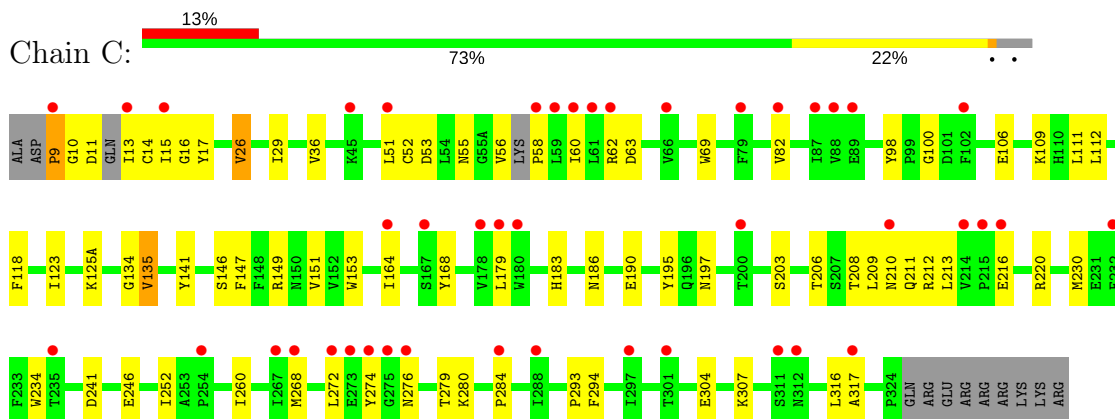
3 Residue-property plots

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

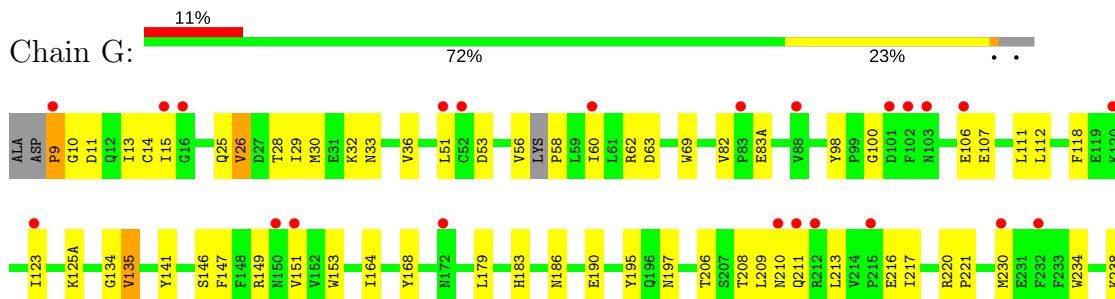
• Molecule 1: Hemagglutinin HA1 chain

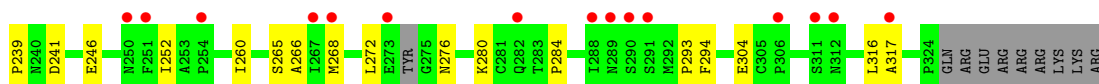


• Molecule 1: Hemagglutinin HA1 chain

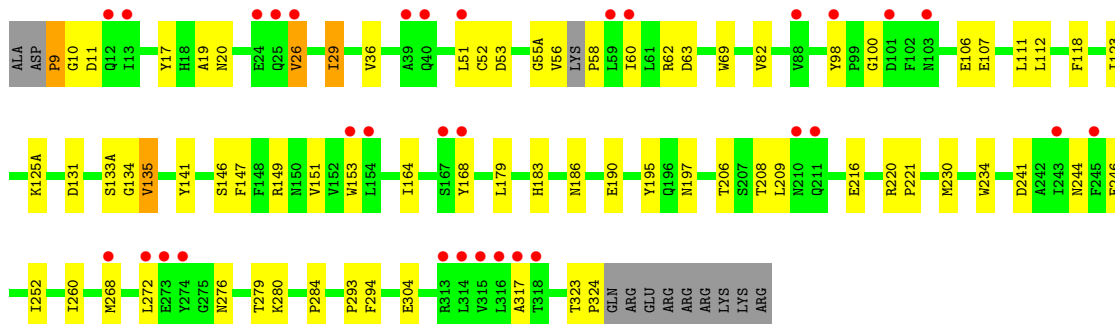
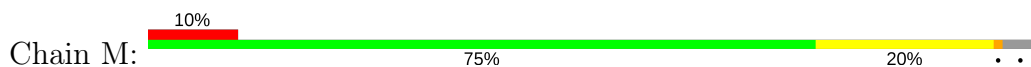


• Molecule 1: Hemagglutinin HA1 chain

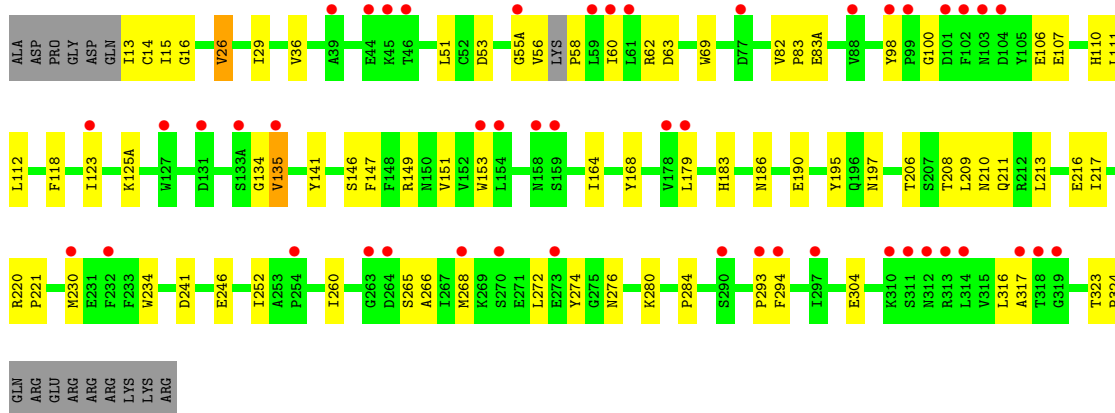




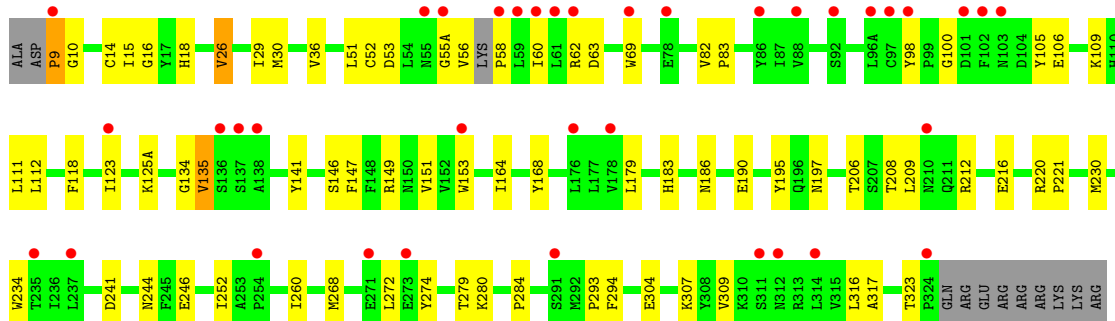
• Molecule 1: Hemagglutinin HA1 chain



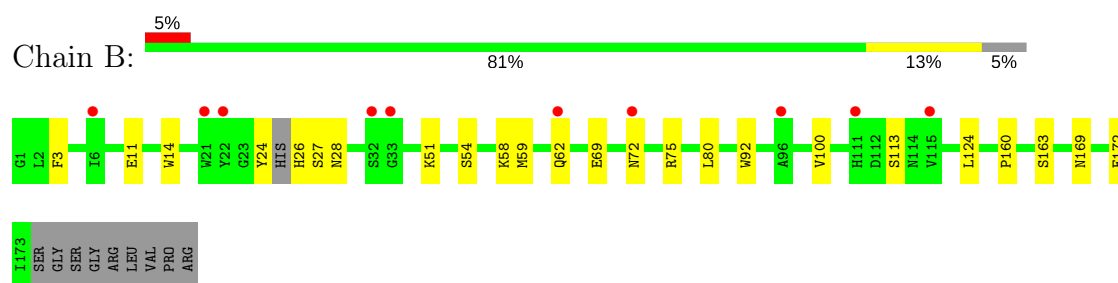
• Molecule 1: Hemagglutinin HA1 chain



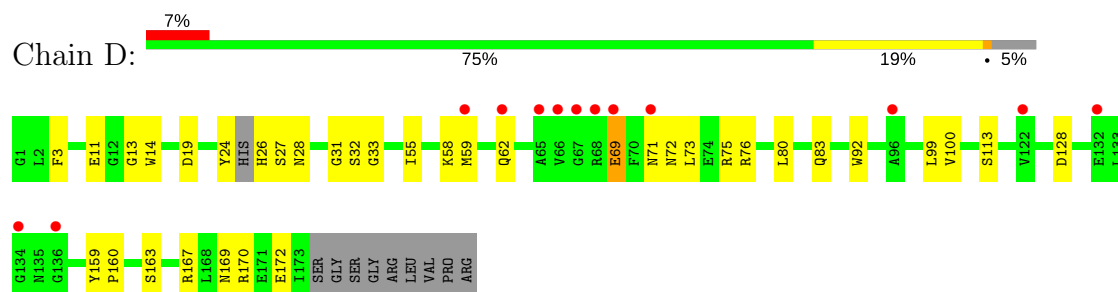
• Molecule 1: Hemagglutinin HA1 chain



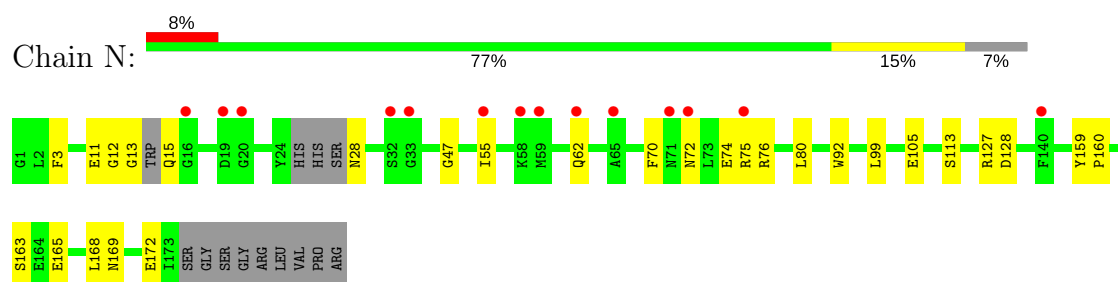
• Molecule 2: Hemagglutinin HA2 chain



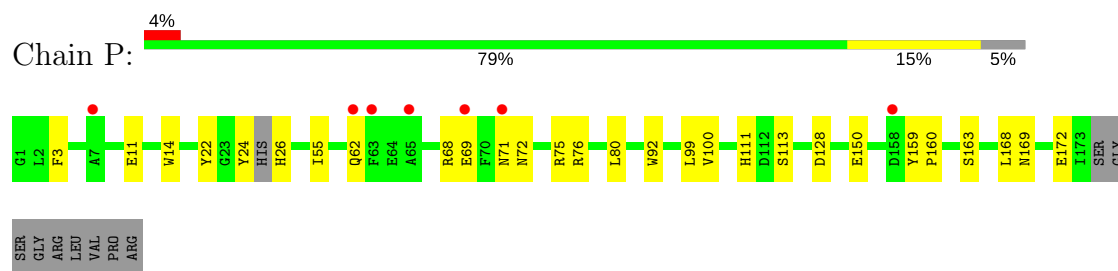
- Molecule 2: Hemagglutinin HA2 chain



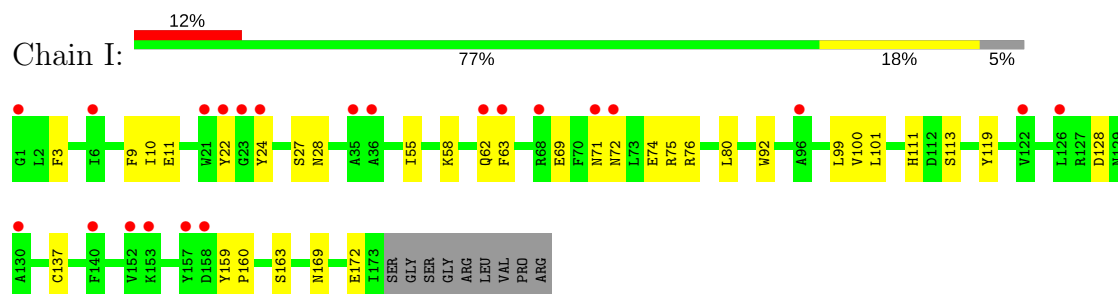
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain

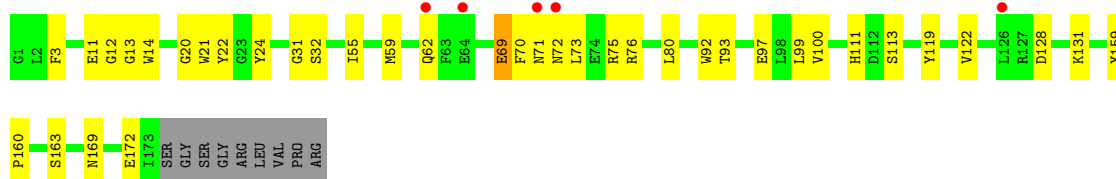


- Molecule 2: Hemagglutinin HA2 chain



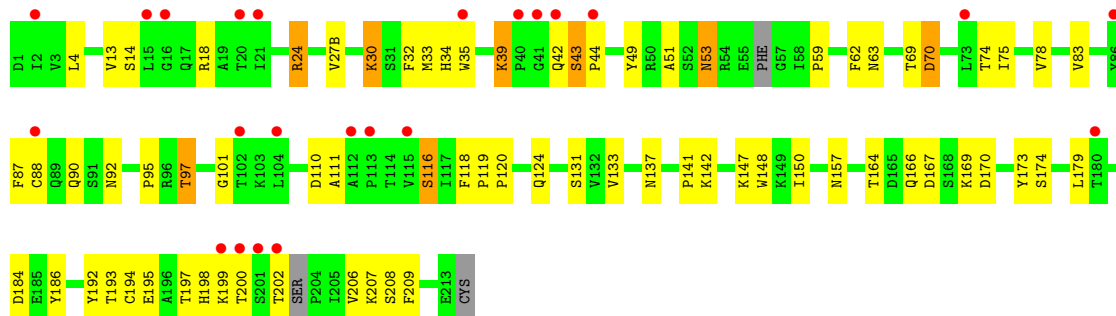
- Molecule 2: Hemagglutinin HA2 chain

Chain U: 3% 74% 20% 5%



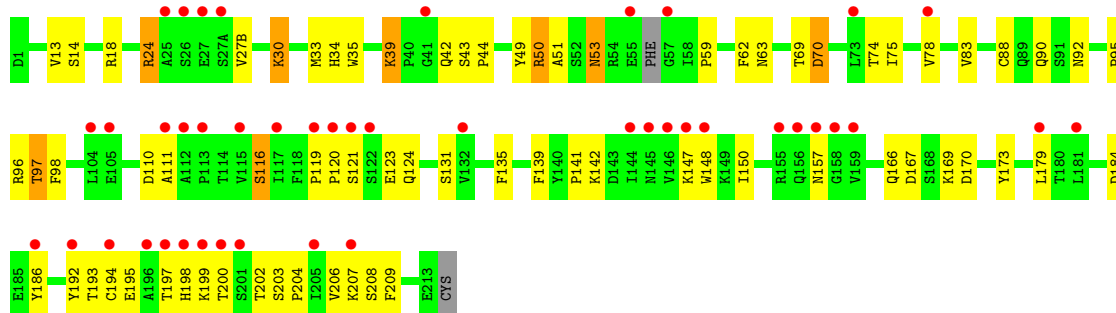
• Molecule 3: H5M9 antibody, light chain (kappa)

Chain L: 11% 65% 30%



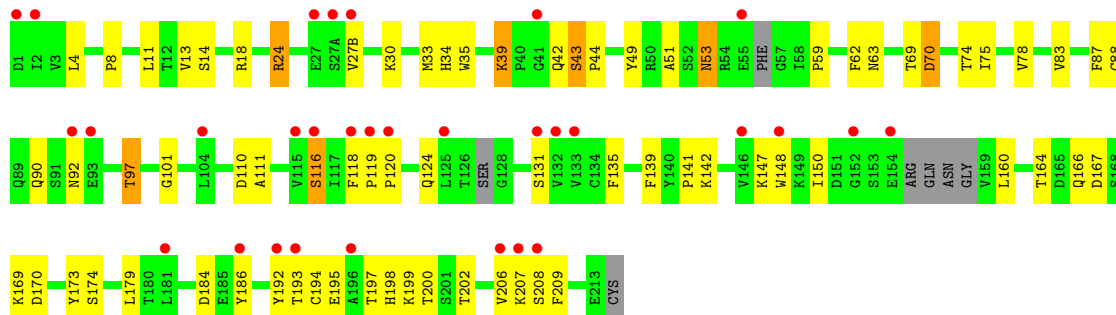
• Molecule 3: H5M9 antibody, light chain (kappa)

Chain E: 20% 66% 30%

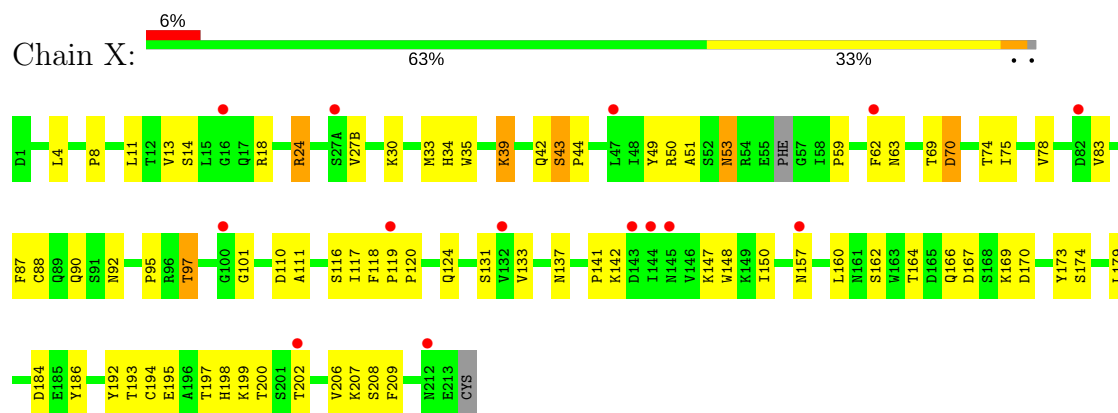


• Molecule 3: H5M9 antibody, light chain (kappa)

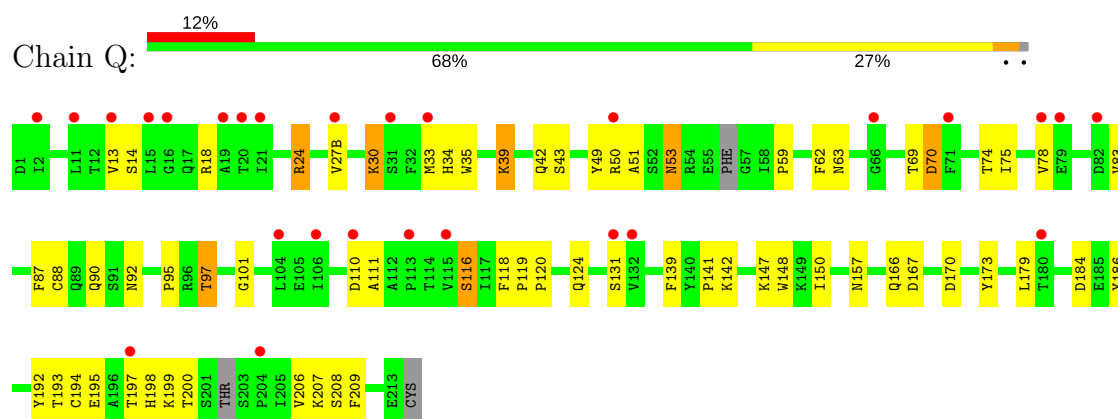
Chain J: 14% 63% 30%



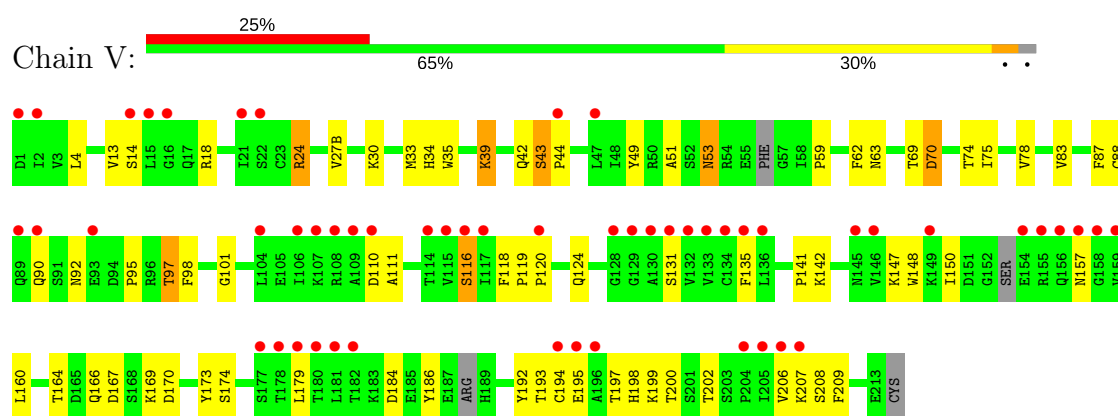
• Molecule 3: H5M9 antibody, light chain (kappa)



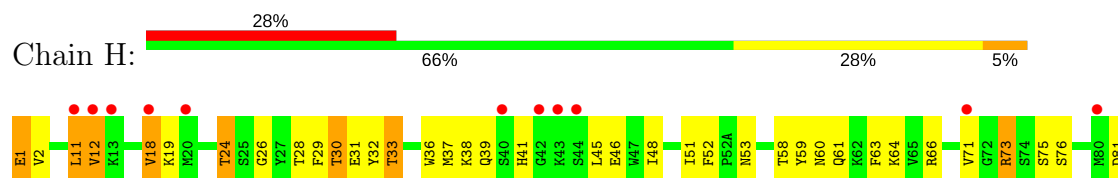
• Molecule 3: H5M9 antibody, light chain (kappa)

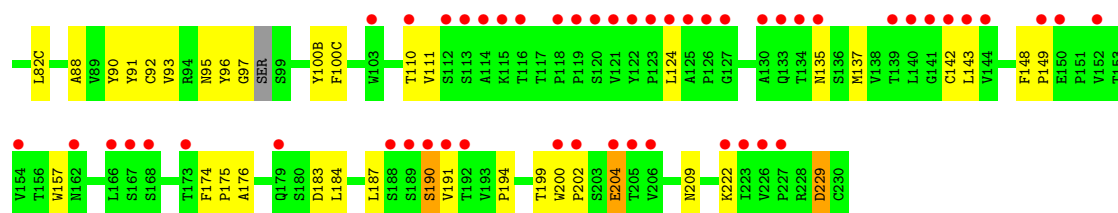


• Molecule 3: H5M9 antibody, light chain (kappa)

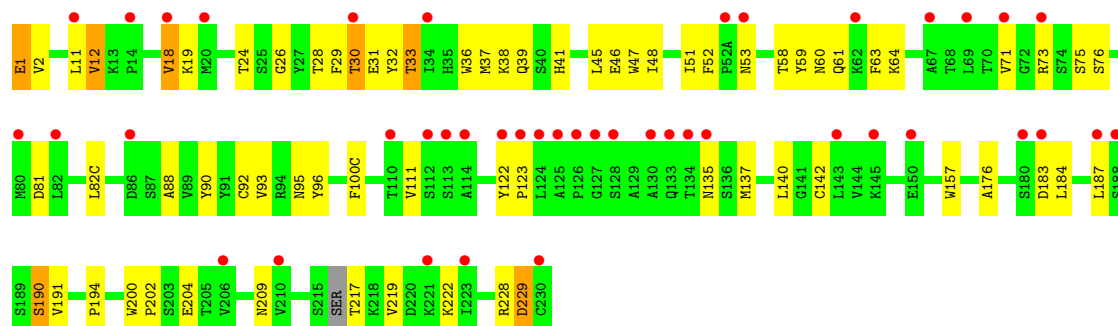


• Molecule 4: H5M9 antibody, heavy chain (IgG1)

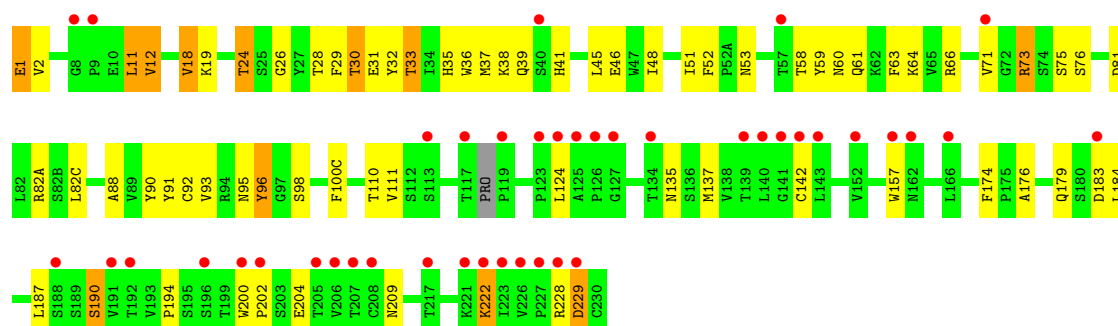




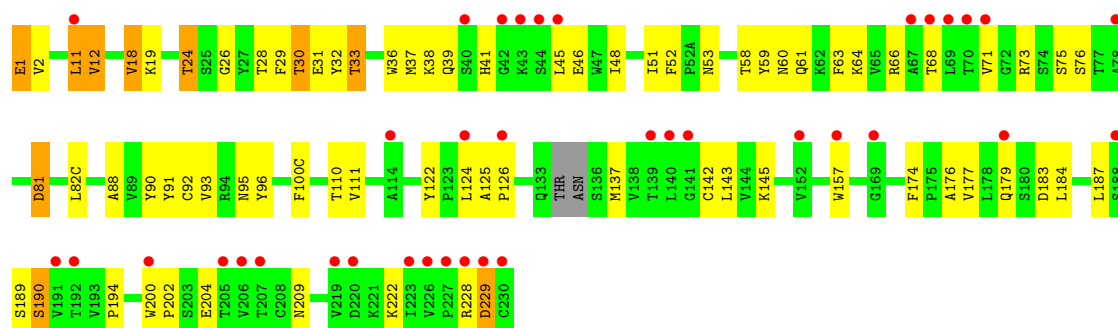
• Molecule 4: H5M9 antibody, heavy chain (IgG1)



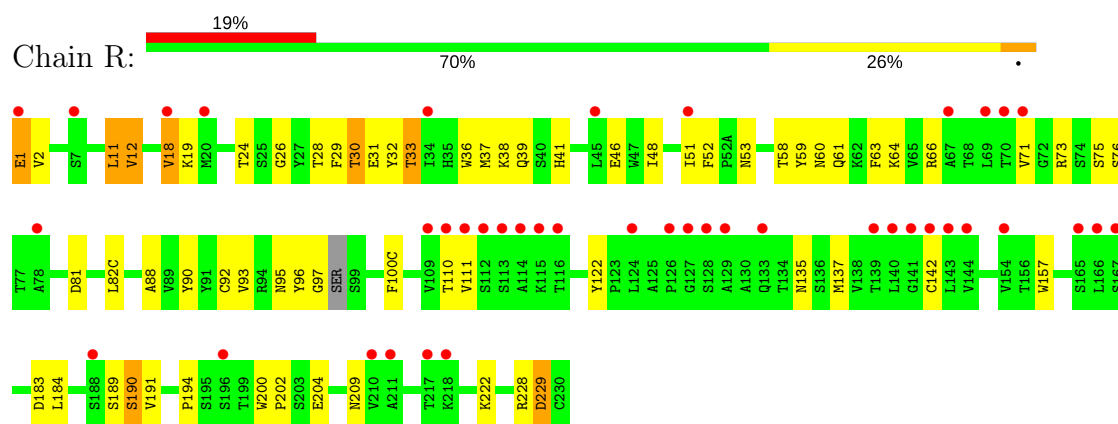
• Molecule 4: H5M9 antibody, heavy chain (IgG1)



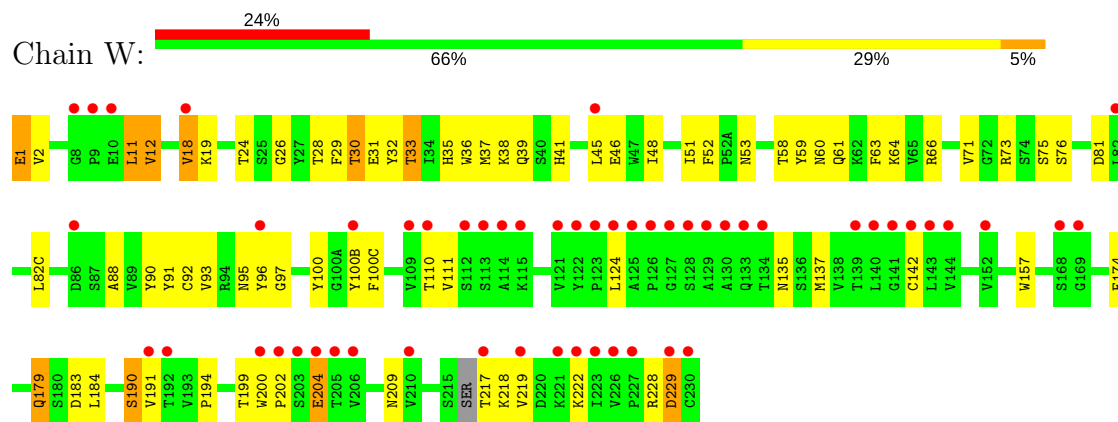
• Molecule 4: H5M9 antibody, heavy chain (IgG1)



• Molecule 4: H5M9 antibody, heavy chain (IgG1)



• Molecule 4: H5M9 antibody, heavy chain (IgG1)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.55Å 199.55Å 466.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.08 – 6.98 50.03 – 6.98	Depositor EDS
% Data completeness (in resolution range)	92.7 (50.08-6.98) 93.0 (50.03-6.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 6.68Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.377 , 0.387 0.368 , 0.364	Depositor DCC
R_{free} test set	843 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	375.9	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 214.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	43995	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/2606	0.67	1/3542 (0.0%)
1	C	0.47	0/2596	0.67	1/3527 (0.0%)
1	G	0.47	0/2592	0.67	1/3521 (0.0%)
1	M	0.47	0/2606	0.67	1/3542 (0.0%)
1	O	0.46	0/2577	0.66	0/3503
1	S	0.47	0/2606	0.67	1/3542 (0.0%)
2	B	0.50	0/1418	0.65	0/1906
2	D	0.50	0/1418	0.65	0/1906
2	I	0.49	0/1430	0.65	0/1924
2	N	0.50	0/1384	0.65	0/1857
2	P	0.50	0/1418	0.65	0/1906
2	U	0.50	0/1430	0.65	0/1924
3	E	0.64	0/1707	0.74	0/2313
3	J	0.64	0/1667	0.75	0/2257
3	L	0.65	0/1700	0.74	0/2301
3	Q	0.65	0/1699	0.74	0/2300
3	V	0.64	0/1688	0.74	0/2285
3	X	0.64	0/1707	0.74	0/2313
4	F	0.62	0/1720	0.77	0/2350
4	H	0.62	0/1720	0.77	0/2350
4	K	0.62	0/1718	0.77	0/2345
4	R	0.62	0/1720	0.77	0/2350
4	T	0.61	0/1711	0.77	0/2337
4	W	0.62	0/1720	0.77	0/2350
All	All	0.55	0/44558	0.71	5/60451 (0.0%)

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
3	E	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	PRO	CA-N-CD	-8.46	99.65	111.50
1	C	9	PRO	CA-N-CD	-8.46	99.66	111.50
1	G	9	PRO	CA-N-CD	-8.46	99.66	111.50
1	M	9	PRO	CA-N-CD	-8.44	99.68	111.50
1	S	9	PRO	CA-N-CD	-8.44	99.68	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	50	ARG	Sidechain

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	2542	0	2464	74	0
1	C	2533	0	2455	75	0
1	G	2530	0	2453	71	0
1	M	2542	0	2464	78	0
1	O	2514	0	2440	76	0
1	S	2542	0	2463	73	0
2	B	1393	0	1295	24	0
2	D	1393	0	1295	55	0
2	I	1403	0	1302	36	0
2	N	1363	0	1272	54	0
2	P	1393	0	1294	35	0
2	U	1403	0	1302	46	0
3	E	1672	0	1597	57	0
3	J	1634	0	1560	77	0
3	L	1666	0	1592	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1665	0	1589	57	0
3	V	1655	0	1577	76	0
3	X	1672	0	1597	77	0
4	F	1675	0	1626	61	0
4	H	1675	0	1626	75	0
4	K	1674	0	1625	79	0
4	R	1675	0	1626	60	0
4	T	1666	0	1618	79	0
4	W	1675	0	1626	100	0
5	A	39	0	34	1	0
5	O	39	0	34	2	0
5	S	39	0	34	2	0
6	A	14	0	13	0	0
6	C	14	0	13	0	0
6	M	14	0	13	0	0
6	O	14	0	13	0	0
6	P	14	0	13	2	0
6	S	14	0	13	0	0
7	C	94	0	79	0	0
8	G	28	0	25	1	0
8	M	28	0	25	1	0
9	G	39	0	34	3	0
10	O	50	0	43	0	0
All	All	43995	0	42144	1209	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 14.

All (1209) 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)
4:H:31:GLU:HG3	4:H:32:TYR:CD1	1.57	1.40
4:K:31:GLU:HG3	4:K:32:TYR:CD1	1.57	1.39
4:W:31:GLU:HG3	4:W:32:TYR:CD1	1.57	1.39
3:V:164:THR:HG23	4:W:174:PHE:CD1	1.59	1.38
4:R:31:GLU:HG3	4:R:32:TYR:CD1	1.57	1.38
4:F:31:GLU:HG3	4:F:32:TYR:CD1	1.57	1.37
4:T:31:GLU:HG3	4:T:32:TYR:CD1	1.57	1.37
4:R:31:GLU:HG3	4:R:32:TYR:CE1	1.79	1.17
1:O:274:TYR:CE2	4:R:97:GLY:HA2	1.81	1.16
4:F:31:GLU:HG3	4:F:32:TYR:CE1	1.79	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:31:GLU:HG3	4:W:32:TYR:CE1	1.79	1.16
4:H:31:GLU:HG3	4:H:32:TYR:CE1	1.79	1.15
4:T:31:GLU:HG3	4:T:32:TYR:CE1	1.79	1.15
4:K:31:GLU:HG3	4:K:32:TYR:CE1	1.79	1.15
1:G:316:LEU:HD21	2:I:100:VAL:HG22	1.29	1.14
3:J:164:THR:HG23	4:K:174:PHE:CD1	1.83	1.12
3:V:43:SER:HB3	4:W:91:TYR:CE1	1.84	1.11
3:X:117:ILE:HG22	3:X:207:LYS:HG3	1.29	1.11
2:D:76:ARG:NH2	2:I:74:GLU:OE2	1.89	1.06
4:W:31:GLU:CG	4:W:32:TYR:CE1	2.39	1.05
4:T:31:GLU:CG	4:T:32:TYR:CE1	2.39	1.05
4:H:31:GLU:CG	4:H:32:TYR:CE1	2.39	1.05
4:R:31:GLU:CG	4:R:32:TYR:CE1	2.39	1.05
4:F:31:GLU:CG	4:F:32:TYR:CE1	2.39	1.04
4:K:31:GLU:CG	4:K:32:TYR:CE1	2.39	1.04
4:K:31:GLU:CD	4:K:32:TYR:CE1	2.32	1.04
1:G:9:PRO:HD2	1:G:10:GLY:H	1.23	1.03
4:W:31:GLU:CD	4:W:32:TYR:CE1	2.32	1.03
1:S:9:PRO:HD2	1:S:10:GLY:H	1.23	1.03
4:F:31:GLU:CD	4:F:32:TYR:CE1	2.32	1.03
4:H:31:GLU:CD	4:H:32:TYR:CE1	2.32	1.03
4:R:31:GLU:CD	4:R:32:TYR:CE1	2.32	1.03
4:T:31:GLU:CD	4:T:32:TYR:CE1	2.32	1.03
1:C:9:PRO:HD2	1:C:10:GLY:H	1.23	1.02
1:O:274:TYR:HE2	4:R:97:GLY:HA2	1.13	1.01
4:T:68:THR:HB	4:T:81:ASP:OD2	1.61	1.01
4:K:31:GLU:CG	4:K:32:TYR:CD1	2.44	1.00
4:W:31:GLU:CG	4:W:32:TYR:CD1	2.44	1.00
4:F:31:GLU:CG	4:F:32:TYR:CD1	2.44	1.00
1:M:9:PRO:HD2	1:M:10:GLY:H	1.23	1.00
4:R:31:GLU:CG	4:R:32:TYR:CD1	2.44	1.00
4:H:31:GLU:CG	4:H:32:TYR:CD1	2.44	1.00
4:T:31:GLU:CG	4:T:32:TYR:CD1	2.44	0.99
4:W:33:THR:HB	4:W:52:PHE:CD1	1.96	0.99
4:R:31:GLU:OE2	4:R:32:TYR:HE1	1.47	0.98
1:A:9:PRO:HD2	1:A:10:GLY:H	1.23	0.98
4:F:31:GLU:OE2	4:F:32:TYR:HE1	1.47	0.98
3:V:164:THR:CG2	4:W:174:PHE:CD1	2.46	0.97
4:K:31:GLU:OE2	4:K:32:TYR:HE1	1.47	0.97
4:W:31:GLU:OE2	4:W:32:TYR:HE1	1.47	0.97
4:T:31:GLU:OE2	4:T:32:TYR:HE1	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:31:GLU:OE2	4:H:32:TYR:HE1	1.47	0.97
1:G:316:LEU:CD2	2:I:100:VAL:HG22	1.94	0.97
2:D:167:ARG:HG2	2:D:170:ARG:NH2	1.80	0.96
1:O:274:TYR:OH	4:R:97:GLY:HA3	1.67	0.95
3:L:43:SER:HB3	4:H:91:TYR:CE1	2.01	0.95
2:N:168:LEU:HD12	2:N:169:ASN:N	1.81	0.94
3:Q:119:PRO:HB2	4:R:228:ARG:HH21	1.31	0.94
1:M:17:TYR:CE2	2:N:13:GLY:CA	2.50	0.94
2:N:76:ARG:HH12	2:P:68:ARG:HG2	1.32	0.93
1:S:274:TYR:HD2	4:W:31:GLU:O	1.51	0.93
1:M:276:ASN:ND2	4:T:52:PHE:CE1	2.38	0.92
3:V:164:THR:HG23	4:W:174:PHE:HD1	1.00	0.92
3:J:8:PRO:HB3	3:X:11:LEU:CD1	1.99	0.92
2:D:32:SER:O	4:W:217:THR:HG23	1.71	0.90
3:X:117:ILE:CG2	3:X:207:LYS:HG3	2.01	0.90
1:O:274:TYR:OH	4:R:97:GLY:CA	2.20	0.89
3:L:44:PRO:HG2	4:H:45:LEU:HD11	1.54	0.88
1:M:17:TYR:CZ	2:N:12:GLY:C	2.47	0.88
1:M:17:TYR:CE2	2:N:13:GLY:HA3	2.07	0.88
2:D:167:ARG:HG2	2:D:170:ARG:HH21	1.36	0.88
3:J:164:THR:HG23	4:K:174:PHE:HD1	1.36	0.88
2:N:76:ARG:NH1	2:P:68:ARG:HG2	1.91	0.86
1:M:9:PRO:HD2	1:M:10:GLY:N	1.91	0.85
1:G:9:PRO:HD2	1:G:10:GLY:N	1.91	0.85
1:S:9:PRO:HD2	1:S:10:GLY:N	1.91	0.85
3:V:174:SER:HB2	4:W:174:PHE:HE1	1.42	0.85
3:J:119:PRO:HB2	4:K:228:ARG:HH21	1.40	0.85
3:J:160:LEU:HD11	4:K:179:GLN:OE1	1.77	0.85
1:A:9:PRO:HD2	1:A:10:GLY:N	1.91	0.84
4:F:31:GLU:CD	4:F:32:TYR:HE1	1.78	0.84
2:U:32:SER:O	4:F:217:THR:HA	1.76	0.84
1:C:9:PRO:HD2	1:C:10:GLY:N	1.91	0.84
1:C:11:ASP:OD1	2:D:28:ASN:HA	1.77	0.84
3:X:117:ILE:HG22	3:X:207:LYS:CG	2.08	0.84
3:V:43:SER:HB3	4:W:91:TYR:HE1	1.34	0.84
3:V:119:PRO:HB2	4:W:228:ARG:HH21	1.44	0.83
4:H:31:GLU:CD	4:H:32:TYR:HE1	1.78	0.83
1:G:11:ASP:OD1	2:I:28:ASN:HA	1.78	0.83
4:W:31:GLU:CD	4:W:32:TYR:HE1	1.78	0.83
1:G:276:ASN:O	4:K:98:SER:HB3	1.78	0.82
3:V:160:LEU:HD21	4:W:179:GLN:HE21	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:160:LEU:HD11	4:T:179:GLN:OE1	1.79	0.82
1:A:83:PRO:CG	4:H:100(B):TYR:OH	2.28	0.82
3:J:43:SER:HB3	4:K:91:TYR:CE1	2.13	0.82
3:X:118:PHE:CD2	4:T:124:LEU:HB3	2.14	0.82
4:R:31:GLU:CD	4:R:32:TYR:HE1	1.78	0.81
1:A:274:TYR:OH	4:H:97:GLY:HA3	1.80	0.81
2:N:165:GLU:HA	2:N:168:LEU:CD2	2.10	0.81
1:A:274:TYR:OH	4:H:97:GLY:CA	2.29	0.81
1:M:17:TYR:CZ	2:N:13:GLY:N	2.48	0.81
3:X:160:LEU:HD11	4:T:179:GLN:CD	2.01	0.81
1:M:107:GLU:OE2	2:U:76:ARG:HG3	1.81	0.81
1:G:25:GLN:OE1	1:G:33:ASN:OD1	1.99	0.80
3:V:44:PRO:HG2	4:W:45:LEU:HD11	1.62	0.80
4:K:28:THR:O	4:K:31:GLU:HG2	1.83	0.79
1:O:274:TYR:CE2	4:R:97:GLY:CA	2.65	0.79
1:S:105:TYR:CZ	1:S:109:LYS:HE3	2.16	0.79
2:N:76:ARG:HG2	2:N:76:ARG:HH11	1.44	0.79
4:F:28:THR:O	4:F:31:GLU:HG2	1.83	0.79
3:J:118:PHE:CD2	4:K:124:LEU:HB3	2.17	0.78
4:T:28:THR:O	4:T:31:GLU:HG2	1.83	0.78
4:R:28:THR:O	4:R:31:GLU:HG2	1.83	0.78
1:S:83:PRO:CG	4:W:100(B):TYR:OH	2.32	0.78
3:V:174:SER:HB2	4:W:174:PHE:CE1	2.18	0.78
3:J:8:PRO:HB3	3:X:11:LEU:HD11	1.64	0.78
4:K:31:GLU:CD	4:K:32:TYR:HE1	1.78	0.78
1:M:118:PHE:HE1	1:M:260:ILE:HD13	1.49	0.78
4:W:28:THR:O	4:W:31:GLU:HG2	1.82	0.78
1:G:118:PHE:HE1	1:G:260:ILE:HD13	1.49	0.78
4:H:28:THR:O	4:H:31:GLU:HG2	1.83	0.78
1:M:206:THR:HB	1:M:209:LEU:HB3	1.66	0.78
1:G:206:THR:HB	1:G:209:LEU:HB3	1.66	0.77
1:S:15:ILE:HD11	2:U:122:VAL:HG21	1.66	0.77
1:M:17:TYR:OH	2:N:12:GLY:C	2.23	0.77
1:G:206:THR:HG22	1:G:208:THR:H	1.50	0.77
4:T:31:GLU:CD	4:T:32:TYR:HE1	1.78	0.77
1:G:316:LEU:HD23	2:I:100:VAL:HG13	1.65	0.77
1:A:206:THR:HG22	1:A:208:THR:H	1.50	0.77
3:J:120:PRO:HB3	3:J:131:SER:H	1.50	0.77
4:W:48:ILE:HA	4:W:63:PHE:HD2	1.49	0.77
1:M:206:THR:HG22	1:M:208:THR:H	1.50	0.77
1:O:118:PHE:HE1	1:O:260:ILE:HD13	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HB	1:A:209:LEU:HB3	1.66	0.77
4:H:48:ILE:HA	4:H:63:PHE:HD2	1.49	0.76
1:O:106:GLU:OE2	2:P:71:ASN:HB3	1.85	0.76
1:C:206:THR:HB	1:C:209:LEU:HB3	1.66	0.76
1:G:106:GLU:CD	2:I:71:ASN:HB3	2.05	0.76
3:L:120:PRO:HB3	3:L:131:SER:H	1.50	0.76
3:Q:120:PRO:HB3	3:Q:131:SER:H	1.50	0.76
1:S:206:THR:HG22	1:S:208:THR:H	1.50	0.76
1:O:206:THR:HG22	1:O:208:THR:H	1.50	0.76
4:T:48:ILE:HA	4:T:63:PHE:HD2	1.50	0.76
4:F:48:ILE:HA	4:F:63:PHE:HD2	1.50	0.76
4:R:48:ILE:HA	4:R:63:PHE:HD2	1.49	0.76
3:X:120:PRO:HB3	3:X:131:SER:H	1.50	0.76
4:K:48:ILE:HA	4:K:63:PHE:HD2	1.49	0.76
1:O:206:THR:HB	1:O:209:LEU:HB3	1.66	0.76
1:S:206:THR:HB	1:S:209:LEU:HB3	1.66	0.76
1:O:316:LEU:HD21	2:P:100:VAL:HG22	1.69	0.75
1:S:118:PHE:HE1	1:S:260:ILE:HD13	1.49	0.75
1:A:118:PHE:HE1	1:A:260:ILE:HD13	1.49	0.75
1:A:11:ASP:OD1	2:B:28:ASN:HA	1.86	0.75
1:C:11:ASP:CG	2:D:28:ASN:HA	2.06	0.75
1:C:118:PHE:HE1	1:C:260:ILE:HD13	1.49	0.75
1:G:276:ASN:ND2	4:K:52:PHE:CE1	2.55	0.75
1:C:206:THR:HG22	1:C:208:THR:H	1.50	0.74
3:E:120:PRO:HB3	3:E:131:SER:H	1.50	0.74
3:L:137:ASN:ND2	4:H:174:PHE:HZ	1.85	0.74
3:V:120:PRO:HB3	3:V:131:SER:H	1.50	0.74
4:W:33:THR:HB	4:W:52:PHE:CE1	2.21	0.74
3:J:8:PRO:CB	3:X:11:LEU:HD12	2.17	0.74
1:M:276:ASN:HD21	4:T:31:GLU:C	1.91	0.74
1:O:216:GLU:O	1:O:220:ARG:NH2	2.21	0.74
1:C:16:GLY:N	2:D:14:TRP:CH2	2.56	0.74
1:M:216:GLU:O	1:M:220:ARG:NH2	2.21	0.73
1:M:11:ASP:CG	2:N:28:ASN:HA	2.09	0.73
1:G:276:ASN:O	4:K:98:SER:CB	2.36	0.73
1:A:56:VAL:HG21	3:L:30:LYS:NZ	2.03	0.73
2:D:76:ARG:NE	1:G:107:GLU:OE2	2.20	0.73
1:S:274:TYR:OH	4:W:97:GLY:HA2	1.88	0.73
2:N:74:GLU:OE2	2:U:76:ARG:NH2	2.21	0.73
1:G:216:GLU:O	1:G:220:ARG:NH2	2.21	0.73
1:O:13:ILE:HA	2:P:26:HIS:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:8:PRO:CB	3:X:11:LEU:CD1	2.67	0.73
1:S:83:PRO:CB	4:W:100(B):TYR:OH	2.36	0.72
1:A:216:GLU:O	1:A:220:ARG:NH2	2.21	0.72
1:C:15:ILE:C	2:D:14:TRP:CH2	2.63	0.72
1:M:17:TYR:CE1	2:N:12:GLY:O	2.43	0.72
2:N:165:GLU:HA	2:N:168:LEU:HD21	1.70	0.72
1:S:216:GLU:O	1:S:220:ARG:NH2	2.21	0.72
1:C:216:GLU:O	1:C:220:ARG:NH2	2.21	0.72
1:C:220:ARG:NE	1:G:210:ASN:OD1	2.22	0.72
3:V:160:LEU:HD11	4:W:179:GLN:HG2	1.73	0.71
2:D:80:LEU:HD11	2:I:80:LEU:HD22	1.72	0.71
1:A:274:TYR:CE2	4:H:97:GLY:HA2	2.26	0.71
1:G:106:GLU:OE2	2:I:71:ASN:HB3	1.91	0.71
1:M:9:PRO:CD	1:M:10:GLY:H	2.02	0.71
1:G:9:PRO:CD	1:G:10:GLY:H	2.02	0.70
1:S:307:LYS:HD3	2:U:59:MET:O	1.91	0.70
1:S:9:PRO:CD	1:S:10:GLY:H	2.02	0.70
1:S:55(A):GLY:HA2	4:W:100:TYR:HB2	1.74	0.70
1:S:106:GLU:OE2	2:U:71:ASN:HB3	1.91	0.70
1:O:274:TYR:CZ	4:R:97:GLY:CA	2.75	0.69
1:M:17:TYR:CD2	2:N:13:GLY:HA3	2.27	0.69
1:C:118:PHE:CE1	1:C:260:ILE:HD13	2.28	0.69
1:C:9:PRO:CD	1:C:10:GLY:H	2.02	0.69
4:K:31:GLU:OE2	4:K:32:TYR:CE1	2.36	0.69
1:M:62:ARG:HG2	1:M:63:ASP:N	2.08	0.69
4:T:31:GLU:OE2	4:T:32:TYR:CE1	2.36	0.69
3:V:43:SER:HA	4:W:91:TYR:OH	1.93	0.69
1:O:118:PHE:CE1	1:O:260:ILE:HD13	2.28	0.68
1:C:62:ARG:HG2	1:C:63:ASP:N	2.08	0.68
1:S:118:PHE:CE1	1:S:260:ILE:HD13	2.28	0.68
4:W:33:THR:HB	4:W:52:PHE:HD1	1.54	0.68
1:S:274:TYR:OH	4:W:97:GLY:CA	2.40	0.68
2:P:150:GLU:HB2	6:P:2001:NAG:H62	1.74	0.68
3:V:98:PHE:CD1	4:W:45:LEU:O	2.46	0.68
1:A:62:ARG:HG2	1:A:63:ASP:N	2.08	0.68
1:G:118:PHE:CE1	1:G:260:ILE:HD13	2.28	0.68
1:G:62:ARG:HG2	1:G:63:ASP:N	2.08	0.68
1:O:56:VAL:HG21	3:Q:30:LYS:NZ	2.08	0.68
1:M:118:PHE:CE1	1:M:260:ILE:HD13	2.28	0.68
1:O:62:ARG:HG2	1:O:63:ASP:N	2.08	0.68
1:S:62:ARG:HG2	1:S:63:ASP:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:OE2	2:I:76:ARG:NE	2.25	0.68
1:A:212:ARG:NH2	1:G:217:ILE:O	2.25	0.68
4:T:68:THR:CB	4:T:81:ASP:OD2	2.41	0.68
2:N:76:ARG:HG2	2:N:76:ARG:NH1	2.08	0.67
3:J:90:GLN:HE21	3:J:97:THR:CG2	2.08	0.67
1:O:15:ILE:C	2:P:14:TRP:CH2	2.67	0.67
3:Q:90:GLN:HE21	3:Q:97:THR:CG2	2.08	0.67
3:X:90:GLN:HE21	3:X:97:THR:CG2	2.08	0.67
1:A:118:PHE:CE1	1:A:260:ILE:HD13	2.28	0.67
3:E:90:GLN:HE21	3:E:97:THR:CG2	2.08	0.67
3:L:90:GLN:HE21	3:L:97:THR:CG2	2.08	0.67
3:V:90:GLN:HE21	3:V:97:THR:CG2	2.08	0.67
2:D:76:ARG:NH1	2:I:74:GLU:OE1	2.27	0.67
3:X:164:THR:HG23	4:T:174:PHE:CD1	2.30	0.67
1:A:83:PRO:HG3	4:H:100(B):TYR:OH	1.94	0.67
1:C:13:ILE:HA	2:D:26:HIS:HA	1.78	0.66
1:S:106:GLU:CD	2:U:71:ASN:HB3	2.16	0.66
1:M:107:GLU:OE2	2:U:76:ARG:CG	2.43	0.66
1:M:17:TYR:CZ	2:N:13:GLY:CA	2.78	0.65
1:A:244:ASN:ND2	1:G:221:PRO:HD3	2.12	0.65
3:X:133:VAL:HG21	4:T:143:LEU:HD13	1.78	0.65
1:M:9:PRO:CD	1:M:10:GLY:N	2.59	0.65
1:M:17:TYR:OH	2:N:12:GLY:CA	2.44	0.65
1:S:274:TYR:CD2	4:W:31:GLU:O	2.42	0.65
1:A:216:GLU:HB3	1:C:212:ARG:HB3	1.79	0.65
3:J:44:PRO:HG2	4:K:45:LEU:HD11	1.79	0.65
1:M:276:ASN:ND2	4:T:52:PHE:HE1	1.94	0.65
1:O:16:GLY:N	2:P:14:TRP:CH2	2.64	0.65
1:C:9:PRO:CD	1:C:10:GLY:N	2.59	0.64
1:O:106:GLU:CD	2:P:71:ASN:HB3	2.17	0.64
2:D:80:LEU:HD21	2:I:80:LEU:HD21	1.79	0.64
4:H:31:GLU:OE2	4:H:32:TYR:CE1	2.36	0.64
1:A:56:VAL:HG21	3:L:30:LYS:HZ2	1.61	0.64
1:G:123:ILE:HD11	1:G:168:TYR:CZ	2.33	0.64
4:K:12:VAL:HG21	4:K:82(C):LEU:HD13	1.80	0.64
1:M:123:ILE:HD11	1:M:168:TYR:CZ	2.33	0.64
4:W:31:GLU:OE2	4:W:32:TYR:CE1	2.36	0.64
1:A:123:ILE:HD11	1:A:168:TYR:CZ	2.33	0.64
4:W:12:VAL:HG21	4:W:82(C):LEU:HD13	1.80	0.64
4:T:12:VAL:HG21	4:T:82(C):LEU:HD13	1.80	0.64
3:E:63:ASN:HB3	3:E:74:THR:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:123:ILE:HD11	1:S:168:TYR:CZ	2.33	0.64
1:A:9:PRO:CD	1:A:10:GLY:N	2.59	0.64
3:V:160:LEU:CD1	4:W:179:GLN:HG2	2.27	0.64
1:C:123:ILE:HD11	1:C:168:TYR:CZ	2.33	0.64
4:H:12:VAL:HG21	4:H:82(C):LEU:HD13	1.80	0.63
1:M:17:TYR:CD2	2:N:13:GLY:CA	2.81	0.63
1:C:316:LEU:HD21	2:D:100:VAL:HG22	1.79	0.63
3:J:43:SER:HB3	4:K:91:TYR:HE1	1.63	0.63
3:J:119:PRO:HB2	4:K:228:ARG:NH2	2.13	0.63
3:V:164:THR:CG2	4:W:174:PHE:HD1	1.94	0.63
1:A:218:ALA:HB2	1:C:203:SER:HB2	1.80	0.63
1:O:123:ILE:HD11	1:O:168:TYR:CZ	2.33	0.63
3:J:119:PRO:CB	4:K:228:ARG:HH21	2.11	0.63
4:W:18:VAL:HG22	4:W:82(C):LEU:HD11	1.81	0.63
4:F:18:VAL:HG22	4:F:82(C):LEU:HD11	1.81	0.63
1:G:9:PRO:CD	1:G:10:GLY:N	2.59	0.63
4:R:18:VAL:HG22	4:R:82(C):LEU:HD11	1.81	0.63
1:A:12:GLN:O	2:B:27:SER:N	2.32	0.63
4:H:18:VAL:HG22	4:H:82(C):LEU:HD11	1.81	0.63
1:A:274:TYR:HE2	4:H:97:GLY:HA2	1.63	0.63
4:F:12:VAL:HG21	4:F:82(C):LEU:HD13	1.80	0.62
2:N:80:LEU:HD22	2:U:80:LEU:HD11	1.81	0.62
3:L:63:ASN:HB3	3:L:74:THR:HB	1.80	0.62
4:R:12:VAL:HG21	4:R:82(C):LEU:HD13	1.80	0.62
3:V:174:SER:CB	4:W:174:PHE:CE1	2.81	0.62
3:X:63:ASN:HB3	3:X:74:THR:HB	1.80	0.62
1:O:55(A):GLY:O	3:Q:50:ARG:NH2	2.33	0.62
3:Q:63:ASN:HB3	3:Q:74:THR:HB	1.80	0.62
4:T:18:VAL:HG22	4:T:82(C):LEU:HD11	1.81	0.62
1:S:9:PRO:CD	1:S:10:GLY:N	2.59	0.62
3:L:118:PHE:CD2	4:H:124:LEU:HB3	2.35	0.62
3:V:63:ASN:HB3	3:V:74:THR:HB	1.80	0.62
3:J:63:ASN:HB3	3:J:74:THR:HB	1.80	0.62
1:C:276:ASN:HD21	4:F:32:TYR:HA	1.64	0.62
3:Q:119:PRO:HB2	4:R:228:ARG:NH2	2.11	0.62
1:S:323:THR:HG21	2:U:12:GLY:HA2	1.82	0.62
4:K:18:VAL:HG22	4:K:82(C):LEU:HD11	1.81	0.61
3:L:137:ASN:HD21	4:H:174:PHE:HZ	1.48	0.61
1:M:17:TYR:CE2	2:N:13:GLY:N	2.68	0.61
2:D:80:LEU:HD21	2:I:80:LEU:CD2	2.30	0.61
1:O:274:TYR:CZ	4:R:97:GLY:HA2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:293:PRO:HG2	1:M:294:PHE:HD1	1.66	0.61
1:A:16:GLY:N	2:B:14:TRP:CH2	2.68	0.61
1:C:293:PRO:HG2	1:C:294:PHE:HD1	1.66	0.61
2:D:32:SER:O	4:W:217:THR:CG2	2.46	0.61
1:O:293:PRO:HG2	1:O:294:PHE:HD1	1.66	0.61
1:G:293:PRO:HG2	1:G:294:PHE:HD1	1.66	0.61
3:L:174:SER:CB	4:H:174:PHE:HE1	2.14	0.61
4:K:200:TRP:CD1	4:K:202:PRO:HA	2.36	0.61
1:O:276:ASN:OD1	4:R:33:THR:HG22	1.99	0.61
4:R:200:TRP:CD1	4:R:202:PRO:HA	2.36	0.61
2:P:80:LEU:HD21	2:U:80:LEU:CD2	2.31	0.61
4:W:48:ILE:HA	4:W:63:PHE:CD2	2.35	0.61
1:S:83:PRO:HB2	4:W:100(B):TYR:OH	2.00	0.60
1:M:186:ASN:ND2	1:M:190:GLU:OE1	2.33	0.60
1:A:293:PRO:HG2	1:A:294:PHE:HD1	1.66	0.60
4:H:200:TRP:CD1	4:H:202:PRO:HA	2.36	0.60
3:J:174:SER:HB2	4:K:174:PHE:CE1	2.36	0.60
3:J:164:THR:CG2	4:K:174:PHE:CD1	2.74	0.60
1:O:217:ILE:O	1:S:212:ARG:NH2	2.31	0.60
1:O:83:PRO:HB3	3:Q:49:TYR:CE2	2.36	0.60
4:K:48:ILE:HA	4:K:63:PHE:CD2	2.35	0.60
2:N:168:LEU:C	2:N:168:LEU:HD12	2.20	0.60
1:O:56:VAL:CG2	3:Q:30:LYS:NZ	2.64	0.60
4:T:200:TRP:CD1	4:T:202:PRO:HA	2.36	0.60
1:A:268:MET:HG3	1:A:284:PRO:HG3	1.84	0.60
3:L:164:THR:HG23	4:H:174:PHE:HD1	1.66	0.60
4:T:48:ILE:HA	4:T:63:PHE:CD2	2.36	0.60
4:W:200:TRP:CD1	4:W:202:PRO:HA	2.36	0.60
3:L:164:THR:HG23	4:H:174:PHE:CD1	2.37	0.60
1:O:14:CYS:O	2:P:24:TYR:HA	2.02	0.60
1:C:268:MET:HG3	1:C:284:PRO:HG3	1.84	0.60
1:A:83(A):GLU:N	3:L:49:TYR:OH	2.28	0.59
3:X:124:GLN:HB2	4:T:122:TYR:CE1	2.37	0.59
3:X:44:PRO:HG2	4:T:45:LEU:HD11	1.84	0.59
3:E:90:GLN:HE21	3:E:97:THR:HG23	1.68	0.59
4:K:1:GLU:O	4:K:26:GLY:HA3	2.03	0.59
3:Q:90:GLN:HE21	3:Q:97:THR:HG23	1.68	0.59
1:S:268:MET:HG3	1:S:284:PRO:HG3	1.84	0.59
1:S:293:PRO:HG2	1:S:294:PHE:HD1	1.66	0.59
4:T:39:GLN:O	4:T:88:ALA:HB1	2.03	0.59
3:V:174:SER:CB	4:W:174:PHE:HE1	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASN:ND2	1:A:190:GLU:OE1	2.33	0.59
3:X:90:GLN:HE21	3:X:97:THR:HG23	1.68	0.59
4:K:19:LYS:NZ	4:K:81:ASP:HB2	2.18	0.59
1:G:268:MET:HG3	1:G:284:PRO:HG3	1.84	0.59
3:J:160:LEU:CD1	4:K:179:GLN:OE1	2.49	0.59
3:X:119:PRO:HB2	4:T:228:ARG:HH21	1.68	0.59
3:E:123:GLU:OE1	4:F:123:PRO:CD	2.51	0.59
1:G:32:LYS:HG2	9:G:2003:NAG:H81	1.85	0.59
2:U:72:ASN:OD1	2:U:75:ARG:NH2	2.36	0.59
3:V:43:SER:CB	4:W:91:TYR:CE1	2.75	0.59
3:J:174:SER:HB2	4:K:174:PHE:HE1	1.68	0.59
4:R:39:GLN:O	4:R:88:ALA:HB1	2.03	0.59
4:W:1:GLU:O	4:W:26:GLY:HA3	2.02	0.59
4:R:19:LYS:NZ	4:R:81:ASP:HB2	2.18	0.59
4:H:19:LYS:NZ	4:H:81:ASP:HB2	2.18	0.59
4:K:200:TRP:CG	4:K:202:PRO:HA	2.38	0.59
4:K:39:GLN:O	4:K:88:ALA:HB1	2.03	0.59
1:O:83:PRO:HB3	3:Q:49:TYR:HE2	1.66	0.59
2:D:72:ASN:OD1	2:D:75:ARG:NH2	2.36	0.58
1:M:268:MET:HG3	1:M:284:PRO:HG3	1.84	0.58
2:N:72:ASN:OD1	2:N:75:ARG:NH2	2.36	0.58
4:F:1:GLU:O	4:F:26:GLY:HA3	2.03	0.58
4:F:200:TRP:CD1	4:F:202:PRO:HA	2.36	0.58
4:F:19:LYS:NZ	4:F:81:ASP:HB2	2.18	0.58
1:O:268:MET:HG3	1:O:284:PRO:HG3	1.84	0.58
4:R:1:GLU:O	4:R:26:GLY:HA3	2.02	0.58
4:H:39:GLN:O	4:H:88:ALA:HB1	2.03	0.58
3:V:164:THR:HG23	4:W:174:PHE:CE1	2.31	0.58
3:L:90:GLN:HE21	3:L:97:THR:HG23	1.68	0.58
4:W:200:TRP:CG	4:W:202:PRO:HA	2.38	0.58
4:W:19:LYS:NZ	4:W:81:ASP:HB2	2.18	0.58
3:X:160:LEU:CD1	4:T:179:GLN:CD	2.70	0.58
4:F:39:GLN:O	4:F:88:ALA:HB1	2.03	0.58
4:H:200:TRP:CG	4:H:202:PRO:HA	2.39	0.58
2:I:72:ASN:OD1	2:I:75:ARG:NH2	2.36	0.58
3:J:90:GLN:HE21	3:J:97:THR:HG23	1.68	0.58
2:P:72:ASN:OD1	2:P:75:ARG:NH2	2.36	0.58
3:V:174:SER:HB3	4:W:174:PHE:CZ	2.39	0.58
4:H:1:GLU:O	4:H:26:GLY:HA3	2.02	0.58
3:Q:124:GLN:HG3	4:R:122:TYR:CE2	2.39	0.58
4:R:200:TRP:CG	4:R:202:PRO:HA	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:107:GLU:OE1	2:U:75:ARG:HB2	2.03	0.58
4:K:190:SER:OG	4:K:190:SER:O	2.22	0.58
4:R:48:ILE:HA	4:R:63:PHE:CD2	2.36	0.58
3:V:90:GLN:HE21	3:V:97:THR:HG23	1.68	0.58
4:F:31:GLU:OE2	4:F:32:TYR:CE1	2.36	0.58
4:R:31:GLU:OE2	4:R:32:TYR:CE1	2.36	0.58
4:T:1:GLU:O	4:T:26:GLY:HA3	2.03	0.58
4:W:190:SER:O	4:W:190:SER:OG	2.22	0.58
1:A:9:PRO:CD	1:A:10:GLY:H	2.02	0.58
1:M:276:ASN:OD1	4:T:32:TYR:HA	2.02	0.58
3:V:118:PHE:CD2	4:W:124:LEU:HB3	2.39	0.58
3:V:135:PHE:CZ	4:W:124:LEU:HD13	2.39	0.58
1:A:316:LEU:HD21	2:B:100:VAL:HG22	1.86	0.57
1:C:62:ARG:HG2	1:C:63:ASP:H	1.70	0.57
2:D:33:GLY:HA2	4:W:217:THR:HA	1.85	0.57
4:F:190:SER:O	4:F:190:SER:OG	2.21	0.57
1:G:186:ASN:ND2	1:G:190:GLU:OE1	2.33	0.57
4:T:200:TRP:CG	4:T:202:PRO:HA	2.38	0.57
4:W:39:GLN:O	4:W:88:ALA:HB1	2.03	0.57
4:F:48:ILE:HA	4:F:63:PHE:CD2	2.36	0.57
1:M:11:ASP:CB	2:N:28:ASN:HA	2.34	0.57
4:F:200:TRP:CG	4:F:202:PRO:HA	2.38	0.57
4:R:59:TYR:HD2	4:R:64:LYS:HD3	1.70	0.57
1:S:307:LYS:NZ	2:U:59:MET:HB2	2.19	0.57
3:V:98:PHE:CD2	4:W:45:LEU:HB2	2.39	0.57
1:G:62:ARG:HG2	1:G:63:ASP:H	1.70	0.57
4:R:157:TRP:HE1	4:R:189:SER:HG	1.52	0.57
3:E:116:SER:HA	3:E:207:LYS:HD2	1.87	0.57
4:H:48:ILE:HA	4:H:63:PHE:CD2	2.36	0.57
2:D:76:ARG:HH12	2:I:74:GLU:CD	2.08	0.57
3:V:116:SER:HA	3:V:207:LYS:HD2	1.87	0.57
3:L:43:SER:HB3	4:H:91:TYR:HE1	1.66	0.57
1:O:186:ASN:ND2	1:O:190:GLU:OE1	2.33	0.57
2:B:72:ASN:OD1	2:B:75:ARG:NH2	2.36	0.57
3:L:116:SER:HA	3:L:207:LYS:HD2	1.87	0.57
3:Q:116:SER:HA	3:Q:207:LYS:HD2	1.87	0.57
3:X:174:SER:CB	4:T:174:PHE:HE1	2.17	0.57
2:P:80:LEU:HD21	2:U:80:LEU:HD21	1.86	0.57
4:H:59:TYR:HD2	4:H:64:LYS:HD3	1.70	0.57
3:V:119:PRO:CB	4:W:228:ARG:HH21	2.16	0.56
1:A:83:PRO:HB3	3:L:49:TYR:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:192:TYR:HB2	3:E:209:PHE:CE1	2.41	0.56
2:B:80:LEU:HD22	2:I:80:LEU:HD11	1.88	0.56
1:O:62:ARG:HG2	1:O:63:ASP:H	1.70	0.56
1:A:83:PRO:HG2	4:H:100(B):TYR:OH	2.05	0.56
3:Q:192:TYR:HB2	3:Q:209:PHE:CE1	2.41	0.56
4:T:59:TYR:HD2	4:T:64:LYS:HD3	1.70	0.56
3:V:192:TYR:HB2	3:V:209:PHE:CE1	2.41	0.56
1:A:11:ASP:CG	2:B:28:ASN:HA	2.25	0.56
1:G:83(A):GLU:OE1	3:J:53:ASN:ND2	2.39	0.56
1:A:307:LYS:HD3	2:B:59:MET:O	2.06	0.56
2:D:33:GLY:CA	4:W:217:THR:HA	2.36	0.56
3:L:192:TYR:HB2	3:L:209:PHE:CE1	2.41	0.56
1:S:62:ARG:HG2	1:S:63:ASP:H	1.70	0.56
3:V:98:PHE:CE2	4:W:45:LEU:HB2	2.41	0.56
3:J:192:TYR:HB2	3:J:209:PHE:CE1	2.41	0.56
1:M:29:ILE:HD12	2:N:105:GLU:OE1	2.06	0.56
1:G:14:CYS:O	2:I:24:TYR:HA	2.06	0.56
3:J:116:SER:HA	3:J:207:LYS:HD2	1.87	0.56
1:M:62:ARG:HG2	1:M:63:ASP:H	1.70	0.56
1:A:293:PRO:HG2	1:A:294:PHE:CD1	2.42	0.55
1:A:15:ILE:C	2:B:14:TRP:CH2	2.79	0.55
1:C:293:PRO:HG2	1:C:294:PHE:CD1	2.41	0.55
3:L:110:ASP:OD2	3:L:199:LYS:HE2	2.07	0.55
4:W:59:TYR:HD2	4:W:64:LYS:HD3	1.70	0.55
1:M:293:PRO:HG2	1:M:294:PHE:CD1	2.42	0.55
4:F:59:TYR:HD2	4:F:64:LYS:HD3	1.70	0.55
3:L:174:SER:HB2	4:H:174:PHE:HE1	1.71	0.55
1:S:186:ASN:ND2	1:S:190:GLU:OE1	2.33	0.55
1:S:293:PRO:HG2	1:S:294:PHE:CD1	2.41	0.55
2:U:31:GLY:HA3	4:F:219:VAL:HG22	1.86	0.55
3:X:192:TYR:HB2	3:X:209:PHE:CE1	2.41	0.55
3:X:110:ASP:OD2	3:X:199:LYS:HE2	2.07	0.55
1:S:18:HIS:N	2:U:21:TRP:O	2.34	0.55
3:E:110:ASP:OD2	3:E:199:LYS:HE2	2.07	0.55
4:H:37:MET:HE3	4:H:46:GLU:O	2.07	0.55
1:S:100:GLY:HA3	1:S:230:MET:O	2.07	0.55
1:G:293:PRO:HG2	1:G:294:PHE:CD1	2.41	0.55
4:K:19:LYS:HZ3	4:K:81:ASP:HB2	1.70	0.55
4:K:59:TYR:HD2	4:K:64:LYS:HD3	1.70	0.55
3:V:119:PRO:HB2	4:W:228:ARG:NH2	2.17	0.55
3:E:123:GLU:OE1	4:F:123:PRO:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:110:ASP:OD2	3:Q:199:LYS:HE2	2.07	0.55
1:S:105:TYR:OH	1:S:109:LYS:HE3	2.06	0.55
1:A:62:ARG:HG2	1:A:63:ASP:H	1.70	0.55
1:O:293:PRO:HG2	1:O:294:PHE:CD1	2.42	0.55
4:T:68:THR:HB	4:T:81:ASP:CG	2.26	0.55
1:S:15:ILE:HG13	2:U:119:TYR:HA	1.89	0.55
1:C:100:GLY:HA3	1:C:230:MET:O	2.07	0.54
4:K:37:MET:HE3	4:K:46:GLU:O	2.06	0.54
1:M:220:ARG:NH2	1:O:210:ASN:OD1	2.40	0.54
3:V:110:ASP:OD2	3:V:199:LYS:HE2	2.07	0.54
1:M:69:TRP:HZ3	1:M:112:LEU:HD21	1.73	0.54
1:M:100:GLY:HA3	1:M:230:MET:O	2.07	0.54
1:C:16:GLY:N	2:D:14:TRP:CZ3	2.76	0.54
2:D:167:ARG:CG	2:D:170:ARG:HH21	2.14	0.54
1:G:69:TRP:HZ3	1:G:112:LEU:HD21	1.73	0.54
1:A:100:GLY:HA3	1:A:230:MET:O	2.07	0.54
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.90	0.54
1:C:186:ASN:ND2	1:C:190:GLU:OE1	2.33	0.54
1:O:183:HIS:HB2	1:O:252:ILE:HD11	1.90	0.54
4:T:81:ASP:C	4:T:81:ASP:OD1	2.45	0.54
3:J:110:ASP:OD2	3:J:199:LYS:HE2	2.07	0.54
3:L:124:GLN:NE2	3:L:131:SER:OG	2.38	0.54
1:O:100:GLY:HA3	1:O:230:MET:O	2.07	0.54
3:X:35:TRP:CZ3	3:X:88:CYS:HB3	2.43	0.54
1:G:100:GLY:HA3	1:G:230:MET:O	2.07	0.54
4:H:190:SER:O	4:H:190:SER:OG	2.22	0.54
3:J:49:TYR:CE1	3:J:53:ASN:HB2	2.43	0.54
1:O:56:VAL:HG21	3:Q:30:LYS:HZ1	1.72	0.54
1:O:274:TYR:CZ	4:R:97:GLY:HA3	2.39	0.54
1:S:69:TRP:HZ3	1:S:112:LEU:HD21	1.73	0.54
3:X:164:THR:HG23	4:T:174:PHE:HD1	1.69	0.54
1:A:51:LEU:HD13	1:A:272:LEU:HB2	1.90	0.54
3:X:160:LEU:CD1	4:T:179:GLN:OE1	2.52	0.54
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.90	0.54
1:S:51:LEU:HD13	1:S:272:LEU:HB2	1.90	0.54
1:M:183:HIS:HB2	1:M:252:ILE:HD11	1.90	0.53
3:Q:49:TYR:CE1	3:Q:53:ASN:HB2	2.43	0.53
3:V:124:GLN:NE2	3:V:131:SER:OG	2.38	0.53
1:C:69:TRP:HZ3	1:C:112:LEU:HD21	1.73	0.53
3:E:35:TRP:CZ3	3:E:88:CYS:HB3	2.43	0.53
3:E:98:PHE:CE1	4:F:37:MET:HE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:35:TRP:CZ3	3:J:88:CYS:HB3	2.43	0.53
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.43	0.53
3:Q:193:THR:HG23	3:Q:208:SER:HB3	1.90	0.53
3:V:193:THR:HG23	3:V:208:SER:HB3	1.90	0.53
3:V:164:THR:HG22	4:W:174:PHE:HA	1.89	0.53
3:X:193:THR:HG23	3:X:208:SER:HB3	1.90	0.53
3:E:49:TYR:CE1	3:E:53:ASN:HB2	2.43	0.53
1:G:51:LEU:HD13	1:G:272:LEU:HB2	1.90	0.53
3:L:49:TYR:CE1	3:L:53:ASN:HB2	2.43	0.53
3:Q:35:TRP:CZ3	3:Q:88:CYS:HB3	2.43	0.53
3:Q:124:GLN:HB2	4:R:122:TYR:CD1	2.43	0.53
3:X:137:ASN:ND2	4:T:174:PHE:HZ	2.06	0.53
3:V:49:TYR:CE1	3:V:53:ASN:HB2	2.43	0.53
3:X:193:THR:HG22	3:X:194:CYS:H	1.74	0.53
1:G:183:HIS:HB2	1:G:252:ILE:HD11	1.90	0.53
1:O:69:TRP:HZ3	1:O:112:LEU:HD21	1.72	0.53
3:X:174:SER:HB2	4:T:174:PHE:HE1	1.74	0.53
3:J:174:SER:HB3	4:K:174:PHE:CZ	2.43	0.53
3:L:193:THR:HG22	3:L:194:CYS:H	1.74	0.53
3:L:147:LYS:HE3	3:L:195:GLU:HB3	1.91	0.53
3:V:35:TRP:CZ3	3:V:88:CYS:HB3	2.43	0.53
3:X:49:TYR:CE1	3:X:53:ASN:HB2	2.43	0.53
1:A:26:VAL:HG11	1:A:317:ALA:HB2	1.91	0.53
1:C:276:ASN:ND2	4:F:52:PHE:CE1	2.76	0.53
3:L:141:PRO:HD2	3:L:198:HIS:HE1	1.74	0.53
3:J:141:PRO:HD2	3:J:198:HIS:HE1	1.74	0.53
1:O:26:VAL:HG11	1:O:317:ALA:HB2	1.91	0.53
1:G:26:VAL:HG11	1:G:317:ALA:HB2	1.91	0.53
1:M:26:VAL:HG11	1:M:317:ALA:HB2	1.91	0.53
4:R:33:THR:CG2	4:R:95:ASN:HD22	2.22	0.53
4:R:37:MET:HE3	4:R:46:GLU:O	2.09	0.53
1:S:26:VAL:HG11	1:S:317:ALA:HB2	1.91	0.53
3:X:147:LYS:HE3	3:X:195:GLU:HB3	1.91	0.53
3:E:147:LYS:HE3	3:E:195:GLU:HB3	1.91	0.52
1:S:183:HIS:HB2	1:S:252:ILE:HD11	1.90	0.52
3:X:141:PRO:HD2	3:X:198:HIS:HE1	1.74	0.52
1:A:69:TRP:HZ3	1:A:112:LEU:HD21	1.73	0.52
3:E:141:PRO:HD2	3:E:198:HIS:HE1	1.74	0.52
3:J:124:GLN:NE2	3:J:131:SER:OG	2.38	0.52
4:K:33:THR:CG2	4:K:95:ASN:HD22	2.22	0.52
3:V:174:SER:HB3	4:W:174:PHE:HZ	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:VAL:HG11	1:C:317:ALA:HB2	1.91	0.52
1:M:244:ASN:ND2	1:S:221:PRO:HD3	2.23	0.52
3:X:124:GLN:HB2	4:T:122:TYR:CZ	2.44	0.52
3:E:193:THR:HG23	3:E:208:SER:HB3	1.91	0.52
2:D:80:LEU:HD11	2:I:80:LEU:CD2	2.38	0.52
3:J:174:SER:CB	4:K:174:PHE:CE1	2.92	0.52
3:L:193:THR:HG23	3:L:208:SER:HB3	1.90	0.52
1:O:51:LEU:HD13	1:O:272:LEU:HB2	1.90	0.52
2:P:160:PRO:HA	2:P:163:SER:HB2	1.92	0.52
4:W:33:THR:CG2	4:W:95:ASN:HD22	2.22	0.52
3:E:193:THR:HG22	3:E:194:CYS:H	1.74	0.52
4:R:38:LYS:HB2	4:R:90:TYR:CE1	2.45	0.52
4:T:157:TRP:HE1	4:T:189:SER:HG	1.58	0.52
1:C:51:LEU:HD13	1:C:272:LEU:HB2	1.90	0.52
3:Q:193:THR:HG22	3:Q:194:CYS:H	1.74	0.52
3:Q:147:LYS:HE3	3:Q:195:GLU:HB3	1.91	0.52
2:U:160:PRO:HA	2:U:163:SER:HB2	1.92	0.52
4:W:38:LYS:HB2	4:W:90:TYR:CE1	2.45	0.52
2:B:160:PRO:HA	2:B:163:SER:HB2	1.92	0.52
4:H:33:THR:CG2	4:H:95:ASN:HD22	2.22	0.52
1:M:51:LEU:HD13	1:M:272:LEU:HB2	1.91	0.52
1:M:55(A):GLY:O	3:X:50:ARG:NH2	2.42	0.52
3:V:147:LYS:HE3	3:V:195:GLU:HB3	1.91	0.52
3:X:118:PHE:CB	4:T:124:LEU:HD22	2.40	0.52
3:J:193:THR:HG23	3:J:208:SER:HB3	1.91	0.52
3:Q:141:PRO:HD2	3:Q:198:HIS:HE1	1.74	0.52
4:T:33:THR:CG2	4:T:95:ASN:HD22	2.23	0.52
4:T:38:LYS:HB2	4:T:90:TYR:CE1	2.45	0.52
3:V:141:PRO:HD2	3:V:198:HIS:HE1	1.74	0.52
4:F:38:LYS:HB2	4:F:90:TYR:CE1	2.45	0.52
1:S:16:GLY:HA3	2:U:14:TRP:CH2	2.44	0.52
2:D:160:PRO:HA	2:D:163:SER:HB2	1.92	0.52
4:K:38:LYS:HB2	4:K:90:TYR:CE1	2.45	0.52
1:O:56:VAL:HG21	3:Q:30:LYS:HZ2	1.73	0.52
1:O:316:LEU:HD23	2:P:100:VAL:HG13	1.92	0.52
1:S:309:VAL:HG22	2:U:93:THR:HA	1.92	0.52
2:B:124:LEU:HD13	2:I:9:PHE:HB2	1.91	0.51
3:J:193:THR:HG22	3:J:194:CYS:H	1.74	0.51
3:V:193:THR:HG22	3:V:194:CYS:H	1.74	0.51
2:D:32:SER:HB2	4:W:218:LYS:O	2.11	0.51
1:O:16:GLY:N	2:P:14:TRP:CZ3	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:38:LYS:HB2	4:H:90:TYR:CE1	2.45	0.51
4:W:37:MET:HE3	4:W:46:GLU:O	2.10	0.51
1:A:13:ILE:HA	2:B:26:HIS:HA	1.91	0.51
1:C:56:VAL:CG2	3:E:50:ARG:NH1	2.74	0.51
3:E:120:PRO:O	4:F:228:ARG:NH2	2.44	0.51
4:F:33:THR:CG2	4:F:95:ASN:HD22	2.22	0.51
3:J:147:LYS:HE3	3:J:195:GLU:HB3	1.91	0.51
1:S:106:GLU:HG2	2:U:70:PHE:CA	2.41	0.51
3:V:13:VAL:HG11	3:V:78:VAL:HG21	1.93	0.51
3:E:13:VAL:HG11	3:E:78:VAL:HG21	1.93	0.51
3:E:95:PRO:HA	4:F:47:TRP:CZ3	2.46	0.51
3:L:13:VAL:HG11	3:L:78:VAL:HG21	1.93	0.51
1:A:56:VAL:CG2	3:L:30:LYS:NZ	2.72	0.51
4:T:12:VAL:HG23	4:T:111:VAL:HG22	1.93	0.51
1:A:83:PRO:HB3	3:L:49:TYR:CE2	2.45	0.51
1:G:11:ASP:HA	2:I:27:SER:O	2.11	0.51
2:N:168:LEU:CD1	2:N:169:ASN:N	2.67	0.51
2:I:160:PRO:HA	2:I:163:SER:HB2	1.92	0.51
1:M:220:ARG:NE	1:O:210:ASN:OD1	2.44	0.51
3:J:174:SER:HB3	4:K:174:PHE:HZ	1.76	0.51
4:W:12:VAL:HG23	4:W:111:VAL:HG22	1.93	0.51
3:Q:13:VAL:HG11	3:Q:78:VAL:HG21	1.93	0.50
4:R:190:SER:OG	4:R:190:SER:O	2.22	0.50
3:X:13:VAL:HG11	3:X:78:VAL:HG21	1.93	0.50
3:E:148:TRP:CE3	3:E:179:LEU:HD13	2.47	0.50
3:E:96:ARG:HB2	4:F:47:TRP:CG	2.47	0.50
2:N:165:GLU:O	2:N:168:LEU:HG	2.12	0.50
3:E:121:SER:HB2	4:F:123:PRO:O	2.12	0.50
4:F:19:LYS:HZ1	4:F:81:ASP:HB2	1.75	0.50
3:J:13:VAL:HG11	3:J:78:VAL:HG21	1.93	0.50
4:K:12:VAL:HG23	4:K:111:VAL:HG22	1.93	0.50
1:O:221:PRO:HD3	1:S:244:ASN:ND2	2.27	0.50
2:B:54:SER:OG	1:G:32:LYS:NZ	2.45	0.50
4:K:93:VAL:HG11	4:K:100(C):PHE:HB3	1.94	0.50
4:R:12:VAL:HG23	4:R:111:VAL:HG22	1.93	0.50
4:T:37:MET:HE3	4:T:46:GLU:O	2.12	0.50
1:G:58:PRO:O	4:K:96:TYR:OH	2.27	0.50
3:J:148:TRP:CE3	3:J:179:LEU:HD13	2.47	0.50
3:J:27(B):VAL:O	3:J:27(B):VAL:HG22	2.12	0.50
1:O:274:TYR:OH	4:R:97:GLY:C	2.50	0.50
3:X:166:GLN:HB2	3:X:173:TYR:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:148:TRP:CE3	3:X:179:LEU:HD13	2.47	0.50
3:L:148:TRP:CE3	3:L:179:LEU:HD13	2.47	0.50
2:N:160:PRO:HA	2:N:163:SER:HB2	1.92	0.50
3:Q:27(B):VAL:HG22	3:Q:27(B):VAL:O	2.12	0.50
3:J:164:THR:HG23	4:K:174:PHE:CE1	2.44	0.49
4:R:93:VAL:HG11	4:R:100(C):PHE:HB3	1.94	0.49
1:S:106:GLU:OE1	2:U:71:ASN:ND2	2.34	0.49
1:M:107:GLU:OE2	2:U:76:ARG:NE	2.45	0.49
3:V:166:GLN:HB2	3:V:173:TYR:CE1	2.48	0.49
3:V:27(B):VAL:HG22	3:V:27(B):VAL:O	2.12	0.49
2:B:51:LYS:HE3	1:G:30:MET:HE2	1.94	0.49
3:L:27(B):VAL:HG22	3:L:27(B):VAL:O	2.12	0.49
3:Q:148:TRP:CE3	3:Q:179:LEU:HD13	2.47	0.49
3:V:148:TRP:CE3	3:V:179:LEU:HD13	2.47	0.49
4:W:93:VAL:HG11	4:W:100(C):PHE:HB3	1.94	0.49
1:C:17:TYR:O	2:D:14:TRP:N	2.36	0.49
4:F:12:VAL:HG23	4:F:111:VAL:HG22	1.93	0.49
1:G:98:TYR:CD1	1:G:230:MET:HG3	2.48	0.49
3:L:137:ASN:ND2	4:H:174:PHE:CZ	2.73	0.49
1:S:106:GLU:HG2	2:U:70:PHE:HA	1.95	0.49
2:P:80:LEU:HD11	2:U:80:LEU:HD22	1.94	0.49
3:E:124:GLN:NE2	3:E:131:SER:OG	2.38	0.49
1:M:98:TYR:CD1	1:M:230:MET:HG3	2.48	0.49
1:O:221:PRO:HB3	5:S:2001:NAG:H81	1.94	0.49
1:O:83:PRO:CB	3:Q:49:TYR:CE2	2.95	0.49
1:S:98:TYR:CD1	1:S:230:MET:HG3	2.48	0.49
4:T:190:SER:O	4:T:190:SER:OG	2.22	0.49
4:H:12:VAL:HG23	4:H:111:VAL:HG22	1.93	0.49
2:N:127:ARG:HH21	2:U:131:LYS:NZ	2.10	0.49
3:X:174:SER:CB	4:T:174:PHE:CE1	2.96	0.49
1:A:98:TYR:CD1	1:A:230:MET:HG3	2.48	0.49
1:C:307:LYS:HD3	2:D:59:MET:O	2.13	0.49
3:E:27(B):VAL:O	3:E:27(B):VAL:HG22	2.12	0.49
4:F:93:VAL:HG11	4:F:100(C):PHE:HB3	1.94	0.49
1:M:147:PHE:CZ	1:M:230:MET:HE1	2.48	0.49
3:Q:124:GLN:NE2	3:Q:131:SER:OG	2.38	0.49
3:V:119:PRO:HG2	4:W:228:ARG:HE	1.78	0.49
4:H:93:VAL:HG11	4:H:100(C):PHE:HB3	1.93	0.49
3:J:135:PHE:CZ	4:K:124:LEU:HD13	2.48	0.49
4:T:93:VAL:HG11	4:T:100(C):PHE:HB3	1.94	0.49
3:J:166:GLN:HB2	3:J:173:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:316:LEU:CD2	2:P:100:VAL:HG22	2.41	0.49
1:O:83(A):GLU:OE1	3:Q:53:ASN:ND2	2.46	0.49
1:A:244:ASN:HD22	1:G:221:PRO:HD3	1.76	0.48
3:E:166:GLN:HB2	3:E:173:TYR:CE1	2.47	0.48
1:O:98:TYR:CD1	1:O:230:MET:HG3	2.48	0.48
3:Q:166:GLN:HB2	3:Q:173:TYR:CE1	2.47	0.48
1:S:307:LYS:HZ2	2:U:59:MET:HB2	1.76	0.48
3:X:27(B):VAL:O	3:X:27(B):VAL:HG22	2.12	0.48
1:C:98:TYR:CD1	1:C:230:MET:HG3	2.48	0.48
1:S:83:PRO:HG2	4:W:100(B):TYR:OH	2.12	0.48
3:L:166:GLN:HB2	3:L:173:TYR:CE1	2.47	0.48
1:M:19:ALA:O	2:N:15:GLN:HA	2.14	0.48
2:B:51:LYS:HE3	1:G:30:MET:CE	2.44	0.48
4:F:51:ILE:HD13	4:F:71:VAL:HG23	1.96	0.48
1:G:179:LEU:HD23	1:G:234:TRP:HB3	1.95	0.48
1:M:17:TYR:CZ	2:N:12:GLY:O	2.65	0.48
1:M:179:LEU:HD23	1:M:234:TRP:HB3	1.95	0.48
4:T:51:ILE:HD13	4:T:71:VAL:HG23	1.96	0.48
4:H:19:LYS:HZ3	4:H:81:ASP:HB2	1.77	0.48
1:M:323:THR:HG21	2:N:13:GLY:H	1.78	0.48
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.96	0.48
1:A:56:VAL:HG21	3:L:30:LYS:HZ1	1.77	0.48
1:C:56:VAL:CG2	3:E:50:ARG:HH12	2.26	0.48
3:J:119:PRO:HG2	4:K:228:ARG:HE	1.79	0.48
3:J:53:ASN:N	3:J:53:ASN:OD1	2.47	0.48
3:Q:195:GLU:HG3	3:Q:206:VAL:HG22	1.96	0.48
3:X:118:PHE:HB3	4:T:124:LEU:HD22	1.95	0.48
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.96	0.48
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.96	0.48
3:E:33:MET:HB3	3:E:51:ALA:HB2	1.96	0.48
1:C:56:VAL:HG22	3:E:50:ARG:NH1	2.28	0.48
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.96	0.48
3:X:124:GLN:NE2	3:X:131:SER:OG	2.38	0.48
1:C:14:CYS:C	2:D:14:TRP:HH2	2.17	0.48
1:G:83(A):GLU:N	3:J:49:TYR:OH	2.29	0.48
2:N:47:GLY:O	1:S:30:MET:HG2	2.14	0.48
1:O:106:GLU:OE1	2:P:71:ASN:ND2	2.28	0.48
1:O:134:GLY:HA3	1:O:153:TRP:HB3	1.96	0.48
4:H:51:ILE:HD13	4:H:71:VAL:HG23	1.96	0.47
4:K:51:ILE:HD13	4:K:71:VAL:HG23	1.96	0.47
3:L:33:MET:HB3	3:L:51:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:179:LEU:HD23	1:O:234:TRP:HB3	1.95	0.47
3:Q:33:MET:HB3	3:Q:51:ALA:HB2	1.96	0.47
1:G:106:GLU:OE1	2:I:71:ASN:ND2	2.24	0.47
3:J:195:GLU:HG3	3:J:206:VAL:HG22	1.96	0.47
3:V:33:MET:HB3	3:V:51:ALA:HB2	1.96	0.47
4:F:183:ASP:O	4:F:184:LEU:HD23	2.15	0.47
1:S:134:GLY:HA3	1:S:153:TRP:HB3	1.96	0.47
1:S:179:LEU:HD23	1:S:234:TRP:HB3	1.95	0.47
4:W:51:ILE:HD13	4:W:71:VAL:HG23	1.96	0.47
1:A:276:ASN:ND2	4:H:52:PHE:CE1	2.82	0.47
1:C:147:PHE:CZ	1:C:230:MET:HE1	2.49	0.47
5:O:2001:NAG:H61	5:O:2002:NAG:N2	2.29	0.47
1:C:147:PHE:HZ	1:C:230:MET:HE1	1.80	0.47
3:L:174:SER:HB3	4:H:174:PHE:CE1	2.49	0.47
1:M:134:GLY:HA3	1:M:153:TRP:HB3	1.96	0.47
4:R:183:ASP:O	4:R:184:LEU:HD23	2.15	0.47
3:X:53:ASN:N	3:X:53:ASN:OD1	2.47	0.47
4:F:37:MET:HE3	4:F:46:GLU:O	2.15	0.47
3:J:33:MET:HB3	3:J:51:ALA:HB2	1.96	0.47
4:K:29:PHE:CD2	4:K:76:SER:HA	2.50	0.47
1:M:147:PHE:HZ	1:M:230:MET:HE1	1.80	0.47
2:N:80:LEU:CD2	2:U:80:LEU:HD11	2.44	0.47
1:O:56:VAL:CG2	3:Q:30:LYS:HZ1	2.27	0.47
3:Q:53:ASN:N	3:Q:53:ASN:OD1	2.47	0.47
1:S:316:LEU:HD21	2:U:100:VAL:HG22	1.95	0.47
4:T:183:ASP:O	4:T:184:LEU:HD23	2.15	0.47
2:D:31:GLY:HA3	4:W:219:VAL:HG22	1.97	0.47
4:F:48:ILE:HG12	4:F:63:PHE:CD2	2.50	0.47
1:C:274:TYR:HD2	4:F:31:GLU:O	1.97	0.47
4:H:183:ASP:O	4:H:184:LEU:HD23	2.15	0.47
4:K:183:ASP:O	4:K:184:LEU:HD23	2.15	0.47
1:M:17:TYR:CE2	2:N:13:GLY:HA2	2.47	0.47
3:V:53:ASN:N	3:V:53:ASN:OD1	2.47	0.47
4:R:29:PHE:CD2	4:R:76:SER:HA	2.50	0.47
3:V:135:PHE:CZ	4:W:124:LEU:CD1	2.98	0.47
3:E:53:ASN:OD1	3:E:53:ASN:N	2.47	0.47
4:F:29:PHE:CD2	4:F:76:SER:HA	2.50	0.47
2:N:165:GLU:HA	2:N:168:LEU:HD23	1.96	0.47
4:R:51:ILE:HD13	4:R:71:VAL:HG23	1.96	0.47
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.95	0.47
3:E:195:GLU:HG3	3:E:206:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:LYS:HB3	9:G:2003:NAG:C8	2.44	0.47
4:T:29:PHE:CD2	4:T:76:SER:HA	2.50	0.47
4:W:19:LYS:HZ3	4:W:81:ASP:HB2	1.78	0.47
4:K:48:ILE:HG12	4:K:63:PHE:CD2	2.50	0.46
4:T:48:ILE:HG12	4:T:63:PHE:CD2	2.50	0.46
3:V:195:GLU:HG3	3:V:206:VAL:HG22	1.96	0.46
3:V:24:ARG:NH1	3:V:70:ASP:HB3	2.31	0.46
3:L:195:GLU:HG3	3:L:206:VAL:HG22	1.96	0.46
1:O:147:PHE:CZ	1:O:230:MET:HE1	2.50	0.46
3:Q:24:ARG:NH1	3:Q:70:ASP:HB3	2.31	0.46
4:W:183:ASP:O	4:W:184:LEU:HD23	2.15	0.46
4:W:29:PHE:CD2	4:W:76:SER:HA	2.50	0.46
3:X:195:GLU:HG3	3:X:206:VAL:HG22	1.96	0.46
3:E:24:ARG:NH1	3:E:70:ASP:HB3	2.31	0.46
4:R:48:ILE:HG12	4:R:63:PHE:CD2	2.49	0.46
3:X:33:MET:HB3	3:X:51:ALA:HB2	1.96	0.46
4:H:29:PHE:CD2	4:H:76:SER:HA	2.50	0.46
2:N:76:ARG:CZ	1:O:110:HIS:HB2	2.46	0.46
3:X:131:SER:OG	4:T:145:LYS:HE2	2.16	0.46
3:E:135:PHE:CE2	4:F:190:SER:HB2	2.50	0.46
1:G:147:PHE:HZ	1:G:230:MET:HE1	1.80	0.46
4:H:48:ILE:HG12	4:H:63:PHE:CD2	2.50	0.46
1:S:147:PHE:HZ	1:S:230:MET:HE1	1.81	0.46
3:X:43:SER:HB3	4:T:91:TYR:CE1	2.51	0.46
4:W:48:ILE:HG12	4:W:63:PHE:CD2	2.50	0.46
4:H:73:ARG:HG2	4:H:73:ARG:H	1.49	0.46
3:J:11:LEU:HD12	3:X:8:PRO:HG3	1.98	0.46
1:S:141:TYR:CZ	1:S:149:ARG:NH2	2.84	0.46
1:A:141:TYR:CZ	1:A:149:ARG:NH2	2.84	0.46
1:A:12:GLN:N	2:B:27:SER:O	2.45	0.46
4:F:60:ASN:OD1	4:F:61:GLN:N	2.49	0.46
1:G:141:TYR:CZ	1:G:149:ARG:NH2	2.84	0.46
3:L:24:ARG:NH1	3:L:70:ASP:HB3	2.31	0.46
1:O:16:GLY:HA3	2:P:14:TRP:CZ3	2.51	0.46
3:V:174:SER:CB	4:W:174:PHE:CZ	2.99	0.46
3:J:167:ASP:HB3	3:J:170:ASP:OD1	2.16	0.46
4:K:60:ASN:OD1	4:K:61:GLN:N	2.49	0.46
4:K:66:ARG:HG3	4:K:66:ARG:H	1.53	0.46
3:L:167:ASP:HB3	3:L:170:ASP:OD1	2.16	0.46
3:Q:167:ASP:HB3	3:Q:170:ASP:OD1	2.16	0.46
1:S:147:PHE:CZ	1:S:230:MET:HE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:169:LYS:HD2	3:V:169:LYS:HA	1.79	0.46
3:X:24:ARG:NH1	3:X:70:ASP:HB3	2.31	0.46
1:A:16:GLY:HA3	2:B:14:TRP:CH2	2.51	0.45
2:D:128:ASP:OD1	2:D:159:TYR:OH	2.22	0.45
1:C:106:GLU:OE2	2:D:71:ASN:HB3	2.15	0.45
1:M:141:TYR:CZ	1:M:149:ARG:NH2	2.84	0.45
3:X:167:ASP:HB3	3:X:170:ASP:OD1	2.16	0.45
1:C:16:GLY:HA3	2:D:14:TRP:CE2	2.51	0.45
1:G:15:ILE:O	2:I:10:ILE:HD13	2.16	0.45
3:L:44:PRO:CG	4:H:45:LEU:HD11	2.38	0.45
3:L:118:PHE:CE2	4:H:124:LEU:HB3	2.52	0.45
1:O:147:PHE:HZ	1:O:230:MET:HE1	1.80	0.45
3:E:50:ARG:HB2	3:E:50:ARG:HE	1.53	0.45
3:J:24:ARG:NH1	3:J:70:ASP:HB3	2.31	0.45
3:L:90:GLN:HE21	3:L:97:THR:HG22	1.82	0.45
1:A:14:CYS:O	2:B:24:TYR:HA	2.17	0.45
1:A:55(A):GLY:HA3	3:L:32:PHE:CZ	2.51	0.45
3:E:167:ASP:HB3	3:E:170:ASP:OD1	2.16	0.45
1:G:147:PHE:CZ	1:G:230:MET:HE1	2.50	0.45
3:L:174:SER:CB	4:H:174:PHE:CE1	2.96	0.45
4:K:73:ARG:HG2	4:K:73:ARG:H	1.49	0.45
2:D:163:SER:O	2:D:167:ARG:HG3	2.17	0.45
3:Q:90:GLN:HE21	3:Q:97:THR:HG22	1.82	0.45
3:V:167:ASP:HB3	3:V:170:ASP:OD1	2.16	0.45
4:W:60:ASN:OD1	4:W:61:GLN:N	2.49	0.45
1:C:11:ASP:HA	2:D:27:SER:O	2.17	0.45
4:H:60:ASN:OD1	4:H:61:GLN:N	2.49	0.45
1:M:244:ASN:HD22	1:S:221:PRO:HD3	1.82	0.45
1:O:141:TYR:CZ	1:O:149:ARG:NH2	2.84	0.45
1:O:14:CYS:C	2:P:14:TRP:HH2	2.19	0.45
1:C:141:TYR:CZ	1:C:149:ARG:NH2	2.84	0.45
1:A:83:PRO:CB	3:L:49:TYR:CE2	3.00	0.45
4:R:30:THR:HB	4:R:53:ASN:HB2	1.99	0.45
4:T:60:ASN:OD1	4:T:61:GLN:N	2.49	0.45
3:V:34:HIS:O	3:V:88:CYS:HA	2.17	0.45
3:E:169:LYS:HD2	3:E:169:LYS:HA	1.80	0.45
1:O:53:ASP:HA	1:O:58:PRO:HD3	1.99	0.45
3:X:111:ALA:O	3:X:200:THR:HG21	2.17	0.45
4:H:30:THR:HB	4:H:53:ASN:HB2	1.99	0.45
1:M:17:TYR:CD2	2:N:13:GLY:HA2	2.52	0.45
1:M:11:ASP:OD1	2:N:28:ASN:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:111:ALA:O	3:Q:200:THR:HG21	2.17	0.45
4:R:142:CYS:HB2	4:R:157:TRP:CH2	2.52	0.45
4:R:19:LYS:HZ3	4:R:81:ASP:HB2	1.80	0.45
1:C:16:GLY:HA3	2:D:14:TRP:CH2	2.52	0.45
3:L:164:THR:HG22	4:H:175:PRO:HD3	1.98	0.45
2:P:128:ASP:OD1	2:P:159:TYR:OH	2.22	0.45
3:E:111:ALA:O	3:E:200:THR:HG21	2.17	0.44
4:F:142:CYS:HB2	4:F:157:TRP:CH2	2.52	0.44
4:F:30:THR:HB	4:F:53:ASN:HB2	1.99	0.44
4:H:142:CYS:HB2	4:H:157:TRP:CH2	2.52	0.44
4:K:30:THR:HB	4:K:53:ASN:HB2	1.99	0.44
2:N:128:ASP:OD1	2:N:159:TYR:OH	2.22	0.44
4:R:60:ASN:OD1	4:R:61:GLN:N	2.49	0.44
3:V:160:LEU:HD21	4:W:179:GLN:NE2	2.21	0.44
3:X:90:GLN:HE21	3:X:97:THR:HG22	1.82	0.44
3:Q:34:HIS:O	3:Q:88:CYS:HA	2.17	0.44
1:A:147:PHE:HZ	1:A:230:MET:HE1	1.81	0.44
2:B:124:LEU:CD1	2:I:9:PHE:HB2	2.47	0.44
3:J:118:PHE:CE2	4:K:124:LEU:HB3	2.50	0.44
4:T:142:CYS:HB2	4:T:157:TRP:CH2	2.52	0.44
3:X:34:HIS:O	3:X:88:CYS:HA	2.17	0.44
2:D:19:ASP:N	2:D:19:ASP:OD1	2.42	0.44
3:J:34:HIS:O	3:J:88:CYS:HA	2.17	0.44
4:K:142:CYS:HB2	4:K:157:TRP:CH2	2.52	0.44
3:L:34:HIS:O	3:L:88:CYS:HA	2.17	0.44
4:W:30:THR:HB	4:W:53:ASN:HB2	1.99	0.44
3:J:39:LYS:NZ	3:J:39:LYS:HB3	2.33	0.44
1:S:62:ARG:CG	1:S:63:ASP:H	2.29	0.44
4:T:30:THR:HB	4:T:53:ASN:HB2	1.99	0.44
2:U:128:ASP:OD1	2:U:159:TYR:OH	2.22	0.44
3:X:124:GLN:HG3	4:T:122:TYR:CE2	2.53	0.44
1:A:53:ASP:HA	1:A:58:PRO:HD3	1.99	0.44
1:A:58:PRO:HG2	1:A:60:ILE:HD11	2.00	0.44
1:C:53:ASP:HA	1:C:58:PRO:HD3	1.99	0.44
3:E:34:HIS:O	3:E:88:CYS:HA	2.17	0.44
3:E:90:GLN:HE21	3:E:97:THR:HG22	1.82	0.44
3:Q:148:TRP:CD2	3:Q:179:LEU:HD13	2.53	0.44
1:S:58:PRO:HG2	1:S:60:ILE:HD11	2.00	0.44
3:V:135:PHE:HZ	4:W:124:LEU:CD1	2.31	0.44
4:W:142:CYS:HB2	4:W:157:TRP:CH2	2.52	0.44
3:L:148:TRP:CD2	3:L:179:LEU:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:16:GLY:HA3	2:P:14:TRP:CH2	2.53	0.44
3:X:124:GLN:HG3	4:T:122:TYR:CZ	2.52	0.44
1:C:62:ARG:CG	1:C:63:ASP:N	2.73	0.44
3:E:98:PHE:CE1	4:F:37:MET:CE	3.00	0.44
1:G:53:ASP:HA	1:G:58:PRO:HD3	1.99	0.44
3:J:148:TRP:CD2	3:J:179:LEU:HD13	2.53	0.44
3:Q:39:LYS:HB3	3:Q:39:LYS:NZ	2.33	0.44
5:S:2001:NAG:H61	5:S:2002:NAG:N2	2.33	0.44
3:V:39:LYS:NZ	3:V:39:LYS:HB3	2.33	0.44
3:E:150:ILE:HG12	3:E:192:TYR:CD1	2.53	0.44
4:F:52:PHE:CE2	4:F:53:ASN:HB3	2.53	0.44
8:M:2001:NAG:H61	8:M:2002:NAG:N2	2.33	0.44
4:T:52:PHE:CE2	4:T:53:ASN:HB3	2.53	0.44
3:V:111:ALA:O	3:V:200:THR:HG21	2.17	0.44
3:J:111:ALA:O	3:J:200:THR:HG21	2.17	0.43
3:J:164:THR:HG22	4:K:174:PHE:HA	2.00	0.43
4:K:52:PHE:CE2	4:K:53:ASN:HB3	2.53	0.43
3:L:150:ILE:HG12	3:L:192:TYR:CD1	2.53	0.43
1:M:53:ASP:HA	1:M:58:PRO:HD3	1.99	0.43
1:O:58:PRO:HG2	1:O:60:ILE:HD11	2.00	0.43
3:Q:150:ILE:HG12	3:Q:192:TYR:CD1	2.53	0.43
3:X:169:LYS:HA	3:X:169:LYS:HD2	1.79	0.43
1:A:147:PHE:CZ	1:A:230:MET:HE1	2.53	0.43
1:A:274:TYR:CZ	4:H:97:GLY:HA2	2.53	0.43
2:I:128:ASP:OD1	2:I:159:TYR:OH	2.22	0.43
4:R:52:PHE:CE2	4:R:53:ASN:HB3	2.53	0.43
3:X:39:LYS:HB3	3:X:39:LYS:NZ	2.33	0.43
1:A:135:VAL:HG22	1:A:146:SER:HA	2.00	0.43
3:J:118:PHE:HA	3:J:119:PRO:HD3	1.87	0.43
1:A:55(A):GLY:HA3	3:L:32:PHE:CE1	2.54	0.43
2:N:76:ARG:HB2	1:O:107:GLU:OE2	2.17	0.43
1:S:53:ASP:HA	1:S:58:PRO:HD3	1.99	0.43
3:X:148:TRP:CD2	3:X:179:LEU:HD13	2.53	0.43
3:L:111:ALA:O	3:L:200:THR:HG21	2.17	0.43
4:R:48:ILE:HG12	4:R:63:PHE:CE2	2.54	0.43
3:V:148:TRP:CD2	3:V:179:LEU:HD13	2.53	0.43
4:W:48:ILE:HG12	4:W:63:PHE:CE2	2.54	0.43
5:A:2001:NAG:H61	5:A:2002:NAG:N2	2.33	0.43
1:C:135:VAL:HG22	1:C:146:SER:HA	2.00	0.43
1:C:55:ASN:O	3:E:30:LYS:HE3	2.19	0.43
3:E:148:TRP:CD2	3:E:179:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:118:PHE:HE2	4:K:124:LEU:O	2.01	0.43
3:J:169:LYS:HD2	3:J:169:LYS:HA	1.80	0.43
3:X:174:SER:HB3	4:T:174:PHE:CE1	2.53	0.43
1:M:276:ASN:ND2	4:T:31:GLU:O	2.50	0.43
3:X:162:SER:HB2	4:T:177:VAL:CG2	2.47	0.43
1:G:135:VAL:HG22	1:G:146:SER:HA	2.00	0.43
1:G:32:LYS:CG	9:G:2003:NAG:H81	2.47	0.43
1:G:58:PRO:HG2	1:G:60:ILE:HD11	2.00	0.43
2:I:58:LYS:HD2	2:I:58:LYS:HA	1.83	0.43
3:L:39:LYS:NZ	3:L:39:LYS:HB3	2.33	0.43
1:O:135:VAL:HG22	1:O:146:SER:HA	2.00	0.43
2:N:3:PHE:CE1	2:P:3:PHE:HE1	2.36	0.43
3:V:150:ILE:HG12	3:V:192:TYR:CD1	2.53	0.43
1:A:206:THR:HG23	1:A:241:ASP:OD2	2.19	0.43
1:A:62:ARG:NH1	1:A:63:ASP:OD2	2.52	0.43
1:C:16:GLY:HA3	2:D:14:TRP:CZ2	2.53	0.43
8:G:2001:NAG:H61	8:G:2002:NAG:N2	2.33	0.43
2:I:169:ASN:O	2:I:172:GLU:OE1	2.37	0.43
3:L:169:LYS:HD2	3:L:169:LYS:HA	1.80	0.43
4:R:66:ARG:HG3	4:R:66:ARG:H	1.53	0.43
3:E:203:SER:HA	3:E:204:PRO:HD3	1.91	0.43
3:J:150:ILE:HG12	3:J:192:TYR:CD1	2.53	0.43
1:S:206:THR:HG23	1:S:241:ASP:OD2	2.19	0.43
2:B:58:LYS:HA	2:B:58:LYS:HD2	1.83	0.43
3:E:39:LYS:NZ	3:E:39:LYS:HB3	2.33	0.43
4:H:137:MET:SD	4:H:194:PRO:HA	2.59	0.43
4:H:48:ILE:HG12	4:H:63:PHE:CE2	2.54	0.43
1:C:11:ASP:CA	2:D:27:SER:O	2.67	0.43
3:L:186:TYR:CE1	3:L:192:TYR:CE2	3.07	0.43
3:Q:186:TYR:CE1	3:Q:192:TYR:CE2	3.07	0.43
4:R:137:MET:SD	4:R:194:PRO:HA	2.59	0.43
1:C:316:LEU:HD23	2:D:100:VAL:HG13	2.01	0.42
3:J:135:PHE:CZ	4:K:124:LEU:CD1	3.02	0.42
4:K:137:MET:SD	4:K:194:PRO:HA	2.59	0.42
4:W:137:MET:SD	4:W:194:PRO:HA	2.59	0.42
3:J:8:PRO:CG	3:X:11:LEU:HD12	2.49	0.42
1:C:16:GLY:CA	2:D:14:TRP:CH2	3.01	0.42
1:C:16:GLY:HA3	2:D:14:TRP:CZ3	2.55	0.42
1:C:109:LYS:NZ	2:D:69:GLU:OE2	2.42	0.42
3:E:186:TYR:CE1	3:E:192:TYR:CE2	3.07	0.42
3:E:59:PRO:HG2	3:E:62:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:193:THR:HG22	3:J:194:CYS:N	2.34	0.42
3:L:4:LEU:HD23	3:L:4:LEU:HA	1.73	0.42
1:M:20:ASN:HA	2:N:15:GLN:OE1	2.19	0.42
2:N:169:ASN:O	2:N:172:GLU:OE1	2.37	0.42
2:P:22:TYR:HH	2:P:111:HIS:HD1	1.64	0.42
2:P:76:ARG:CZ	2:U:69:GLU:H	2.32	0.42
3:Q:59:PRO:HG2	3:Q:62:PHE:CE2	2.55	0.42
3:X:4:LEU:HD23	3:X:4:LEU:HA	1.73	0.42
4:H:52:PHE:CE2	4:H:53:ASN:HB3	2.53	0.42
3:J:62:PHE:CD1	3:J:75:ILE:HG12	2.55	0.42
4:K:48:ILE:HG12	4:K:63:PHE:CE2	2.54	0.42
3:L:133:VAL:HG21	4:H:143:LEU:HD13	2.00	0.42
1:M:58:PRO:HG2	1:M:60:ILE:HD11	2.00	0.42
1:O:323:THR:HA	1:O:324:PRO:HD3	1.77	0.42
3:Q:118:PHE:HA	3:Q:119:PRO:HD3	1.87	0.42
4:T:48:ILE:HG12	4:T:63:PHE:CE2	2.54	0.42
3:X:150:ILE:HG12	3:X:192:TYR:CD1	2.53	0.42
1:C:58:PRO:HG2	1:C:60:ILE:HD11	2.00	0.42
1:C:17:TYR:CE2	2:D:13:GLY:HA3	2.55	0.42
2:D:169:ASN:O	2:D:172:GLU:OE1	2.37	0.42
1:C:14:CYS:O	2:D:24:TYR:HA	2.19	0.42
1:G:28:THR:HA	2:I:101:LEU:HD22	2.01	0.42
3:J:119:PRO:HB3	3:J:209:PHE:CE2	2.55	0.42
1:M:135:VAL:HG22	1:M:146:SER:HA	2.00	0.42
4:T:19:LYS:NZ	4:T:81:ASP:HB3	2.34	0.42
3:X:119:PRO:HB3	3:X:209:PHE:CE2	2.55	0.42
1:O:206:THR:HG23	1:O:241:ASP:OD2	2.19	0.42
3:Q:119:PRO:HB3	3:Q:209:PHE:CE2	2.55	0.42
4:R:19:LYS:HE2	4:R:81:ASP:OD1	2.20	0.42
3:V:59:PRO:HG2	3:V:62:PHE:CE2	2.55	0.42
3:X:186:TYR:CE1	3:X:192:TYR:CE2	3.07	0.42
1:A:280:LYS:HE3	1:A:304:GLU:CG	2.50	0.42
1:C:206:THR:HG23	1:C:241:ASP:OD2	2.19	0.42
3:E:62:PHE:CD1	3:E:75:ILE:HG12	2.55	0.42
3:J:186:TYR:CE1	3:J:192:TYR:CE2	3.07	0.42
4:K:19:LYS:HE2	4:K:81:ASP:OD1	2.20	0.42
2:P:169:ASN:O	2:P:172:GLU:OE1	2.37	0.42
3:Q:62:PHE:CD1	3:Q:75:ILE:HG12	2.55	0.42
3:V:186:TYR:CE1	3:V:192:TYR:CE2	3.07	0.42
1:C:280:LYS:HE3	1:C:304:GLU:CG	2.50	0.42
2:D:3:PHE:CE2	2:D:113:SER:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:119:PRO:HG3	3:E:209:PHE:CD2	2.55	0.42
4:F:19:LYS:HE2	4:F:81:ASP:OD1	2.20	0.42
3:E:44:PRO:HG2	4:F:45:LEU:HD11	2.02	0.42
1:M:323:THR:HA	1:M:324:PRO:HD3	1.77	0.42
4:T:137:MET:SD	4:T:194:PRO:HA	2.59	0.42
4:T:93:VAL:CG1	4:T:100(C):PHE:HB3	2.50	0.42
3:V:119:PRO:HG3	3:V:209:PHE:CD2	2.55	0.42
2:B:169:ASN:O	2:B:172:GLU:OE1	2.37	0.42
1:C:16:GLY:CA	2:D:14:TRP:CZ3	3.03	0.42
3:E:27(B):VAL:HG23	3:E:92:ASN:HB2	2.02	0.42
1:G:206:THR:HG23	1:G:241:ASP:OD2	2.19	0.42
3:L:119:PRO:HB3	3:L:209:PHE:CE2	2.55	0.42
4:T:125:ALA:HA	4:T:126:PRO:HD3	1.85	0.42
2:P:76:ARG:NH1	2:U:69:GLU:H	2.17	0.42
3:V:27(B):VAL:HG23	3:V:92:ASN:HB2	2.02	0.42
4:W:33:THR:HG1	4:W:35:HIS:HE2	1.66	0.42
3:X:18:ARG:HG3	3:X:18:ARG:O	2.20	0.42
3:X:62:PHE:CD1	3:X:75:ILE:HG12	2.55	0.42
3:E:119:PRO:HB3	3:E:209:PHE:CE2	2.55	0.42
4:F:48:ILE:HG12	4:F:63:PHE:CE2	2.54	0.42
3:J:174:SER:CB	4:K:174:PHE:HE1	2.28	0.42
4:K:33:THR:HG1	4:K:35:HIS:HE2	1.67	0.42
3:L:59:PRO:HG2	3:L:62:PHE:CE2	2.55	0.42
1:M:280:LYS:HE3	1:M:304:GLU:CG	2.50	0.42
2:N:3:PHE:CE2	2:N:113:SER:HB2	2.55	0.42
1:O:280:LYS:HE3	1:O:304:GLU:CG	2.50	0.42
1:S:135:VAL:HG22	1:S:146:SER:HA	2.00	0.42
1:S:14:CYS:O	2:U:24:TYR:HA	2.20	0.42
1:S:18:HIS:HB2	2:U:20:GLY:O	2.20	0.42
3:V:119:PRO:HB3	3:V:209:PHE:CE2	2.55	0.42
1:G:280:LYS:HE3	1:G:304:GLU:CG	2.50	0.42
4:H:199:THR:O	4:H:204:GLU:N	2.50	0.42
3:L:174:SER:HB2	4:H:174:PHE:CE1	2.54	0.42
3:L:62:PHE:CD1	3:L:75:ILE:HG12	2.55	0.42
1:M:11:ASP:CG	2:N:28:ASN:CA	2.85	0.42
1:M:17:TYR:OH	2:N:13:GLY:N	2.52	0.42
1:M:206:THR:HG23	1:M:241:ASP:OD2	2.19	0.42
2:N:168:LEU:HD12	2:N:169:ASN:CA	2.48	0.42
1:O:62:ARG:CG	1:O:63:ASP:H	2.29	0.42
3:X:124:GLN:CB	4:T:122:TYR:CZ	3.03	0.42
2:U:73:LEU:HA	2:U:73:LEU:HD23	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:62:PHE:CD1	3:V:75:ILE:HG12	2.55	0.42
3:V:98:PHE:CZ	4:W:45:LEU:HB3	2.55	0.42
4:W:19:LYS:HE2	4:W:81:ASP:OD1	2.20	0.42
3:X:59:PRO:HG2	3:X:62:PHE:CE2	2.55	0.42
3:E:193:THR:HG22	3:E:194:CYS:N	2.34	0.41
4:F:137:MET:SD	4:F:194:PRO:HA	2.59	0.41
4:H:19:LYS:HE2	4:H:81:ASP:OD1	2.20	0.41
3:J:4:LEU:HA	3:J:4:LEU:HD23	1.73	0.41
3:J:119:PRO:CG	4:K:228:ARG:HH21	2.33	0.41
2:N:62:GLN:HG3	2:N:92:TRP:CD2	2.55	0.41
4:T:95:ASN:HA	4:T:100(C):PHE:HA	2.02	0.41
1:S:323:THR:HG21	2:U:13:GLY:H	1.85	0.41
2:N:74:GLU:CD	2:U:76:ARG:HH12	2.23	0.41
3:V:18:ARG:HG3	3:V:18:ARG:O	2.20	0.41
1:C:164:ILE:O	1:C:246:GLU:HA	2.20	0.41
2:D:73:LEU:HD23	2:D:73:LEU:HA	1.91	0.41
4:F:95:ASN:HA	4:F:100(C):PHE:HA	2.02	0.41
3:J:119:PRO:HG3	3:J:209:PHE:CD2	2.55	0.41
1:M:221:PRO:HB3	5:O:2001:NAG:H81	2.02	0.41
1:O:16:GLY:CA	2:P:14:TRP:CZ3	3.03	0.41
2:P:3:PHE:CE2	2:P:113:SER:HB2	2.55	0.41
3:Q:18:ARG:O	3:Q:18:ARG:HG3	2.20	0.41
3:Q:87:PHE:CE1	3:Q:101:GLY:HA3	2.56	0.41
2:U:169:ASN:O	2:U:172:GLU:OE1	2.37	0.41
3:V:135:PHE:CE2	4:W:124:LEU:HD13	2.55	0.41
4:W:66:ARG:H	4:W:66:ARG:HG3	1.53	0.41
1:C:16:GLY:HA3	2:D:14:TRP:CD2	2.55	0.41
3:E:18:ARG:O	3:E:18:ARG:HG3	2.20	0.41
4:H:66:ARG:HG3	4:H:66:ARG:H	1.53	0.41
3:J:90:GLN:HE21	3:J:97:THR:HG22	1.82	0.41
1:S:307:LYS:HB3	2:U:62:GLN:NE2	2.36	0.41
2:U:3:PHE:CE2	2:U:113:SER:HB2	2.55	0.41
3:X:87:PHE:CE1	3:X:101:GLY:HA3	2.56	0.41
2:B:3:PHE:CE2	2:B:113:SER:HB2	2.55	0.41
3:E:124:GLN:HG3	4:F:122:TYR:CE2	2.54	0.41
1:G:238:LYS:HA	1:G:239:PRO:HD3	1.94	0.41
4:H:11:LEU:HA	4:H:110:THR:O	2.21	0.41
3:J:59:PRO:HG2	3:J:62:PHE:CE2	2.54	0.41
3:L:27(B):VAL:HG23	3:L:92:ASN:HB2	2.02	0.41
3:V:4:LEU:HA	3:V:4:LEU:HD23	1.73	0.41
4:W:93:VAL:CG1	4:W:100(C):PHE:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:SER:OG	1:A:266:ALA:N	2.53	0.41
3:E:24:ARG:HH11	3:E:70:ASP:HB3	1.86	0.41
4:F:93:VAL:CG1	4:F:100(C):PHE:HB3	2.50	0.41
4:H:148:PHE:HA	4:H:149:PRO:HA	1.85	0.41
2:I:62:GLN:HG3	2:I:92:TRP:CD2	2.55	0.41
3:J:18:ARG:HG3	3:J:18:ARG:O	2.20	0.41
3:J:27(B):VAL:HG23	3:J:92:ASN:HB2	2.02	0.41
3:L:18:ARG:O	3:L:18:ARG:HG3	2.20	0.41
4:W:19:LYS:HZ1	4:W:81:ASP:HB2	1.86	0.41
1:C:17:TYR:CE2	2:D:13:GLY:CA	3.04	0.41
1:G:13:ILE:O	2:I:137:CYS:HA	2.21	0.41
4:K:95:ASN:HA	4:K:100(C):PHE:HA	2.03	0.41
2:D:58:LYS:HA	2:D:58:LYS:HD2	1.83	0.41
4:F:176:ALA:HA	4:F:187:LEU:HB3	2.03	0.41
1:G:164:ILE:O	1:G:246:GLU:HA	2.20	0.41
4:K:33:THR:HG23	4:K:95:ASN:HD22	1.86	0.41
2:N:11:GLU:O	2:N:11:GLU:HG3	2.21	0.41
2:N:55:ILE:HG23	2:N:99:LEU:HD23	2.03	0.41
1:S:18:HIS:HB2	2:U:21:TRP:HA	2.01	0.41
4:T:11:LEU:HA	4:T:110:THR:O	2.21	0.41
3:V:193:THR:HG22	3:V:194:CYS:N	2.34	0.41
4:W:199:THR:O	4:W:204:GLU:N	2.51	0.41
3:X:95:PRO:O	3:X:97:THR:HG22	2.21	0.41
2:B:62:GLN:HG3	2:B:92:TRP:CD2	2.55	0.41
3:E:139:PHE:HD2	3:E:198:HIS:HE2	1.69	0.41
4:F:140:LEU:HD23	4:F:140:LEU:HA	1.90	0.41
4:H:157:TRP:CZ2	4:H:191:VAL:HG12	2.56	0.41
2:I:3:PHE:CE2	2:I:113:SER:HB2	2.55	0.41
4:K:11:LEU:HA	4:K:110:THR:O	2.21	0.41
3:L:87:PHE:CE1	3:L:101:GLY:HA3	2.56	0.41
1:O:164:ILE:O	1:O:246:GLU:HA	2.20	0.41
1:O:265:SER:OG	1:O:266:ALA:N	2.53	0.41
2:P:11:GLU:O	2:P:11:GLU:HG3	2.21	0.41
2:P:62:GLN:HG3	2:P:92:TRP:CD2	2.55	0.41
1:S:164:ILE:O	1:S:246:GLU:HA	2.21	0.41
1:S:280:LYS:HE3	1:S:304:GLU:CG	2.50	0.41
4:W:11:LEU:HA	4:W:110:THR:O	2.21	0.41
4:W:157:TRP:CZ2	4:W:191:VAL:HG12	2.56	0.41
4:F:33:THR:HG23	4:F:95:ASN:HD22	1.86	0.41
4:H:176:ALA:HA	4:H:187:LEU:HB3	2.03	0.41
2:I:11:GLU:HG3	2:I:11:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:GLN:NE2	2:I:63:PHE:CZ	2.89	0.41
3:L:119:PRO:HG3	3:L:209:PHE:CD2	2.55	0.41
1:M:52:CYS:HB2	1:M:279:THR:HG22	2.03	0.41
2:P:150:GLU:CB	6:P:2001:NAG:H62	2.47	0.41
2:P:55:ILE:HG23	2:P:99:LEU:HD23	2.03	0.41
3:Q:193:THR:HG22	3:Q:194:CYS:N	2.35	0.41
4:T:176:ALA:HA	4:T:187:LEU:HB3	2.03	0.41
2:U:11:GLU:HG3	2:U:11:GLU:O	2.21	0.41
2:U:55:ILE:HG23	2:U:99:LEU:HD23	2.03	0.41
3:X:119:PRO:HG3	3:X:209:PHE:CD2	2.55	0.41
3:X:193:THR:HG22	3:X:194:CYS:N	2.34	0.41
3:X:24:ARG:HH11	3:X:70:ASP:HB3	1.86	0.41
1:A:218:ALA:CB	1:C:203:SER:HB2	2.46	0.41
1:C:62:ARG:NH1	1:C:63:ASP:OD2	2.53	0.41
1:G:265:SER:OG	1:G:266:ALA:N	2.53	0.41
4:H:36:TRP:CZ3	4:H:92:CYS:HB2	2.56	0.41
3:J:87:PHE:CE1	3:J:101:GLY:HA3	2.56	0.41
4:K:36:TRP:CZ3	4:K:92:CYS:HB2	2.56	0.41
1:S:52:CYS:HB2	1:S:279:THR:HG22	2.03	0.41
2:U:62:GLN:HG3	2:U:92:TRP:CD2	2.55	0.41
3:V:87:PHE:CE1	3:V:101:GLY:HA3	2.56	0.41
3:V:95:PRO:O	3:V:97:THR:HG22	2.21	0.41
2:B:11:GLU:O	2:B:11:GLU:HG3	2.21	0.41
1:C:211:GLN:NE2	1:C:213:LEU:HD11	2.36	0.41
4:F:36:TRP:CZ3	4:F:92:CYS:HB2	2.56	0.41
1:G:62:ARG:NH1	1:G:63:ASP:OD2	2.53	0.41
4:H:93:VAL:CG1	4:H:100(C):PHE:HB3	2.50	0.41
4:H:33:THR:HG23	4:H:95:ASN:HD22	1.86	0.41
1:M:106:GLU:HG2	2:N:70:PHE:HA	2.03	0.41
1:M:164:ILE:O	1:M:246:GLU:HA	2.20	0.41
2:P:168:LEU:HA	2:P:168:LEU:HD23	1.96	0.41
3:Q:119:PRO:HG3	3:Q:209:PHE:CD2	2.55	0.41
4:R:93:VAL:CG1	4:R:100(C):PHE:HB3	2.50	0.41
4:R:11:LEU:HA	4:R:110:THR:O	2.21	0.41
3:Q:124:GLN:HB2	4:R:122:TYR:CG	2.56	0.41
4:R:157:TRP:CZ2	4:R:191:VAL:HG12	2.56	0.41
4:R:33:THR:HG23	4:R:95:ASN:HD22	1.86	0.41
1:A:211:GLN:NE2	1:A:213:LEU:HD11	2.36	0.40
1:C:52:CYS:HB2	1:C:279:THR:HG22	2.03	0.40
1:G:211:GLN:NE2	1:G:213:LEU:HD11	2.36	0.40
1:G:28:THR:CA	2:I:101:LEU:HD22	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:22:TYR:OH	2:I:111:HIS:ND1	2.40	0.40
2:I:55:ILE:HG23	2:I:99:LEU:HD23	2.03	0.40
4:K:93:VAL:CG1	4:K:100(C):PHE:HB3	2.50	0.40
3:L:24:ARG:HH11	3:L:70:ASP:HB3	1.86	0.40
1:M:62:ARG:NH1	1:M:63:ASP:OD2	2.53	0.40
1:S:53:ASP:OD1	1:S:56:VAL:C	2.60	0.40
2:U:22:TYR:OH	2:U:111:HIS:ND1	2.40	0.40
4:W:95:ASN:HA	4:W:100(C):PHE:HA	2.02	0.40
4:F:157:TRP:CZ2	4:F:191:VAL:HG12	2.56	0.40
1:G:62:ARG:CG	1:G:63:ASP:H	2.29	0.40
4:H:24:THR:HG22	4:H:76:SER:OG	2.21	0.40
1:G:15:ILE:HG13	2:I:119:TYR:HA	2.03	0.40
3:L:193:THR:HG22	3:L:194:CYS:N	2.34	0.40
3:L:95:PRO:O	3:L:97:THR:HG22	2.21	0.40
1:M:323:THR:HG21	2:N:12:GLY:HA2	2.02	0.40
1:O:211:GLN:NE2	1:O:213:LEU:HD11	2.36	0.40
3:Q:139:PHE:HD2	3:Q:198:HIS:HE2	1.69	0.40
4:T:36:TRP:CH2	4:T:92:CYS:HB2	2.56	0.40
3:X:162:SER:HB2	4:T:177:VAL:HG21	2.04	0.40
3:X:27(B):VAL:HG23	3:X:92:ASN:HB2	2.02	0.40
1:C:62:ARG:CG	1:C:63:ASP:H	2.29	0.40
2:D:11:GLU:O	2:D:11:GLU:HG3	2.21	0.40
2:D:55:ILE:HG23	2:D:99:LEU:HD23	2.03	0.40
1:G:53:ASP:OD1	1:G:56:VAL:C	2.60	0.40
3:L:118:PHE:HA	3:L:119:PRO:HD3	1.87	0.40
1:M:131:ASP:OD2	1:M:133(A):SER:OG	2.37	0.40
1:O:62:ARG:NH1	1:O:63:ASP:OD2	2.53	0.40
3:Q:27(B):VAL:HG23	3:Q:92:ASN:HB2	2.02	0.40
3:Q:24:ARG:HH11	3:Q:70:ASP:HB3	1.86	0.40
3:Q:95:PRO:O	3:Q:97:THR:HG22	2.21	0.40
4:R:19:LYS:HZ1	4:R:81:ASP:HB2	1.85	0.40
4:T:66:ARG:H	4:T:66:ARG:HG3	1.53	0.40
3:V:24:ARG:HH11	3:V:70:ASP:HB3	1.86	0.40
4:W:36:TRP:CH2	4:W:92:CYS:HB2	2.57	0.40
1:A:164:ILE:O	1:A:246:GLU:HA	2.21	0.40
2:D:62:GLN:HG3	2:D:92:TRP:CD2	2.55	0.40
4:F:36:TRP:CH2	4:F:92:CYS:HB2	2.56	0.40
3:J:139:PHE:HD2	3:J:198:HIS:HE2	1.69	0.40
3:J:24:ARG:HH11	3:J:70:ASP:HB3	1.86	0.40
4:K:176:ALA:HA	4:K:187:LEU:HB3	2.03	0.40
4:R:36:TRP:CZ3	4:R:92:CYS:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:36:TRP:CZ3	4:W:92:CYS:HB2	2.56	0.40
1:A:53:ASP:OD1	1:A:56:VAL:C	2.60	0.40
1:C:53:ASP:OD1	1:C:56:VAL:C	2.60	0.40
4:K:222:LYS:H	4:K:222:LYS:HG2	1.69	0.40
4:K:24:THR:HG22	4:K:76:SER:OG	2.21	0.40
4:K:82(A):ARG:NH1	4:K:82(A):ARG:HB3	2.37	0.40
1:M:53:ASP:OD1	1:M:56:VAL:C	2.60	0.40
1:S:62:ARG:NH1	1:S:63:ASP:OD2	2.53	0.40
4:T:24:THR:HG22	4:T:76:SER:OG	2.22	0.40
4:W:33:THR:HG23	4:W:95:ASN:HD22	1.86	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	318/334 (95%)	309 (97%)	9 (3%)	0	100	100
1	C	315/334 (94%)	305 (97%)	10 (3%)	0	100	100
1	G	315/334 (94%)	306 (97%)	9 (3%)	0	100	100
1	M	318/334 (95%)	309 (97%)	9 (3%)	0	100	100
1	O	314/334 (94%)	305 (97%)	9 (3%)	0	100	100
1	S	318/334 (95%)	308 (97%)	10 (3%)	0	100	100
2	B	168/182 (92%)	164 (98%)	4 (2%)	0	100	100
2	D	168/182 (92%)	164 (98%)	4 (2%)	0	100	100
2	I	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	N	163/182 (90%)	160 (98%)	3 (2%)	0	100	100
2	P	168/182 (92%)	164 (98%)	4 (2%)	0	100	100
2	U	171/182 (94%)	167 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	212/218 (97%)	194 (92%)	18 (8%)	0	100	100
3	J	203/218 (93%)	185 (91%)	18 (9%)	0	100	100
3	L	209/218 (96%)	191 (91%)	18 (9%)	0	100	100
3	Q	209/218 (96%)	191 (91%)	18 (9%)	0	100	100
3	V	206/218 (94%)	189 (92%)	17 (8%)	0	100	100
3	X	212/218 (97%)	194 (92%)	18 (8%)	0	100	100
4	F	217/222 (98%)	187 (86%)	26 (12%)	4 (2%)	10	49
4	H	217/222 (98%)	189 (87%)	24 (11%)	4 (2%)	10	49
4	K	217/222 (98%)	188 (87%)	25 (12%)	4 (2%)	10	49
4	R	217/222 (98%)	189 (87%)	24 (11%)	4 (2%)	10	49
4	T	216/222 (97%)	188 (87%)	25 (12%)	3 (1%)	13	54
4	W	217/222 (98%)	188 (87%)	25 (12%)	4 (2%)	10	49
All	All	5459/5736 (95%)	5101 (93%)	335 (6%)	23 (0%)	38	77

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	135	ASN
4	F	135	ASN
4	K	135	ASN
4	R	135	ASN
4	W	135	ASN
4	H	229	ASP
4	F	229	ASP
4	K	229	ASP
4	T	229	ASP
4	R	229	ASP
4	W	229	ASP
4	H	96	TYR
4	F	96	TYR
4	K	96	TYR
4	T	96	TYR
4	R	96	TYR
4	W	96	TYR
4	H	41	HIS
4	F	41	HIS
4	K	41	HIS
4	T	41	HIS

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Mol	Chain	Res	Type
4	R	41	HIS
4	W	41	HIS

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	286/297 (96%)	276 (96%)	10 (4%)	41	69
1	C	285/297 (96%)	274 (96%)	11 (4%)	37	66
1	G	285/297 (96%)	275 (96%)	10 (4%)	41	69
1	M	286/297 (96%)	276 (96%)	10 (4%)	41	69
1	O	283/297 (95%)	273 (96%)	10 (4%)	41	69
1	S	286/297 (96%)	276 (96%)	10 (4%)	41	69
2	B	147/155 (95%)	146 (99%)	1 (1%)	87	93
2	D	147/155 (95%)	146 (99%)	1 (1%)	87	93
2	I	148/155 (96%)	147 (99%)	1 (1%)	87	93
2	N	144/155 (93%)	144 (100%)	0	100	100
2	P	147/155 (95%)	146 (99%)	1 (1%)	87	93
2	U	148/155 (96%)	146 (99%)	2 (1%)	71	86
3	E	189/191 (99%)	172 (91%)	17 (9%)	11	38
3	J	185/191 (97%)	169 (91%)	16 (9%)	12	42
3	L	188/191 (98%)	171 (91%)	17 (9%)	11	38
3	Q	188/191 (98%)	172 (92%)	16 (8%)	12	42
3	V	187/191 (98%)	170 (91%)	17 (9%)	11	38
3	X	189/191 (99%)	172 (91%)	17 (9%)	11	38
4	F	192/193 (100%)	176 (92%)	16 (8%)	13	43
4	H	192/193 (100%)	176 (92%)	16 (8%)	13	43
4	K	192/193 (100%)	176 (92%)	16 (8%)	13	43
4	R	192/193 (100%)	176 (92%)	16 (8%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	T	191/193 (99%)	174 (91%)	17 (9%)	11	39
4	W	192/193 (100%)	175 (91%)	17 (9%)	11	39
All	All	4869/5016 (97%)	4604 (95%)	265 (5%)	26	58

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	29	ILE
1	A	36	VAL
1	A	82	VAL
1	A	111	LEU
1	A	125(A)	LYS
1	A	135	VAL
1	A	151	VAL
1	A	195	TYR
1	A	197	ASN
2	B	69	GLU
1	C	26	VAL
1	C	29	ILE
1	C	36	VAL
1	C	82	VAL
1	C	111	LEU
1	C	125(A)	LYS
1	C	135	VAL
1	C	151	VAL
1	C	195	TYR
1	C	197	ASN
1	C	210	ASN
2	D	69	GLU
1	G	26	VAL
1	G	29	ILE
1	G	36	VAL
1	G	82	VAL
1	G	111	LEU
1	G	125(A)	LYS
1	G	135	VAL
1	G	151	VAL
1	G	195	TYR
1	G	197	ASN
1	M	26	VAL

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Mol	Chain	Res	Type
1	M	29	ILE
1	M	36	VAL
1	M	82	VAL
1	M	111	LEU
1	M	125(A)	LYS
1	M	135	VAL
1	M	151	VAL
1	M	195	TYR
1	M	197	ASN
1	O	26	VAL
1	O	29	ILE
1	O	36	VAL
1	O	82	VAL
1	O	111	LEU
1	O	125(A)	LYS
1	O	135	VAL
1	O	151	VAL
1	O	195	TYR
1	O	197	ASN
2	P	69	GLU
1	S	26	VAL
1	S	29	ILE
1	S	36	VAL
1	S	82	VAL
1	S	111	LEU
1	S	125(A)	LYS
1	S	135	VAL
1	S	151	VAL
1	S	195	TYR
1	S	197	ASN
3	L	14	SER
3	L	24	ARG
3	L	30	LYS
3	L	39	LYS
3	L	42	GLN
3	L	43	SER
3	L	53	ASN
3	L	69	THR
3	L	70	ASP
3	L	83	VAL
3	L	97	THR
3	L	116	SER

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Mol	Chain	Res	Type
3	L	142	LYS
3	L	157	ASN
3	L	184	ASP
3	L	197	THR
3	L	202	THR
3	E	14	SER
3	E	24	ARG
3	E	30	LYS
3	E	39	LYS
3	E	42	GLN
3	E	43	SER
3	E	53	ASN
3	E	69	THR
3	E	70	ASP
3	E	83	VAL
3	E	97	THR
3	E	116	SER
3	E	142	LYS
3	E	157	ASN
3	E	184	ASP
3	E	197	THR
3	E	202	THR
3	J	14	SER
3	J	24	ARG
3	J	30	LYS
3	J	39	LYS
3	J	42	GLN
3	J	43	SER
3	J	53	ASN
3	J	69	THR
3	J	70	ASP
3	J	83	VAL
3	J	97	THR
3	J	116	SER
3	J	142	LYS
3	J	184	ASP
3	J	197	THR
3	J	202	THR
3	X	14	SER
3	X	24	ARG
3	X	30	LYS
3	X	39	LYS

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Mol	Chain	Res	Type
3	X	42	GLN
3	X	43	SER
3	X	53	ASN
3	X	69	THR
3	X	70	ASP
3	X	83	VAL
3	X	97	THR
3	X	116	SER
3	X	142	LYS
3	X	157	ASN
3	X	184	ASP
3	X	197	THR
3	X	202	THR
3	Q	14	SER
3	Q	24	ARG
3	Q	30	LYS
3	Q	39	LYS
3	Q	42	GLN
3	Q	43	SER
3	Q	53	ASN
3	Q	69	THR
3	Q	70	ASP
3	Q	83	VAL
3	Q	97	THR
3	Q	116	SER
3	Q	142	LYS
3	Q	157	ASN
3	Q	184	ASP
3	Q	197	THR
3	V	14	SER
3	V	24	ARG
3	V	30	LYS
3	V	39	LYS
3	V	42	GLN
3	V	43	SER
3	V	53	ASN
3	V	69	THR
3	V	70	ASP
3	V	83	VAL
3	V	97	THR
3	V	116	SER
3	V	142	LYS

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Mol	Chain	Res	Type
3	V	157	ASN
3	V	184	ASP
3	V	197	THR
3	V	202	THR
2	I	69	GLU
2	U	69	GLU
2	U	97	GLU
4	H	1	GLU
4	H	2	VAL
4	H	11	LEU
4	H	12	VAL
4	H	18	VAL
4	H	24	THR
4	H	30	THR
4	H	33	THR
4	H	58	THR
4	H	73	ARG
4	H	75	SER
4	H	190	SER
4	H	204	GLU
4	H	209	ASN
4	H	222	LYS
4	H	229	ASP
4	F	1	GLU
4	F	2	VAL
4	F	11	LEU
4	F	12	VAL
4	F	18	VAL
4	F	24	THR
4	F	30	THR
4	F	33	THR
4	F	58	THR
4	F	73	ARG
4	F	75	SER
4	F	190	SER
4	F	204	GLU
4	F	209	ASN
4	F	222	LYS
4	F	229	ASP
4	K	1	GLU
4	K	2	VAL
4	K	11	LEU

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Mol	Chain	Res	Type
4	K	12	VAL
4	K	18	VAL
4	K	24	THR
4	K	30	THR
4	K	33	THR
4	K	58	THR
4	K	73	ARG
4	K	75	SER
4	K	190	SER
4	K	204	GLU
4	K	209	ASN
4	K	222	LYS
4	K	229	ASP
4	T	1	GLU
4	T	2	VAL
4	T	11	LEU
4	T	12	VAL
4	T	18	VAL
4	T	24	THR
4	T	30	THR
4	T	33	THR
4	T	58	THR
4	T	73	ARG
4	T	75	SER
4	T	81	ASP
4	T	190	SER
4	T	204	GLU
4	T	209	ASN
4	T	222	LYS
4	T	229	ASP
4	R	1	GLU
4	R	2	VAL
4	R	11	LEU
4	R	12	VAL
4	R	18	VAL
4	R	24	THR
4	R	30	THR
4	R	33	THR
4	R	58	THR
4	R	73	ARG
4	R	75	SER
4	R	190	SER

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Mol	Chain	Res	Type
4	R	204	GLU
4	R	209	ASN
4	R	222	LYS
4	R	229	ASP
4	W	1	GLU
4	W	2	VAL
4	W	11	LEU
4	W	12	VAL
4	W	18	VAL
4	W	24	THR
4	W	30	THR
4	W	33	THR
4	W	58	THR
4	W	73	ARG
4	W	75	SER
4	W	179	GLN
4	W	190	SER
4	W	204	GLU
4	W	209	ASN
4	W	222	LYS
4	W	229	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	C	211	GLN
1	C	276	ASN
1	G	211	GLN
1	M	211	GLN
1	M	276	ASN
1	O	211	GLN
1	S	211	GLN
3	V	38	GLN
4	H	95	ASN
4	F	95	ASN
4	K	95	ASN
4	K	172	HIS
4	T	95	ASN
4	R	95	ASN
4	W	39	GLN
4	W	95	ASN

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 ⓘ

28 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$
5	NAG	A	2001	1,5	14,14,15	1.31	2 (14%)	15,19,21	2.07	4 (26%)
5	NAG	A	2002	5	14,14,15	1.87	4 (28%)	15,19,21	1.61	2 (13%)
5	MAN	A	2003	5	11,11,12	1.99	3 (27%)	13,15,17	1.87	4 (30%)
7	NAG	C	2002	1,7	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
7	NAG	C	2003	7	14,14,15	0.49	0	15,19,21	1.19	2 (13%)
7	BMA	C	2004	7	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
7	MAN	C	2005	7	11,11,12	0.60	0	13,15,17	2.60	3 (23%)
7	MAN	C	2006	7	11,11,12	0.57	0	13,15,17	2.05	5 (38%)
7	MAN	C	2007	7	11,11,12	0.58	0	13,15,17	2.00	5 (38%)
7	MAN	C	2008	7	11,11,12	0.59	0	13,15,17	2.41	6 (46%)
7	MAN	C	2009	7	11,11,12	0.60	0	13,15,17	2.46	6 (46%)
8	NAG	G	2001	1,8	14,14,15	1.38	3 (21%)	15,19,21	1.97	4 (26%)
8	NAG	G	2002	8	14,14,15	1.74	4 (28%)	15,19,21	1.88	5 (33%)
9	NAG	G	2003	1,9	14,14,15	0.54	0	15,19,21	1.33	3 (20%)
9	NAG	G	2004	9	14,14,15	0.44	0	15,19,21	0.61	0
9	BMA	G	2005	9	11,11,12	0.61	0	13,15,17	0.65	0
8	NAG	M	2001	1,8	14,14,15	1.30	2 (14%)	15,19,21	2.06	4 (26%)
8	NAG	M	2002	8	14,14,15	1.85	4 (28%)	15,19,21	1.61	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	O	2001	1,5	14,14,15	1.28	1 (7%)	15,19,21	1.85	4 (26%)
5	NAG	O	2002	5	14,14,15	1.81	4 (28%)	15,19,21	1.86	6 (40%)
5	MAN	O	2003	5	11,11,12	1.87	3 (27%)	13,15,17	1.95	4 (30%)
10	NAG	O	2005	1,10	14,14,15	0.58	0	15,19,21	1.35	2 (13%)
10	NAG	O	2006	10	14,14,15	0.47	0	15,19,21	1.19	2 (13%)
10	BMA	O	2007	10	11,11,12	0.75	0	13,15,17	0.69	0
10	MAN	O	2008	10	11,11,12	0.62	0	13,15,17	1.09	1 (7%)
5	NAG	S	2001	1,5	14,14,15	1.38	3 (21%)	15,19,21	1.99	5 (33%)
5	NAG	S	2002	5	14,14,15	1.74	4 (28%)	15,19,21	1.89	5 (33%)
5	MAN	S	2003	5	11,11,12	1.84	3 (27%)	13,15,17	2.04	4 (30%)

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	2001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2002	5	-	0/6/23/26	0/1/1/1
5	MAN	A	2003	5	-	0/2/19/22	0/1/1/1
7	NAG	C	2002	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	2003	7	-	0/6/23/26	0/1/1/1
7	BMA	C	2004	7	-	0/2/19/22	0/1/1/1
7	MAN	C	2005	7	-	0/2/19/22	0/1/1/1
7	MAN	C	2006	7	-	0/2/19/22	0/1/1/1
7	MAN	C	2007	7	-	0/2/19/22	0/1/1/1
7	MAN	C	2008	7	-	0/2/19/22	0/1/1/1
7	MAN	C	2009	7	-	0/2/19/22	0/1/1/1
8	NAG	G	2001	1,8	-	0/6/23/26	0/1/1/1
8	NAG	G	2002	8	-	0/6/23/26	0/1/1/1
9	NAG	G	2003	1,9	-	0/6/23/26	0/1/1/1
9	NAG	G	2004	9	-	0/6/23/26	0/1/1/1
9	BMA	G	2005	9	-	0/2/19/22	0/1/1/1
8	NAG	M	2001	1,8	-	0/6/23/26	0/1/1/1
8	NAG	M	2002	8	-	0/6/23/26	0/1/1/1
5	NAG	O	2001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2002	5	-	0/6/23/26	0/1/1/1
5	MAN	O	2003	5	-	0/2/19/22	0/1/1/1
10	NAG	O	2005	1,10	-	0/6/23/26	0/1/1/1
10	NAG	O	2006	10	-	0/6/23/26	0/1/1/1
10	BMA	O	2007	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	O	2008	10	-	0/2/19/22	0/1/1/1
5	NAG	S	2001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2002	5	-	0/6/23/26	0/1/1/1
5	MAN	S	2003	5	-	0/2/19/22	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	2001	NAG	C4-C5	2.08	1.57	1.53
8	G	2001	NAG	C4-C5	2.08	1.57	1.53
8	M	2001	NAG	C3-C2	2.13	1.57	1.52
8	G	2001	NAG	C3-C2	2.13	1.57	1.52
5	A	2001	NAG	C3-C2	2.16	1.57	1.52
5	S	2001	NAG	C3-C2	2.16	1.57	1.52
5	A	2003	MAN	C1-C2	2.19	1.57	1.52
8	G	2001	NAG	C1-C2	2.23	1.55	1.52
8	G	2002	NAG	O4-C4	2.26	1.48	1.43
5	A	2002	NAG	C4-C5	2.27	1.57	1.53
8	M	2002	NAG	C4-C5	2.27	1.57	1.53
5	S	2002	NAG	O4-C4	2.27	1.48	1.43
5	O	2003	MAN	C4-C3	2.29	1.58	1.52
5	S	2003	MAN	C4-C3	2.29	1.58	1.52
5	S	2001	NAG	C1-C2	2.29	1.55	1.52
5	S	2003	MAN	C1-C2	2.30	1.57	1.52
5	O	2002	NAG	C4-C3	2.34	1.58	1.52
8	G	2002	NAG	C3-C2	2.43	1.57	1.52
5	O	2002	NAG	C4-C5	2.45	1.58	1.53
5	A	2001	NAG	O3-C3	2.46	1.48	1.43
5	S	2002	NAG	C3-C2	2.47	1.57	1.52
8	M	2001	NAG	O3-C3	2.52	1.48	1.43
8	G	2002	NAG	C4-C3	2.70	1.59	1.52
5	S	2002	NAG	C4-C3	2.75	1.59	1.52
5	O	2001	NAG	C1-C2	2.75	1.56	1.52
5	O	2003	MAN	C1-C2	2.80	1.58	1.52
8	M	2002	NAG	O4-C4	2.88	1.49	1.43
5	A	2002	NAG	O4-C4	2.89	1.49	1.43
8	M	2002	NAG	C4-C3	3.00	1.60	1.52
5	A	2002	NAG	C4-C3	3.01	1.60	1.52
5	A	2003	MAN	C4-C3	3.05	1.60	1.52
5	O	2002	NAG	C1-C2	3.11	1.56	1.52
5	O	2003	MAN	C2-C3	3.19	1.56	1.52
5	A	2003	MAN	C2-C3	3.20	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	2002	NAG	O4-C4	3.21	1.50	1.43
5	S	2003	MAN	C2-C3	3.36	1.57	1.52
5	S	2002	NAG	C1-C2	3.59	1.57	1.52
8	G	2002	NAG	C1-C2	3.62	1.57	1.52
8	M	2002	NAG	C1-C2	3.64	1.57	1.52
5	A	2002	NAG	C1-C2	3.75	1.57	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	2002	NAG	O5-C1-C2	-8.48	99.67	111.47
7	C	2008	MAN	C6-C5-C4	-5.05	101.18	113.00
7	C	2006	MAN	O4-C4-C3	-4.18	101.27	110.36
7	C	2005	MAN	C2-C3-C4	-4.06	103.80	110.88
7	C	2008	MAN	O4-C4-C3	-3.81	102.07	110.36
5	S	2001	NAG	C8-C7-N2	-3.76	109.32	116.11
8	G	2001	NAG	C8-C7-N2	-3.69	109.44	116.11
7	C	2007	MAN	O4-C4-C3	-3.63	102.46	110.36
7	C	2005	MAN	O5-C1-C2	-3.43	105.41	110.79
7	C	2008	MAN	C3-C4-C5	-3.17	104.64	110.22
5	S	2002	NAG	C3-C4-C5	-3.12	104.72	110.22
8	G	2002	NAG	C3-C4-C5	-3.11	104.73	110.22
7	C	2008	MAN	O2-C2-C3	-3.04	104.19	110.17
9	G	2003	NAG	C2-N2-C7	-2.98	118.60	122.94
8	M	2002	NAG	C3-C4-C5	-2.82	105.24	110.22
9	G	2003	NAG	O5-C1-C2	-2.82	107.55	111.47
7	C	2002	NAG	O7-C7-C8	-2.79	116.98	122.06
5	A	2001	NAG	C8-C7-N2	-2.78	111.09	116.11
5	A	2002	NAG	C3-C4-C5	-2.77	105.33	110.22
8	M	2001	NAG	C8-C7-N2	-2.75	111.15	116.11
7	C	2003	NAG	O5-C1-C2	-2.70	107.71	111.47
5	O	2001	NAG	C8-C7-N2	-2.70	111.23	116.11
7	C	2002	NAG	C4-C3-C2	-2.68	107.09	111.02
7	C	2004	BMA	O4-C4-C5	-2.58	102.79	109.28
7	C	2004	BMA	C6-C5-C4	-2.42	107.34	113.00
7	C	2006	MAN	O3-C3-C2	-2.37	105.72	110.02
9	G	2003	NAG	O3-C3-C2	-2.35	104.35	109.39
5	O	2002	NAG	C8-C7-N2	-2.35	111.87	116.11
7	C	2003	NAG	C4-C3-C2	-2.20	107.80	111.02
7	C	2009	MAN	C1-C2-C3	-2.14	106.94	109.65
10	O	2006	NAG	O4-C4-C3	-2.11	105.77	110.36
7	C	2009	MAN	O4-C4-C3	-2.10	105.79	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	2002	NAG	C3-C4-C5	-2.01	106.67	110.22
5	S	2001	NAG	O7-C7-N2	2.00	125.77	121.92
8	G	2001	NAG	O3-C3-C4	2.01	114.73	110.36
5	O	2003	MAN	C3-C4-C5	2.02	113.77	110.22
10	O	2006	NAG	C1-O5-C5	2.03	114.96	112.17
5	S	2001	NAG	O3-C3-C4	2.03	114.78	110.36
5	A	2003	MAN	C3-C4-C5	2.08	113.88	110.22
5	O	2001	NAG	C2-N2-C7	2.09	126.00	122.94
7	C	2008	MAN	C2-C3-C4	2.09	114.52	110.88
7	C	2006	MAN	O3-C3-C4	2.10	114.92	110.36
5	O	2001	NAG	O3-C3-C2	2.15	114.00	109.39
7	C	2007	MAN	C1-O5-C5	2.16	115.14	112.17
5	O	2002	NAG	O4-C4-C3	2.21	115.17	110.36
7	C	2006	MAN	C1-O5-C5	2.26	115.28	112.17
5	S	2003	MAN	C3-C4-C5	2.27	114.22	110.22
5	S	2002	NAG	C1-C2-N2	2.29	114.41	110.49
8	G	2002	NAG	C1-C2-N2	2.31	114.43	110.49
8	G	2002	NAG	O4-C4-C3	2.37	115.52	110.36
5	S	2002	NAG	O4-C4-C3	2.41	115.59	110.36
8	M	2001	NAG	O3-C3-C2	2.42	114.56	109.39
7	C	2008	MAN	O2-C2-C1	2.42	114.11	109.18
5	A	2001	NAG	O3-C3-C2	2.48	114.70	109.39
8	G	2001	NAG	O3-C3-C2	2.51	114.76	109.39
5	S	2001	NAG	O3-C3-C2	2.54	114.84	109.39
10	O	2005	NAG	C1-C2-N2	2.56	114.86	110.49
7	C	2007	MAN	O5-C1-C2	2.56	114.81	110.79
5	O	2002	NAG	C2-N2-C7	2.60	126.73	122.94
7	C	2007	MAN	O3-C3-C2	2.61	114.77	110.02
5	A	2003	MAN	C2-C3-C4	2.65	115.51	110.88
7	C	2009	MAN	O4-C4-C5	2.75	116.22	109.28
7	C	2009	MAN	O2-C2-C1	2.95	115.19	109.18
5	O	2002	NAG	C4-C3-C2	2.97	115.37	111.02
5	S	2003	MAN	O2-C2-C1	2.98	115.23	109.18
8	G	2002	NAG	C1-O5-C5	3.00	116.30	112.17
7	C	2004	BMA	O2-C2-C3	3.01	116.08	110.17
5	S	2002	NAG	C1-O5-C5	3.06	116.39	112.17
10	O	2005	NAG	C1-O5-C5	3.07	116.39	112.17
5	O	2003	MAN	C2-C3-C4	3.10	116.28	110.88
5	A	2001	NAG	C2-N2-C7	3.14	127.52	122.94
8	M	2002	NAG	O3-C3-C4	3.15	117.21	110.36
8	M	2001	NAG	C2-N2-C7	3.15	127.54	122.94
5	A	2002	NAG	O3-C3-C4	3.18	117.28	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	2002	NAG	O3-C3-C4	3.18	117.28	110.36
7	C	2006	MAN	O4-C4-C5	3.18	117.31	109.28
8	G	2002	NAG	O3-C3-C4	3.20	117.33	110.36
10	O	2008	MAN	C1-O5-C5	3.22	116.60	112.17
7	C	2007	MAN	C2-C3-C4	3.23	116.51	110.88
5	S	2003	MAN	C2-C3-C4	3.25	116.55	110.88
7	C	2009	MAN	C3-C4-C5	3.45	116.30	110.22
5	A	2003	MAN	O2-C2-C1	3.47	116.24	109.18
5	O	2003	MAN	C1-O5-C5	3.58	117.09	112.17
5	O	2002	NAG	O3-C3-C4	3.77	118.57	110.36
5	A	2003	MAN	C1-O5-C5	4.10	117.82	112.17
5	O	2003	MAN	O2-C2-C1	4.21	117.73	109.18
5	O	2001	NAG	C1-O5-C5	4.34	118.15	112.17
8	G	2001	NAG	C1-O5-C5	4.52	118.39	112.17
5	S	2001	NAG	C1-O5-C5	4.53	118.41	112.17
5	S	2003	MAN	C1-O5-C5	4.83	118.82	112.17
5	A	2001	NAG	C1-O5-C5	5.01	119.07	112.17
8	M	2001	NAG	C1-O5-C5	5.03	119.10	112.17
7	C	2009	MAN	C1-O5-C5	5.70	120.02	112.17
7	C	2005	MAN	C1-C2-C3	6.79	118.25	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2001	NAG	1	0
5	A	2002	NAG	1	0
8	G	2001	NAG	1	0
8	G	2002	NAG	1	0
9	G	2003	NAG	3	0
8	M	2001	NAG	1	0
8	M	2002	NAG	1	0
5	O	2001	NAG	2	0
5	O	2002	NAG	1	0
5	S	2001	NAG	2	0
5	S	2002	NAG	1	0

5.6 Ligand geometry

6 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$
6	NAG	A	2004	1	14,14,15	1.97	4 (28%)	15,19,21	2.53	5 (33%)
6	NAG	C	2001	1	14,14,15	1.29	1 (7%)	15,19,21	1.85	4 (26%)
6	NAG	M	2003	1	14,14,15	1.96	4 (28%)	15,19,21	2.51	5 (33%)
6	NAG	O	2004	1	14,14,15	1.90	4 (28%)	15,19,21	2.52	8 (53%)
6	NAG	P	2001	2	14,14,15	2.19	5 (35%)	15,19,21	2.82	7 (46%)
6	NAG	S	2004	1	14,14,15	1.87	5 (35%)	15,19,21	2.43	7 (46%)

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	2004	1	-	0/6/23/26	0/1/1/1
6	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
6	NAG	M	2003	1	-	0/6/23/26	0/1/1/1
6	NAG	O	2004	1	-	0/6/23/26	0/1/1/1
6	NAG	P	2001	2	-	0/6/23/26	0/1/1/1
6	NAG	S	2004	1	-	0/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	2004	NAG	O3-C3	2.03	1.47	1.43
6	P	2001	NAG	C4-C3	2.09	1.57	1.52
6	S	2004	NAG	C2-N2	2.24	1.50	1.46
6	P	2001	NAG	C3-C2	2.35	1.57	1.52
6	O	2004	NAG	O3-C3	2.62	1.49	1.43
6	O	2004	NAG	O4-C4	2.81	1.49	1.43
6	C	2001	NAG	C1-C2	2.85	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	2004	NAG	C4-C3	2.91	1.59	1.52
6	S	2004	NAG	C4-C3	2.94	1.59	1.52
6	S	2004	NAG	C1-C2	2.95	1.56	1.52
6	A	2004	NAG	O4-C4	3.02	1.49	1.43
6	M	2003	NAG	O4-C4	3.03	1.49	1.43
6	M	2003	NAG	C4-C3	3.04	1.60	1.52
6	A	2004	NAG	C4-C3	3.07	1.60	1.52
6	A	2004	NAG	O3-C3	3.07	1.50	1.43
6	M	2003	NAG	O3-C3	3.11	1.50	1.43
6	P	2001	NAG	C4-C5	3.11	1.59	1.53
6	P	2001	NAG	C2-N2	3.19	1.51	1.46
6	S	2004	NAG	O4-C4	3.38	1.50	1.43
6	M	2003	NAG	C1-C2	3.74	1.57	1.52
6	O	2004	NAG	C1-C2	3.76	1.57	1.52
6	A	2004	NAG	C1-C2	3.78	1.57	1.52
6	P	2001	NAG	C1-C2	4.60	1.58	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	2004	NAG	O4-C4-C5	-2.71	102.47	109.28
6	C	2001	NAG	C8-C7-N2	-2.70	111.23	116.11
6	O	2004	NAG	O5-C1-C2	-2.31	108.26	111.47
6	S	2004	NAG	O4-C4-C5	-2.02	104.19	109.28
6	O	2004	NAG	O4-C4-C3	2.07	114.86	110.36
6	P	2001	NAG	C4-C3-C2	2.08	114.06	111.02
6	C	2001	NAG	C2-N2-C7	2.08	125.98	122.94
6	S	2004	NAG	O4-C4-C3	2.09	114.90	110.36
6	M	2003	NAG	O4-C4-C3	2.14	115.02	110.36
6	P	2001	NAG	O4-C4-C5	2.15	114.70	109.28
6	C	2001	NAG	O3-C3-C2	2.15	113.99	109.39
6	A	2004	NAG	O4-C4-C3	2.15	115.04	110.36
6	O	2004	NAG	O3-C3-C4	2.24	115.23	110.36
6	S	2004	NAG	C3-C4-C5	2.43	114.50	110.22
6	P	2001	NAG	O3-C3-C2	2.47	114.68	109.39
6	S	2004	NAG	C2-N2-C7	2.58	126.71	122.94
6	P	2001	NAG	O7-C7-N2	2.73	127.18	121.92
6	O	2004	NAG	C3-C4-C5	2.76	115.08	110.22
6	P	2001	NAG	C1-O5-C5	2.80	116.02	112.17
6	M	2003	NAG	C3-C4-C5	2.96	115.43	110.22
6	A	2004	NAG	C3-C4-C5	2.98	115.47	110.22
6	O	2004	NAG	C1-O5-C5	3.18	116.55	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	2003	NAG	O3-C3-C4	3.33	117.60	110.36
6	A	2004	NAG	O3-C3-C4	3.36	117.67	110.36
6	P	2001	NAG	O5-C1-C2	3.44	116.26	111.47
6	S	2004	NAG	O3-C3-C4	3.48	117.92	110.36
6	S	2004	NAG	C1-C2-N2	3.82	117.01	110.49
6	O	2004	NAG	C4-C3-C2	3.84	116.65	111.02
6	C	2001	NAG	C1-O5-C5	4.36	118.18	112.17
6	M	2003	NAG	C4-C3-C2	4.91	118.22	111.02
6	A	2004	NAG	C4-C3-C2	4.94	118.26	111.02
6	M	2003	NAG	C1-C2-N2	5.04	119.11	110.49
6	A	2004	NAG	C1-C2-N2	5.08	119.16	110.49
6	S	2004	NAG	C4-C3-C2	5.62	119.26	111.02
6	O	2004	NAG	C1-C2-N2	5.69	120.21	110.49
6	P	2001	NAG	C2-N2-C7	7.84	134.38	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	2001	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/334 (96%)	0.71	30 (9%) 9 16	60, 90, 90, 90	0
1	C	321/334 (96%)	0.84	44 (13%) 3 11	60, 90, 90, 90	0
1	G	321/334 (96%)	0.80	38 (11%) 5 13	60, 90, 90, 90	0
1	M	322/334 (96%)	0.71	32 (9%) 8 15	60, 90, 90, 90	0
1	O	318/334 (95%)	0.90	47 (14%) 3 10	90, 90, 90, 90	0
1	S	322/334 (96%)	0.69	37 (11%) 5 13	60, 90, 90, 90	0
2	B	172/182 (94%)	0.36	10 (5%) 24 27	90, 90, 90, 90	0
2	D	172/182 (94%)	0.49	13 (7%) 15 20	90, 90, 90, 90	0
2	I	173/182 (95%)	0.97	22 (12%) 4 12	90, 90, 90, 90	0
2	N	169/182 (92%)	0.57	14 (8%) 12 18	90, 90, 90, 90	0
2	P	172/182 (94%)	0.50	7 (4%) 38 38	90, 90, 90, 90	0
2	U	173/182 (95%)	0.29	5 (2%) 52 50	90, 90, 90, 90	0
3	E	216/218 (99%)	1.18	44 (20%) 1 8	90, 90, 90, 90	0
3	J	211/218 (96%)	1.02	31 (14%) 3 10	90, 90, 90, 90	0
3	L	215/218 (98%)	0.68	23 (10%) 7 14	90, 90, 90, 90	0
3	Q	215/218 (98%)	0.80	27 (12%) 4 12	90, 90, 90, 90	0
3	V	214/218 (98%)	1.22	54 (25%) 1 7	90, 90, 90, 90	0
3	X	216/218 (99%)	0.62	14 (6%) 20 24	90, 90, 90, 90	0
4	F	221/222 (99%)	0.95	43 (19%) 1 8	90, 90, 90, 90	1 (0%)
4	H	221/222 (99%)	1.36	62 (28%) 1 6	90, 90, 90, 90	1 (0%)
4	K	221/222 (99%)	1.17	42 (19%) 1 8	90, 90, 90, 90	1 (0%)
4	R	221/222 (99%)	1.00	42 (19%) 1 8	90, 90, 90, 90	1 (0%)
4	T	220/222 (99%)	0.99	37 (16%) 2 9	90, 90, 90, 90	1 (0%)
4	W	221/222 (99%)	1.37	54 (24%) 1 7	90, 90, 90, 90	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5569/5736 (97%)	0.85	772 (13%) 3 11	60, 90, 90, 90	6 (0%)

All (772) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	W	130	ALA	14.5
3	E	157	ASN	10.0
1	C	273	GLU	8.6
4	W	129	ALA	8.2
4	W	123	PRO	8.1
3	J	120	PRO	7.9
3	E	155	ARG	7.7
3	E	146	VAL	7.4
3	V	181	LEU	7.4
3	V	115	VAL	7.2
4	K	123	PRO	7.2
3	E	156	GLN	7.1
4	W	128	SER	6.7
1	C	60	ILE	6.6
4	W	223	ILE	6.5
3	E	145	ASN	6.4
4	W	227	PRO	6.4
4	K	227	PRO	6.3
3	V	116	SER	6.2
4	H	11	LEU	6.0
3	V	130	ALA	5.9
4	K	124	LEU	5.9
4	T	140	LEU	5.9
4	W	202	PRO	5.9
1	C	272	LEU	5.9
4	K	206	VAL	5.8
1	S	273	GLU	5.8
3	V	180	THR	5.8
1	A	273	GLU	5.7
1	O	60	ILE	5.7
3	L	200	THR	5.7
4	W	121	VAL	5.7
4	K	205	THR	5.5
3	J	1	ASP	5.5
4	H	139	THR	5.5
3	E	200	THR	5.4
4	W	140	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
4	K	125	ALA	5.4
4	W	124	LEU	5.4
4	T	206	VAL	5.3
1	M	317	ALA	5.2
3	E	113	PRO	5.1
3	V	135	PHE	5.1
2	P	62	GLN	5.1
1	M	273	GLU	5.1
3	J	119	PRO	5.0
4	W	203	SER	5.0
1	S	60	ILE	5.0
4	T	69	LEU	5.0
1	C	274	TYR	4.9
4	H	130	ALA	4.9
4	W	122	TYR	4.9
1	O	133(A)	SER	4.9
4	R	69	LEU	4.8
1	O	98	TYR	4.8
1	O	103	ASN	4.8
4	H	168	SER	4.8
4	H	123	PRO	4.8
4	W	141	GLY	4.8
4	H	120	SER	4.8
2	N	62	GLN	4.7
1	A	317	ALA	4.7
4	H	121	VAL	4.7
4	H	227	PRO	4.7
4	R	71	VAL	4.6
1	G	273	GLU	4.6
1	G	312	ASN	4.6
1	G	289	ASN	4.6
3	E	115	VAL	4.6
1	O	311	SER	4.5
2	N	32	SER	4.5
4	K	226	VAL	4.5
4	K	202	PRO	4.5
4	W	126	PRO	4.5
3	E	27	GLU	4.5
4	H	124	LEU	4.5
4	F	30	THR	4.5
3	J	27	GLU	4.4
4	T	126	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
3	Q	79	GLU	4.4
3	E	207	LYS	4.4
3	V	157	ASN	4.4
4	T	139	THR	4.4
3	Q	110	ASP	4.4
3	V	182	THR	4.3
4	R	78	ALA	4.3
4	H	206	VAL	4.3
4	H	12	VAL	4.3
4	W	200	TRP	4.2
4	H	125	ALA	4.2
4	T	223	ILE	4.2
4	T	229	ASP	4.2
4	W	226	VAL	4.2
4	T	227	PRO	4.2
4	T	219	VAL	4.1
4	R	142	CYS	4.1
1	O	312	ASN	4.1
4	R	20	MET	4.1
4	K	223	ILE	4.1
3	V	129	GLY	4.1
3	V	146	VAL	4.1
4	W	204	GLU	4.1
3	V	15	LEU	4.0
1	M	153	TRP	4.0
4	K	228	ARG	4.0
4	H	226	VAL	4.0
4	W	125	ALA	4.0
1	S	98	TYR	4.0
3	Q	19	ALA	4.0
4	W	127	GLY	4.0
1	O	45	LYS	4.0
1	O	318	THR	4.0
4	H	126	PRO	4.0
3	V	205	ILE	4.0
2	N	72	ASN	3.9
2	B	32	SER	3.9
4	F	53	ASN	3.9
4	K	8	GLY	3.9
4	H	189	SER	3.9
4	W	115	LYS	3.9
4	F	114	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
4	K	141	GLY	3.9
4	K	126	PRO	3.9
4	K	142	CYS	3.9
4	F	126	PRO	3.8
1	M	210	ASN	3.8
4	R	140	LEU	3.8
3	V	114	THR	3.8
4	F	134	THR	3.8
4	T	67	ALA	3.8
4	H	223	ILE	3.8
3	L	201	SER	3.8
4	W	139	THR	3.8
3	Q	2	ILE	3.8
4	H	166	LEU	3.8
4	H	112	SER	3.8
4	H	167	SER	3.8
4	K	119	PRO	3.8
1	C	61	LEU	3.8
4	R	70	THR	3.8
2	I	23	GLY	3.8
3	V	16	GLY	3.8
3	E	112	ALA	3.8
4	W	221	LYS	3.8
4	T	220	ASP	3.7
3	V	131	SER	3.7
3	Q	131	SER	3.7
1	C	216	GLU	3.7
4	T	68	THR	3.7
3	J	132	VAL	3.7
1	O	123	ILE	3.7
2	N	19	ASP	3.7
3	E	27(A)	SER	3.7
2	D	68	ARG	3.7
4	H	141	GLY	3.7
3	J	207	LYS	3.7
3	V	108	ARG	3.6
4	K	188	SER	3.6
1	C	276	ASN	3.6
3	V	107	LYS	3.6
4	H	71	VAL	3.6
4	R	116	THR	3.6
1	G	15	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	51	LEU	3.6
1	G	103	ASN	3.6
4	F	11	LEU	3.6
4	T	207	THR	3.6
4	T	45	LEU	3.6
1	M	12	GLN	3.6
1	M	318	THR	3.6
1	S	9	PRO	3.5
4	F	135	ASN	3.5
1	G	290	SER	3.5
4	H	114	ALA	3.5
2	I	72	ASN	3.5
1	C	88	VAL	3.5
4	W	222	LYS	3.5
4	W	230	CYS	3.5
1	O	317	ALA	3.5
1	G	250	ASN	3.5
3	E	197	THR	3.5
3	E	148	TRP	3.5
3	L	113	PRO	3.5
3	J	208	SER	3.5
3	L	202	THR	3.5
1	G	51	LEU	3.4
4	F	127	GLY	3.4
4	T	44	SER	3.4
2	B	33	GLY	3.4
3	E	159	VAL	3.4
2	I	62	GLN	3.4
1	M	272	LEU	3.4
1	O	61	LEU	3.4
1	O	268	MET	3.4
1	O	159	SER	3.4
4	F	230	CYS	3.4
4	R	210	VAL	3.4
4	W	18	VAL	3.4
2	D	67	GLY	3.4
1	A	147	PHE	3.4
4	W	45	LEU	3.4
4	W	191	VAL	3.4
1	M	60	ILE	3.4
3	Q	78	VAL	3.4
4	F	133	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
3	E	144	ILE	3.3
4	H	113	SER	3.3
1	O	154	LEU	3.3
3	V	158	GLY	3.3
4	H	205	THR	3.3
3	V	134	CYS	3.3
4	T	169	GLY	3.3
2	I	158	ASP	3.3
2	I	126	LEU	3.3
3	E	158	GLY	3.3
3	V	109	ALA	3.3
4	H	119	PRO	3.3
3	V	159	VAL	3.3
1	C	13	ILE	3.3
2	D	62	GLN	3.3
4	F	124	LEU	3.3
3	Q	82	ASP	3.3
3	V	14	SER	3.3
2	D	65	ALA	3.3
3	Q	11	LEU	3.3
4	W	114	ALA	3.3
4	W	143	LEU	3.3
3	J	27(A)	SER	3.3
1	C	62	ARG	3.3
1	M	25	GLN	3.3
4	F	223	ILE	3.3
4	R	114	ALA	3.3
2	N	65	ALA	3.3
3	V	156	GLN	3.3
4	R	143	LEU	3.3
4	W	219	VAL	3.2
3	J	93	GLU	3.2
4	H	140	LEU	3.2
4	T	200	TRP	3.2
4	T	230	CYS	3.2
2	B	22	TYR	3.2
4	R	139	THR	3.2
3	V	21	ILE	3.2
1	G	210	ASN	3.2
2	N	71	ASN	3.2
2	P	63	PHE	3.2
2	P	65	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	288	ILE	3.2
3	Q	50	ARG	3.2
4	F	20	MET	3.2
2	B	21	TRP	3.2
1	S	55	ASN	3.2
2	I	122	VAL	3.2
4	W	142	CYS	3.2
4	T	226	VAL	3.2
3	E	199	LYS	3.2
4	F	123	PRO	3.2
4	F	52(A)	PRO	3.2
1	O	101	ASP	3.2
4	W	205	THR	3.2
3	E	196	ALA	3.2
4	F	71	VAL	3.2
3	Q	20	THR	3.2
1	O	273	GLU	3.2
1	O	153	TRP	3.2
4	H	142	CYS	3.2
4	K	113	SER	3.2
3	V	47	LEU	3.2
1	C	311	SER	3.2
1	O	158	ASN	3.1
1	O	127	TRP	3.1
4	T	191	VAL	3.1
4	K	222	LYS	3.1
3	Q	132	VAL	3.1
4	H	144	VAL	3.1
3	E	111	ALA	3.1
4	R	218	LYS	3.1
1	G	60	ILE	3.1
3	L	2	ILE	3.1
1	C	267	ILE	3.1
4	H	202	PRO	3.1
1	O	230	MET	3.1
3	Q	33	MET	3.1
4	R	34	ILE	3.1
4	H	222	LYS	3.1
3	J	146	VAL	3.1
1	M	39	ALA	3.1
4	F	73	ARG	3.1
1	S	86	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	I	1	GLY	3.1
4	H	133	GLN	3.1
4	H	191	VAL	3.1
1	M	51	LEU	3.1
4	K	134	THR	3.1
4	W	100(B)	TYR	3.1
4	K	229	ASP	3.1
3	V	204	PRO	3.0
4	H	134	THR	3.0
3	E	25	ALA	3.0
1	G	9	PRO	3.0
4	W	133	GLN	3.0
3	E	194	CYS	3.0
1	C	178	VAL	3.0
1	M	211	GLN	3.0
3	V	120	PRO	3.0
4	T	152	VAL	3.0
1	A	313	ARG	3.0
1	C	214	VAL	3.0
3	V	128	GLY	3.0
3	L	104	LEU	3.0
2	D	122	VAL	3.0
1	C	89	GLU	3.0
2	I	71	ASN	3.0
3	X	212	ASN	3.0
4	F	80	MET	2.9
2	I	157	TYR	2.9
4	F	206	VAL	2.9
4	H	188	SER	2.9
1	G	254	PRO	2.9
1	C	164	ILE	2.9
1	C	297	ILE	2.9
3	J	131	SER	2.9
1	O	55(A)	GLY	2.9
3	V	155	ARG	2.9
1	A	10	GLY	2.9
3	E	57	GLY	2.9
1	A	39	ALA	2.9
3	V	132	VAL	2.9
2	I	35	ALA	2.9
1	C	179	LEU	2.9
3	L	21	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
3	Q	21	ILE	2.9
4	H	43	LYS	2.9
4	R	113	SER	2.9
1	A	55(A)	GLY	2.9
2	D	66	VAL	2.9
1	O	314	LEU	2.9
3	J	186	TYR	2.9
3	J	148	TRP	2.9
4	R	141	GLY	2.9
1	G	101	ASP	2.9
4	R	126	PRO	2.9
3	V	1	ASP	2.9
1	C	312	ASN	2.9
1	A	210	ASN	2.9
1	S	103	ASN	2.9
4	W	217	THR	2.8
2	I	140	PHE	2.8
1	S	97	CYS	2.8
2	B	111	HIS	2.8
4	R	51	ILE	2.8
4	H	154	VAL	2.8
4	R	211	ALA	2.8
1	C	82	VAL	2.8
4	H	190	SER	2.8
3	E	120	PRO	2.8
1	O	297	ILE	2.8
3	J	154	GLU	2.8
4	K	191	VAL	2.8
1	A	316	LEU	2.8
2	I	63	PHE	2.8
4	K	196	SER	2.8
3	V	179	LEU	2.8
4	T	78	ALA	2.8
2	P	71	ASN	2.8
4	H	20	MET	2.8
4	W	82	LEU	2.8
1	M	315	VAL	2.8
4	R	154	VAL	2.8
3	V	178	THR	2.8
4	T	205	THR	2.8
3	J	115	VAL	2.8
2	N	16	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	J	206	VAL	2.8
1	O	59	LEU	2.8
4	H	179	GLN	2.8
4	F	67	ALA	2.8
1	M	313	ARG	2.8
2	U	126	LEU	2.8
4	K	152	VAL	2.8
2	D	136	GLY	2.8
1	O	270	SER	2.7
4	W	109	VAL	2.7
4	W	192	THR	2.7
1	M	103	ASN	2.7
4	F	34	ILE	2.7
1	A	274	TYR	2.7
2	U	64	GLU	2.7
4	R	188	SER	2.7
4	F	183	ASP	2.7
1	O	102	PHE	2.7
4	T	188	SER	2.7
1	G	232	PHE	2.7
1	O	46	THR	2.7
1	C	58	PRO	2.7
3	E	192	TYR	2.7
3	Q	204	PRO	2.7
1	S	78	GLU	2.7
1	G	120	LYS	2.7
4	R	112	SER	2.7
2	U	62	GLN	2.7
1	A	9	PRO	2.7
4	H	110	THR	2.7
2	N	75	ARG	2.7
4	H	116	THR	2.7
3	L	112	ALA	2.7
3	E	119	PRO	2.7
1	S	92	SER	2.7
2	D	132	GLU	2.7
1	C	275	GLY	2.6
3	J	118	PHE	2.6
1	M	88	VAL	2.6
3	L	88	CYS	2.6
3	X	100	GLY	2.6
4	K	200	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	59	LEU	2.6
4	H	152	VAL	2.6
4	W	152	VAL	2.6
1	S	176	LEU	2.6
2	B	62	GLN	2.6
3	J	133	VAL	2.6
3	J	92	ASN	2.6
1	A	60	ILE	2.6
1	S	314	LEU	2.6
2	N	33	GLY	2.6
3	V	206	VAL	2.6
1	S	324	PRO	2.6
1	C	59	LEU	2.6
1	O	88	VAL	2.6
3	Q	27(B)	VAL	2.6
4	F	180	SER	2.6
4	T	40	SER	2.6
1	G	317	ALA	2.6
2	I	21	TRP	2.6
4	R	115	LYS	2.6
1	G	251	PHE	2.6
1	O	313	ARG	2.6
1	O	77	ASP	2.6
2	P	158	ASP	2.6
1	A	289	ASN	2.6
1	A	267	ILE	2.6
3	E	121	SER	2.6
3	X	82	ASP	2.6
4	R	166	LEU	2.6
3	X	202	THR	2.6
4	K	162	ASN	2.6
4	K	166	LEU	2.6
3	V	177	SER	2.6
1	G	282	GLN	2.6
3	V	89	GLN	2.6
4	F	18	VAL	2.6
1	S	61	LEU	2.6
3	L	41	GLY	2.6
3	E	117	ILE	2.6
4	H	40	SER	2.6
1	C	79	PHE	2.6
4	H	200	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	P	7	ALA	2.6
1	G	212	ARG	2.6
3	L	44	PRO	2.6
4	W	168	SER	2.6
1	M	168	TYR	2.5
2	N	58	LYS	2.5
3	E	41	GLY	2.5
3	J	181	LEU	2.5
1	C	301	THR	2.5
4	T	192	THR	2.5
1	A	230	MET	2.5
1	S	138	ALA	2.5
3	V	154	GLU	2.5
3	V	136	LEU	2.5
3	L	115	VAL	2.5
3	Q	16	GLY	2.5
4	R	18	VAL	2.5
1	A	148	PHE	2.5
1	M	101	ASP	2.5
4	F	125	ALA	2.5
4	W	110	THR	2.5
1	O	39	ALA	2.5
3	Q	197	THR	2.5
3	V	117	ILE	2.5
1	M	243	ILE	2.5
2	I	152	VAL	2.5
4	T	70	THR	2.5
3	V	149	LYS	2.5
3	V	207	LYS	2.5
1	C	45	LYS	2.5
1	A	288	ILE	2.5
1	C	167	SER	2.5
3	Q	13	VAL	2.5
3	J	116	SER	2.5
4	H	115	LYS	2.5
3	J	27(B)	VAL	2.5
1	G	52	CYS	2.5
4	W	113	SER	2.5
1	S	210	ASN	2.5
1	C	254	PRO	2.5
1	S	58	PRO	2.5
1	C	210	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	134	GLY	2.5
4	H	127	GLY	2.5
4	K	183	ASP	2.5
1	C	268	MET	2.4
3	V	44	PRO	2.4
3	X	27(A)	SER	2.4
1	A	66	VAL	2.4
1	A	272	LEU	2.4
3	E	147	LYS	2.4
1	S	312	ASN	2.4
1	M	154	LEU	2.4
1	O	104	ASP	2.4
1	C	9	PRO	2.4
3	J	196	ALA	2.4
1	C	180	TRP	2.4
4	K	9	PRO	2.4
4	R	196	SER	2.4
4	K	143	LEU	2.4
4	T	141	GLY	2.4
1	S	137	SER	2.4
4	K	57	THR	2.4
1	G	268	MET	2.4
4	T	179	GLN	2.4
1	C	284	PRO	2.4
4	F	122	TYR	2.4
1	A	153	TRP	2.4
3	J	193	THR	2.4
1	A	55	ASN	2.4
1	O	263	GLY	2.4
4	H	192	THR	2.4
1	A	314	LEU	2.4
1	G	306	PRO	2.4
2	N	140	PHE	2.4
4	T	228	ARG	2.4
3	Q	115	VAL	2.4
4	F	210	VAL	2.4
4	H	143	LEU	2.4
2	N	59	MET	2.4
3	E	181	LEU	2.3
3	E	198	HIS	2.3
3	V	194	CYS	2.3
3	E	179	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	T	114	ALA	2.3
4	W	206	VAL	2.3
4	H	13	LYS	2.3
1	O	293	PRO	2.3
4	K	127	GLY	2.3
4	F	150	GLU	2.3
3	V	133	VAL	2.3
1	O	232	PHE	2.3
2	N	55	ILE	2.3
1	M	26	VAL	2.3
4	T	43	LYS	2.3
1	C	87	ILE	2.3
1	S	254	PRO	2.3
4	F	110	THR	2.3
4	F	130	ALA	2.3
1	C	102	PHE	2.3
3	E	26	SER	2.3
4	R	111	VAL	2.3
2	D	71	ASN	2.3
4	R	128	SER	2.3
2	I	153	LYS	2.3
4	F	14	PRO	2.3
4	F	62	LYS	2.3
2	D	59	MET	2.3
2	B	72	ASN	2.3
4	W	86	ASP	2.3
3	V	104	LEU	2.3
4	F	69	LEU	2.3
4	F	86	ASP	2.3
4	F	112	SER	2.3
4	R	167	SER	2.3
3	X	62	PHE	2.3
3	Q	15	LEU	2.3
1	G	150	ASN	2.3
1	O	44	GLU	2.3
1	S	153	TRP	2.3
2	P	69	GLU	2.3
3	L	73	LEU	2.3
3	X	47	LEU	2.3
3	Q	66	GLY	2.3
3	L	42	GLN	2.3
3	L	86	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	S	59	LEU	2.3
3	J	41	GLY	2.3
2	I	68	ARG	2.3
1	O	264	ASP	2.3
1	M	245	PHE	2.3
4	H	173	THR	2.3
4	R	127	GLY	2.3
1	O	179	LEU	2.2
3	L	40	PRO	2.2
3	X	157	ASN	2.2
1	A	178	VAL	2.2
3	E	78	VAL	2.2
1	A	96(A)	LEU	2.2
1	S	96(A)	LEU	2.2
4	F	143	LEU	2.2
4	H	44	SER	2.2
1	O	254	PRO	2.2
4	K	140	LEU	2.2
4	F	82	LEU	2.2
4	T	11	LEU	2.2
4	R	67	ALA	2.2
4	R	129	ALA	2.2
4	H	204	GLU	2.2
1	G	83	PRO	2.2
3	E	201	SER	2.2
3	E	186	TYR	2.2
1	O	99	PRO	2.2
4	K	221	LYS	2.2
1	A	275	GLY	2.2
1	M	268	MET	2.2
2	B	96	ALA	2.2
2	N	20	GLY	2.2
1	O	294	PHE	2.2
3	E	105	GLU	2.2
3	Q	180	THR	2.2
1	O	178	VAL	2.2
3	Q	31	SER	2.2
1	S	271	GLU	2.2
4	W	96	TYR	2.2
4	W	229	ASP	2.2
2	U	71	ASN	2.2
1	S	178	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	V	106	ILE	2.2
1	O	310	LYS	2.2
4	H	103	TRP	2.2
2	D	96	ALA	2.2
3	E	55	GLU	2.2
1	M	98	TYR	2.2
3	X	16	GLY	2.2
4	W	8	GLY	2.2
1	C	66	VAL	2.2
1	G	88	VAL	2.2
1	G	172	ASN	2.2
1	G	211	GLN	2.2
1	M	13	ILE	2.2
4	R	133	GLN	2.2
2	I	22	TYR	2.2
4	R	124	LEU	2.2
1	G	230	MET	2.2
3	L	15	LEU	2.2
3	X	119	PRO	2.2
4	R	1	GLU	2.2
4	R	45	LEU	2.2
1	G	106	GLU	2.2
4	T	42	GLY	2.2
3	X	144	ILE	2.2
1	A	152	VAL	2.2
4	K	207	THR	2.2
1	G	102	PHE	2.2
1	C	200	THR	2.2
1	S	235	THR	2.2
2	D	69	GLU	2.2
4	R	144	VAL	2.2
1	S	62	ARG	2.2
3	E	205	ILE	2.2
4	K	192	THR	2.2
4	R	109	VAL	2.2
1	G	267	ILE	2.2
3	L	16	GLY	2.2
3	E	132	VAL	2.2
4	F	128	SER	2.2
1	C	235	THR	2.1
1	O	131	ASP	2.1
1	C	15	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	X	132	VAL	2.1
4	T	157	TRP	2.1
1	S	123	ILE	2.1
3	Q	106	ILE	2.1
4	R	217	THR	2.1
4	W	134	THR	2.1
3	L	35	TRP	2.1
3	V	22	SER	2.1
4	W	10	GLU	2.1
3	L	199	LYS	2.1
1	S	55(A)	GLY	2.1
4	W	144	VAL	2.1
4	W	9	PRO	2.1
1	O	319	GLY	2.1
1	S	101	ASP	2.1
1	M	314	LEU	2.1
1	S	237	LEU	2.1
3	Q	104	LEU	2.1
3	L	20	THR	2.1
1	G	311	SER	2.1
1	M	167	SER	2.1
4	H	80	MET	2.1
4	K	40	SER	2.1
2	I	96	ALA	2.1
3	J	104	LEU	2.1
1	G	215	PRO	2.1
1	O	135	VAL	2.1
1	S	88	VAL	2.1
4	H	118	PRO	2.1
4	H	149	PRO	2.1
1	A	211	GLN	2.1
3	L	102	THR	2.1
3	J	2	ILE	2.1
1	O	290	SER	2.1
3	J	55	GLU	2.1
2	U	72	ASN	2.1
4	H	135	ASN	2.1
4	W	112	SER	2.1
3	V	2	ILE	2.1
3	V	195	GLU	2.1
1	C	232	PHE	2.1
1	S	69	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	130	ALA	2.1
4	H	162	ASN	2.1
3	E	122	SER	2.1
1	M	274	TYR	2.1
4	F	145	LYS	2.1
3	V	145	ASN	2.1
4	K	217	THR	2.1
1	G	123	ILE	2.1
3	J	192	TYR	2.1
4	T	71	VAL	2.1
1	S	311	SER	2.1
3	E	104	LEU	2.1
3	V	90	GLN	2.1
1	S	102	PHE	2.1
3	J	152	GLY	2.1
3	Q	71	PHE	2.1
4	F	221	LYS	2.1
1	M	316	LEU	2.1
1	C	288	ILE	2.1
2	I	24	TYR	2.1
1	G	16	GLY	2.1
2	B	115	VAL	2.1
3	L	180	THR	2.1
4	K	208	CYS	2.1
3	V	93	GLU	2.1
4	F	113	SER	2.1
4	K	71	VAL	2.1
1	M	40	GLN	2.1
4	K	157	TRP	2.1
1	C	215	PRO	2.0
4	F	187	LEU	2.0
4	K	117	THR	2.0
2	I	36	ALA	2.0
4	H	42	GLY	2.0
3	X	143	ASP	2.0
4	F	188	SER	2.0
4	R	7	SER	2.0
1	A	112	LEU	2.0
2	B	6	ILE	2.0
1	G	291	SER	2.0
3	V	110	ASP	2.0
1	M	24	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	Q	113	PRO	2.0
4	H	122	TYR	2.0
4	R	110	THR	2.0
4	W	169	GLY	2.0
1	S	136	SER	2.0
1	C	317	ALA	2.0
1	S	291	SER	2.0
4	W	210	VAL	2.0
3	V	196	ALA	2.0
4	H	150	GLU	2.0
1	G	151	VAL	2.0
4	K	139	THR	2.0
3	J	125	LEU	2.0
4	T	124	LEU	2.0
1	A	315	VAL	2.0
4	H	18	VAL	2.0
2	I	6	ILE	2.0
1	A	154	LEU	2.0
3	E	73	LEU	2.0
3	X	145	ASN	2.0
4	R	165	SER	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	NAG	M	2001	14/15	0.80	0.48	1.12	90,90,90,90	0
5	NAG	A	2001	14/15	0.80	0.42	1.01	90,90,90,90	0
5	NAG	O	2001	14/15	0.77	0.44	0.54	90,90,90,90	0
5	NAG	S	2001	14/15	0.68	0.33	-0.29	90,90,90,90	0
8	NAG	G	2001	14/15	0.76	0.23	-0.36	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MAN	C	2008	11/12	0.91	0.35	-	90,90,90,90	0
5	MAN	O	2003	11/12	0.57	0.41	-	90,90,90,90	0
8	NAG	G	2002	14/15	0.69	0.31	-	90,90,90,90	0
10	BMA	O	2007	11/12	0.71	0.37	-	43,47,56,63	0
7	BMA	C	2004	11/12	0.84	0.35	-	90,90,90,90	0
8	NAG	M	2002	14/15	0.76	0.40	-	90,90,90,90	0
7	MAN	C	2005	11/12	0.82	0.31	-	90,90,90,90	0
5	NAG	S	2002	14/15	0.77	0.26	-	90,90,90,90	0
10	MAN	O	2008	11/12	0.56	0.41	-	47,49,50,52	0
7	MAN	C	2006	11/12	0.77	0.48	-	90,90,90,90	0
7	MAN	C	2009	11/12	0.78	0.32	-	90,90,90,90	0
10	NAG	O	2005	14/15	0.57	0.46	-	32,37,44,45	0
10	NAG	O	2006	14/15	0.83	0.41	-	37,38,39,42	0
5	NAG	A	2002	14/15	0.66	0.51	-	90,90,90,90	0
7	NAG	C	2003	14/15	0.77	0.32	-	90,90,90,90	0
9	NAG	G	2003	14/15	0.88	0.25	-	38,47,53,63	0
9	NAG	G	2004	14/15	0.70	0.40	-	48,62,76,87	0
7	MAN	C	2007	11/12	0.59	0.28	-	90,90,90,90	0
5	MAN	A	2003	11/12	0.49	0.51	-	90,90,90,90	0
7	NAG	C	2002	14/15	0.66	0.38	-	90,90,90,90	0
5	NAG	O	2002	14/15	0.69	0.40	-	90,90,90,90	0
5	MAN	S	2003	11/12	0.66	0.23	-	90,90,90,90	0
9	BMA	G	2005	11/12	0.57	0.40	-	102,115,122,126	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	C	2001	14/15	0.81	0.39	2.30	90,90,90,90	0
6	NAG	M	2003	14/15	0.68	0.40	-	90,90,90,90	0
6	NAG	O	2004	14/15	0.86	0.24	-	90,90,90,90	0
6	NAG	S	2004	14/15	0.67	0.43	-	90,90,90,90	0
6	NAG	A	2004	14/15	0.70	0.42	-	90,90,90,90	0
6	NAG	P	2001	14/15	0.73	0.42	-	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.