Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2018 – 05:45 PM EST

PDB ID	:	5W08
Title	:	A/Texas/50/2012(H3N2) Influenza hemagglutinin in complex with K03.12 Fab
Authors	:	McCarthy, K.R.; Harrison, S.C.
Deposited on	:	2017-05-30
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

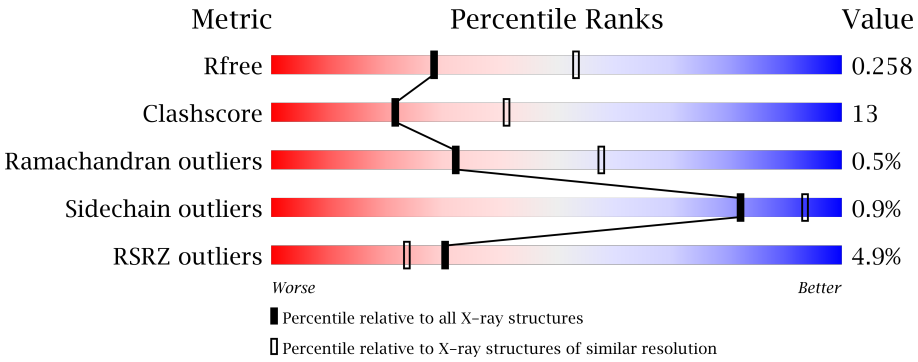
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	291	3% 72% 21% • 7%
1	B	291	2% 74% 20% • 6%
1	C	291	4% 66% 27% 7%
1	D	291	3% 73% 21% 6%
1	E	291	2% 72% 21% • 6%

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Mol	Chain	Length	Quality of chain
1	F	291	8% 68% 26% 6%
2	G	244	.% 78% 19% •
2	I	244	2% 77% 20% ••
2	K	244	.% 77% 19% ••
2	M	244	5% 81% 15% •
2	O	244	6% 80% 15% ••
2	Q	244	7% 79% 16% ••
3	H	214	6% 84% 14% •
3	J	214	7% 82% 18%
3	L	214	8% 74% 24% •
3	N	214	8% 80% 17% ••
3	P	214	6% 85% 14% ••
3	R	214	10% 76% 22% ••

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	403	-	-	X	-
4	NAG	A	406	-	-	X	-
4	NAG	A	407	-	-	-	X
4	NAG	D	405	-	-	X	-
4	NAG	D	406	-	-	X	-
4	NAG	E	404	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34382 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2159	1362	383	404	10			
1	B	274	Total	C	N	O	S	0	0	0
			2171	1369	385	407	10			
1	C	272	Total	C	N	O	S	0	0	0
			2159	1362	383	404	10			
1	D	273	Total	C	N	O	S	0	0	0
			2166	1366	384	406	10			
1	E	273	Total	C	N	O	S	0	0	0
			2166	1366	384	406	10			
1	F	274	Total	C	N	O	S	0	0	0
			2171	1369	385	407	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLY	-	expression tag	UNP R4L1D1
A	321	ALA	-	expression tag	UNP R4L1D1
A	322	LEU	-	expression tag	UNP R4L1D1
A	323	GLU	-	expression tag	UNP R4L1D1
A	324	VAL	-	expression tag	UNP R4L1D1
A	325	LEU	-	expression tag	UNP R4L1D1
A	326	PHE	-	expression tag	UNP R4L1D1
A	327	GLN	-	expression tag	UNP R4L1D1
B	320	GLY	-	expression tag	UNP R4L1D1
B	321	ALA	-	expression tag	UNP R4L1D1
B	322	LEU	-	expression tag	UNP R4L1D1
B	323	GLU	-	expression tag	UNP R4L1D1
B	324	VAL	-	expression tag	UNP R4L1D1
B	325	LEU	-	expression tag	UNP R4L1D1
B	326	PHE	-	expression tag	UNP R4L1D1
B	327	GLN	-	expression tag	UNP R4L1D1
C	320	GLY	-	expression tag	UNP R4L1D1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	321	ALA	-	expression tag	UNP R4L1D1
C	322	LEU	-	expression tag	UNP R4L1D1
C	323	GLU	-	expression tag	UNP R4L1D1
C	324	VAL	-	expression tag	UNP R4L1D1
C	325	LEU	-	expression tag	UNP R4L1D1
C	326	PHE	-	expression tag	UNP R4L1D1
C	327	GLN	-	expression tag	UNP R4L1D1
D	320	GLY	-	expression tag	UNP R4L1D1
D	321	ALA	-	expression tag	UNP R4L1D1
D	322	LEU	-	expression tag	UNP R4L1D1
D	323	GLU	-	expression tag	UNP R4L1D1
D	324	VAL	-	expression tag	UNP R4L1D1
D	325	LEU	-	expression tag	UNP R4L1D1
D	326	PHE	-	expression tag	UNP R4L1D1
D	327	GLN	-	expression tag	UNP R4L1D1
E	320	GLY	-	expression tag	UNP R4L1D1
E	321	ALA	-	expression tag	UNP R4L1D1
E	322	LEU	-	expression tag	UNP R4L1D1
E	323	GLU	-	expression tag	UNP R4L1D1
E	324	VAL	-	expression tag	UNP R4L1D1
E	325	LEU	-	expression tag	UNP R4L1D1
E	326	PHE	-	expression tag	UNP R4L1D1
E	327	GLN	-	expression tag	UNP R4L1D1
F	320	GLY	-	expression tag	UNP R4L1D1
F	321	ALA	-	expression tag	UNP R4L1D1
F	322	LEU	-	expression tag	UNP R4L1D1
F	323	GLU	-	expression tag	UNP R4L1D1
F	324	VAL	-	expression tag	UNP R4L1D1
F	325	LEU	-	expression tag	UNP R4L1D1
F	326	PHE	-	expression tag	UNP R4L1D1
F	327	GLN	-	expression tag	UNP R4L1D1

- Molecule 2 is a protein called K03.12 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	236	Total	C	N	O	S	0	0	0
			1790	1132	300	349	9			
2	I	238	Total	C	N	O	S	0	0	0
			1807	1142	303	353	9			
2	K	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			
2	M	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			
2	Q	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	239	HIS	-	expression tag	UNP S6C4S0
G	240	HIS	-	expression tag	UNP S6C4S0
G	241	HIS	-	expression tag	UNP S6C4S0
G	242	HIS	-	expression tag	UNP S6C4S0
G	243	HIS	-	expression tag	UNP S6C4S0
G	244	HIS	-	expression tag	UNP S6C4S0
I	239	HIS	-	expression tag	UNP S6C4S0
I	240	HIS	-	expression tag	UNP S6C4S0
I	241	HIS	-	expression tag	UNP S6C4S0
I	242	HIS	-	expression tag	UNP S6C4S0
I	243	HIS	-	expression tag	UNP S6C4S0
I	244	HIS	-	expression tag	UNP S6C4S0
K	239	HIS	-	expression tag	UNP S6C4S0
K	240	HIS	-	expression tag	UNP S6C4S0
K	241	HIS	-	expression tag	UNP S6C4S0
K	242	HIS	-	expression tag	UNP S6C4S0
K	243	HIS	-	expression tag	UNP S6C4S0
K	244	HIS	-	expression tag	UNP S6C4S0
M	239	HIS	-	expression tag	UNP S6C4S0
M	240	HIS	-	expression tag	UNP S6C4S0
M	241	HIS	-	expression tag	UNP S6C4S0
M	242	HIS	-	expression tag	UNP S6C4S0
M	243	HIS	-	expression tag	UNP S6C4S0
M	244	HIS	-	expression tag	UNP S6C4S0
O	239	HIS	-	expression tag	UNP S6C4S0
O	240	HIS	-	expression tag	UNP S6C4S0
O	241	HIS	-	expression tag	UNP S6C4S0
O	242	HIS	-	expression tag	UNP S6C4S0
O	243	HIS	-	expression tag	UNP S6C4S0
O	244	HIS	-	expression tag	UNP S6C4S0
Q	239	HIS	-	expression tag	UNP S6C4S0
Q	240	HIS	-	expression tag	UNP S6C4S0
Q	241	HIS	-	expression tag	UNP S6C4S0
Q	242	HIS	-	expression tag	UNP S6C4S0

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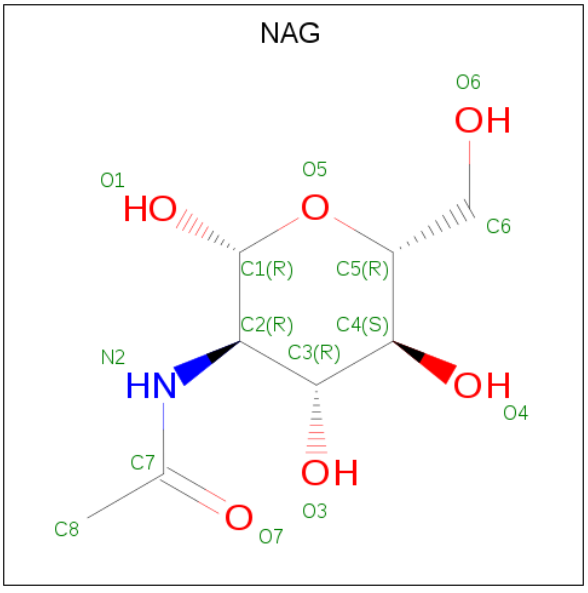
Chain	Residue	Modelled	Actual	Comment	Reference
Q	243	HIS	-	expression tag	UNP S6C4S0
Q	244	HIS	-	expression tag	UNP S6C4S0

- Molecule 3 is a protein called K03.12 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	212	Total	C	N	O	S	0	0	0
			1561	973	258	325	5			
3	J	213	Total	C	N	O	S	0	0	0
			1568	978	259	326	5			
3	L	211	Total	C	N	O	S	0	0	0
			1555	970	257	324	4			
3	N	212	Total	C	N	O	S	0	0	0
			1562	975	258	325	4			
3	P	212	Total	C	N	O	S	0	0	0
			1562	975	258	325	4			
3	R	212	Total	C	N	O	S	0	0	0
			1562	975	258	325	4			

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



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

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

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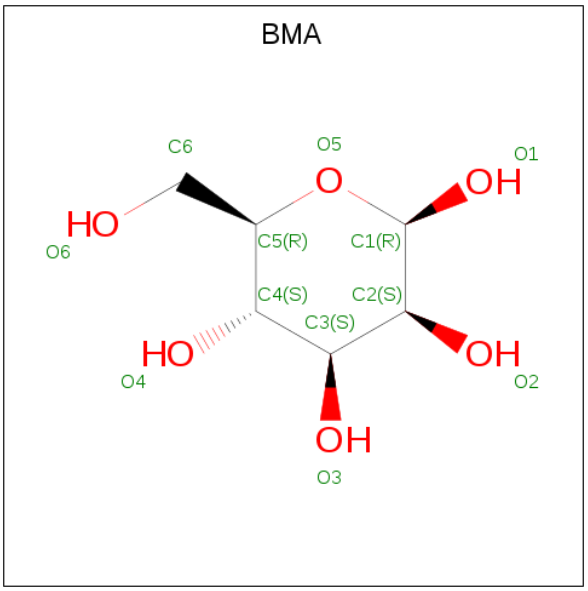
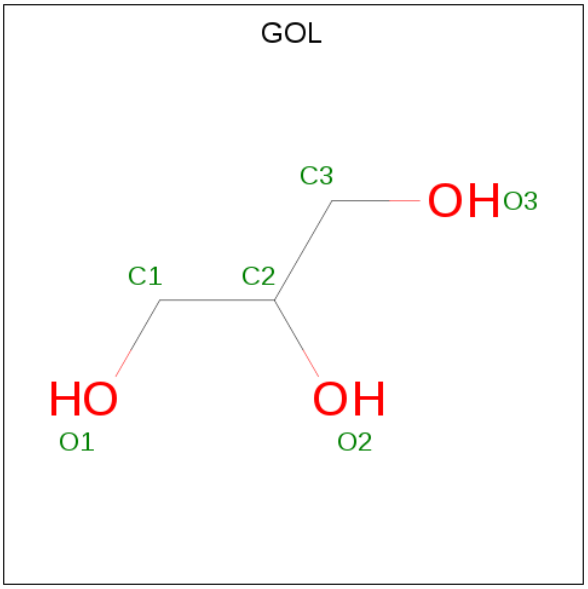
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1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

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0
5	C	1	Total C O 11 6 5	0	0
5	E	1	Total C O 11 6 5	0	0
5	F	1	Total C O 11 6 5	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total C O 6 3 3	0	0

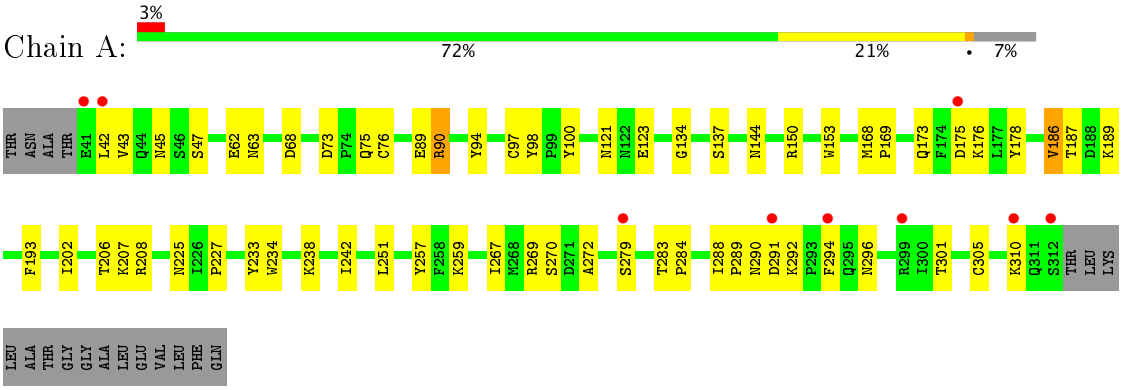
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	58	Total O 58 58	0	0
7	B	79	Total O 79 79	0	0
7	C	48	Total O 48 48	0	0
7	D	49	Total O 49 49	0	0
7	E	46	Total O 46 46	0	0
7	F	37	Total O 37 37	0	0
7	G	45	Total O 45 45	0	0
7	H	41	Total O 41 41	0	0
7	I	55	Total O 55 55	0	0
7	J	43	Total O 43 43	0	0
7	K	29	Total O 29 29	0	0
7	L	23	Total O 23 23	0	0
7	M	28	Total O 28 28	0	0
7	N	40	Total O 40 40	0	0
7	O	30	Total O 30 30	0	0
7	P	22	Total O 22 22	0	0
7	Q	24	Total O 24 24	0	0
7	R	25	Total O 25 25	0	0

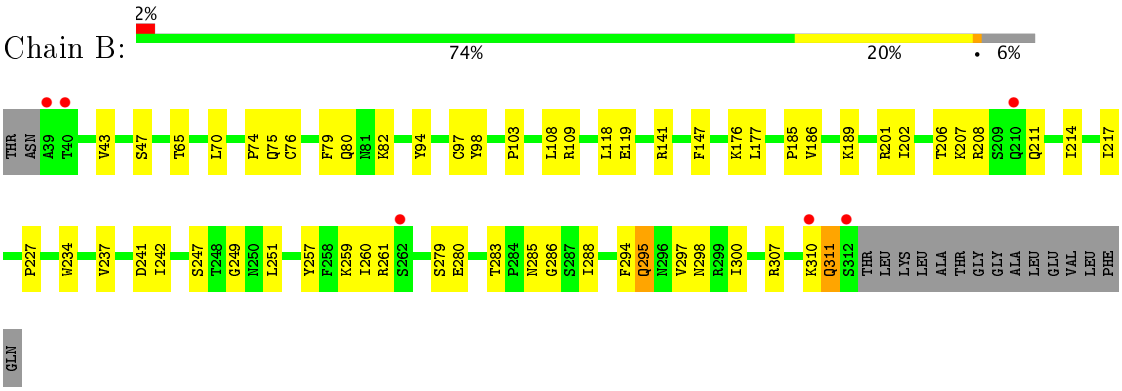
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

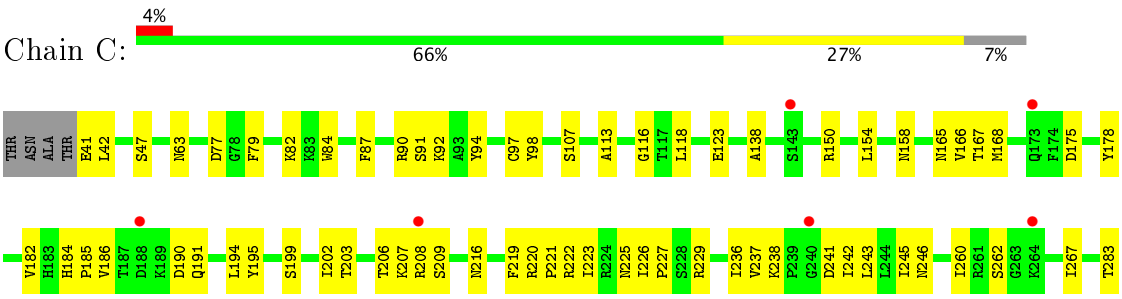
- Molecule 1: Hemagglutinin HA1

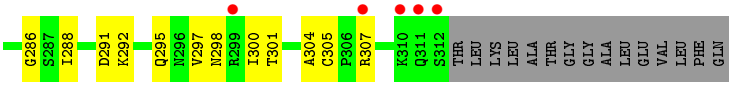


- Molecule 1: Hemagglutinin HA1



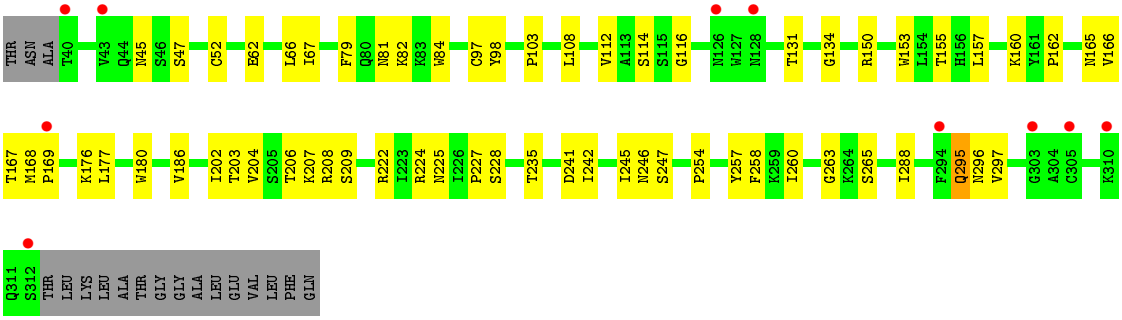
- Molecule 1: Hemagglutinin HA1

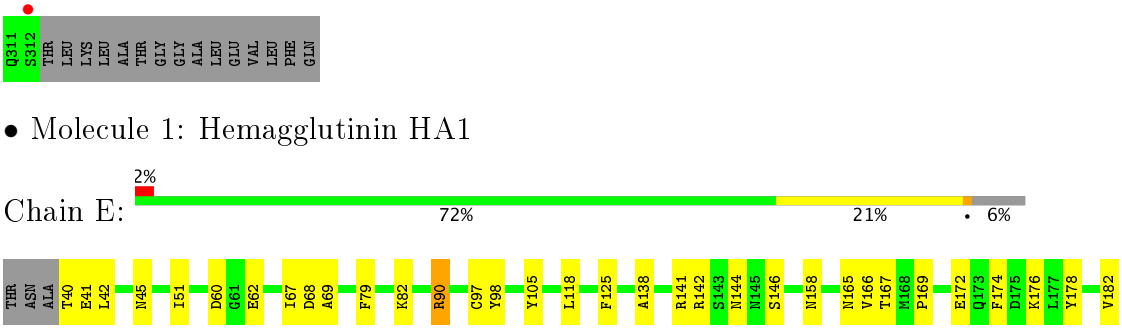


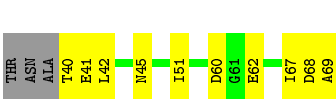


• Molecule 1: Hemagglutinin HA1

Chain D:

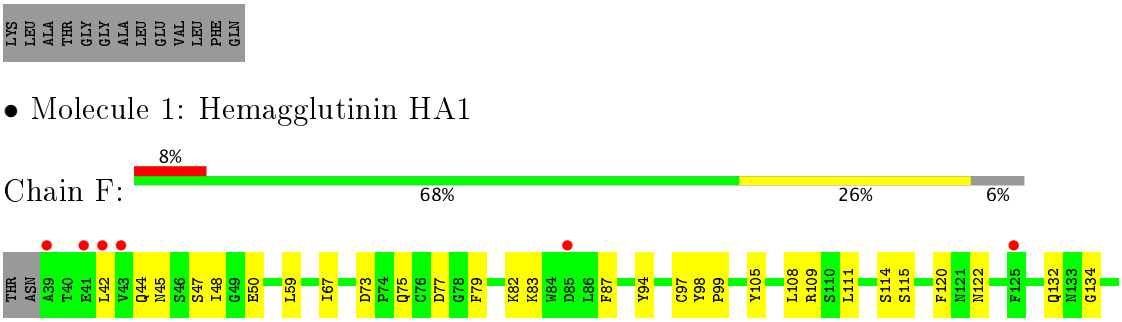


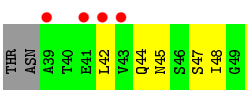




• Molecule 1: Hemagglutinin HA1

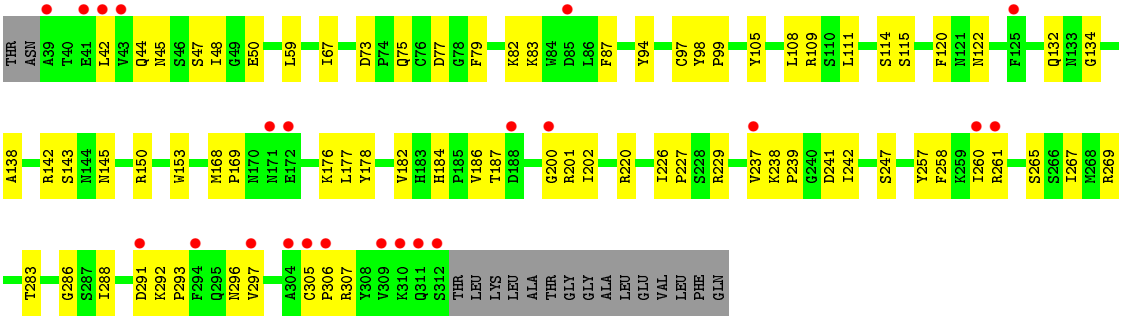
Chain E:

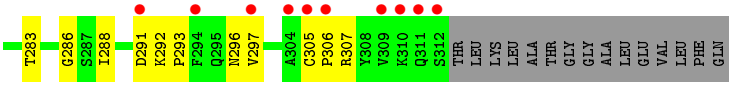




• Molecule 1: Hemagglutinin HA1

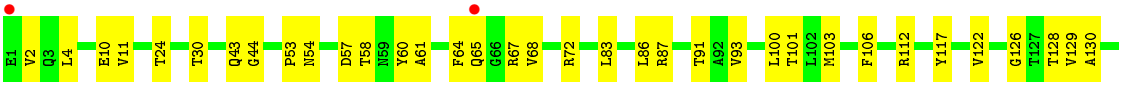
Chain F:



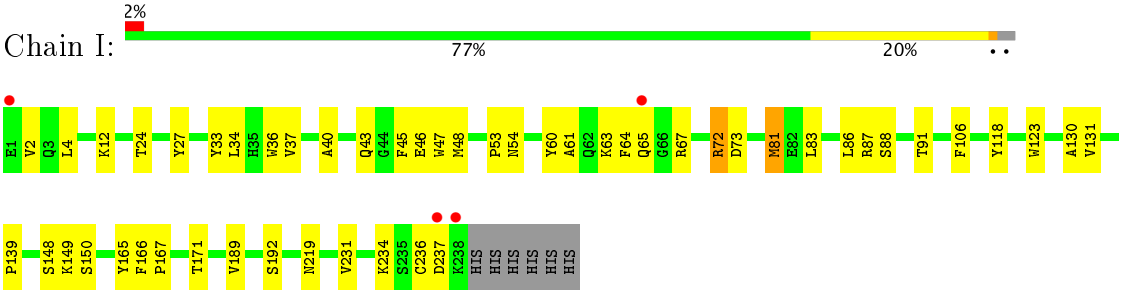


• Molecule 2: K03.12 antibody heavy chain

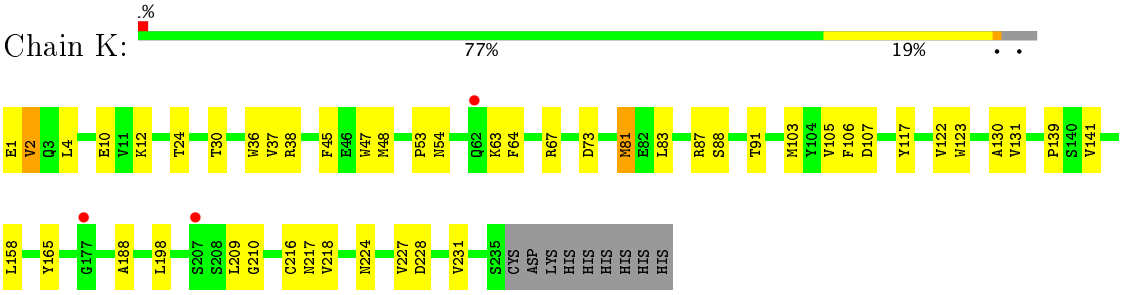
Chain G:



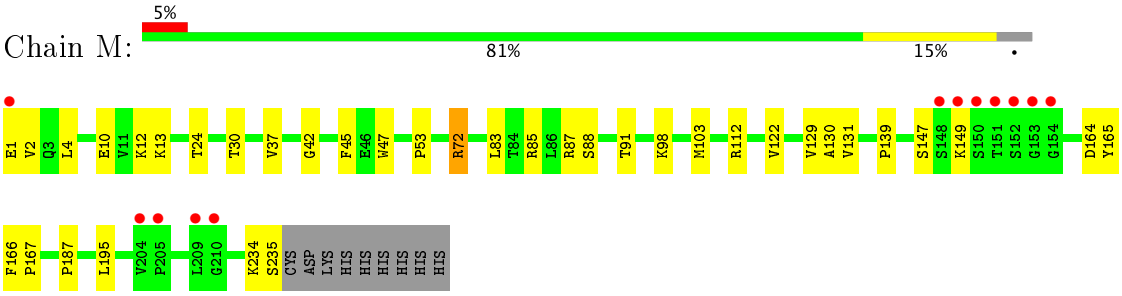
• Molecule 2: K03.12 antibody heavy chain



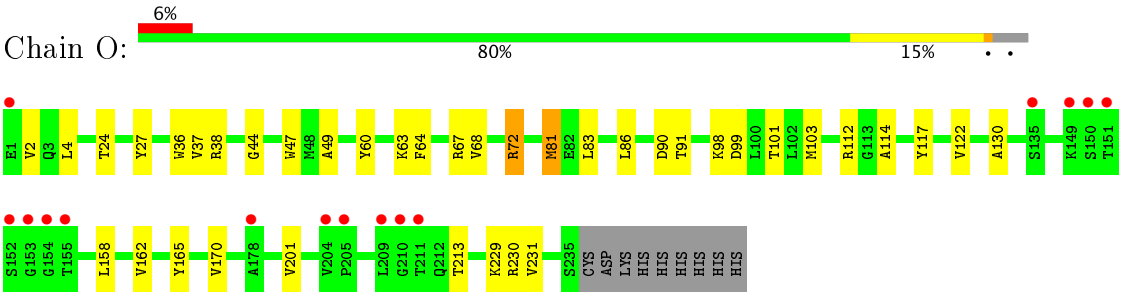
• Molecule 2: K03.12 antibody heavy chain



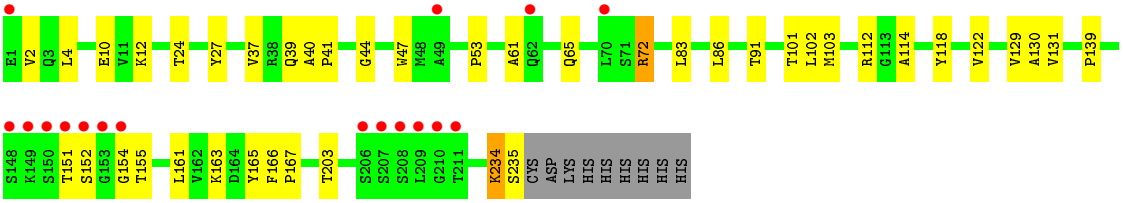
• Molecule 2: K03.12 antibody heavy chain



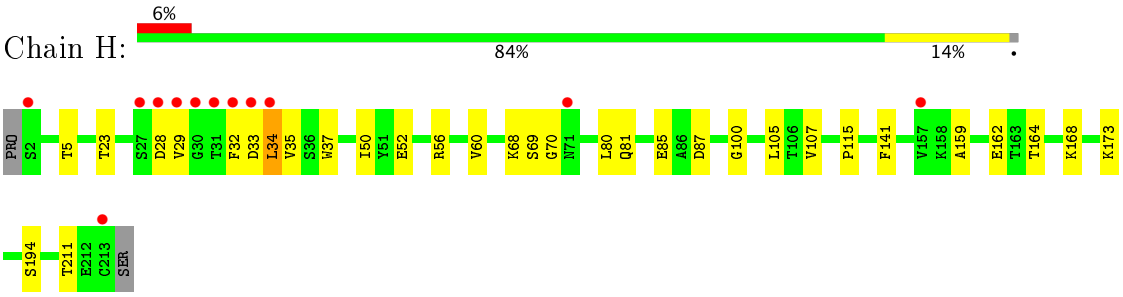
• Molecule 2: K03.12 antibody heavy chain



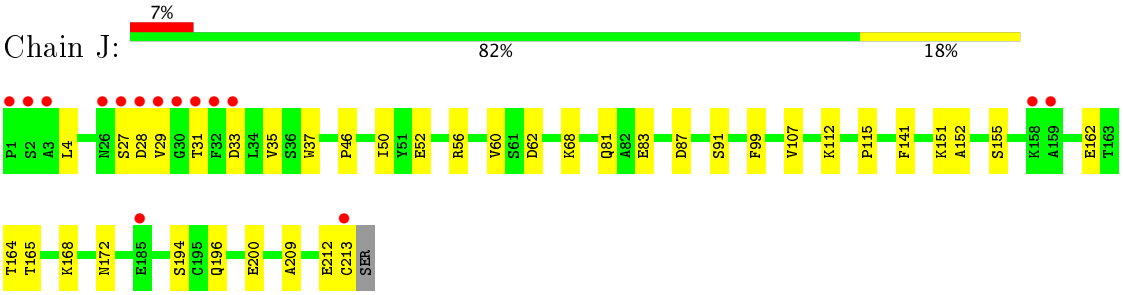
• Molecule 2: K03.12 antibody heavy chain



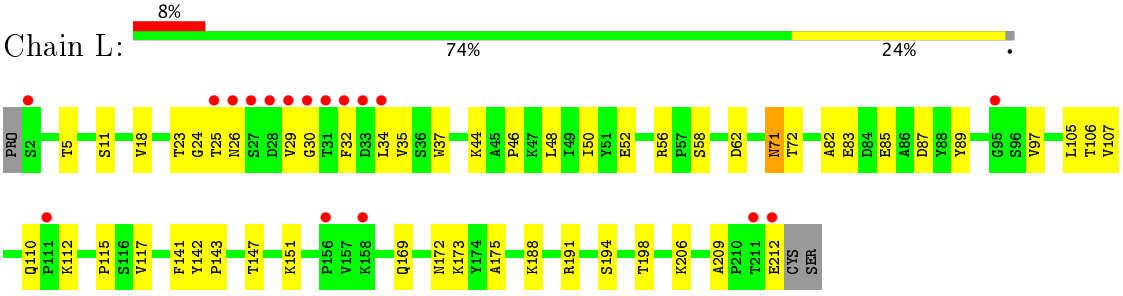
• Molecule 3: K03.12 antibody light chain



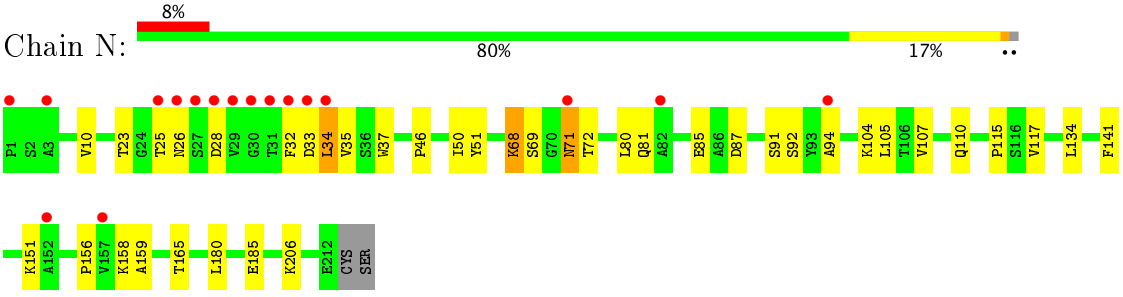
• Molecule 3: K03.12 antibody light chain



• Molecule 3: K03.12 antibody light chain

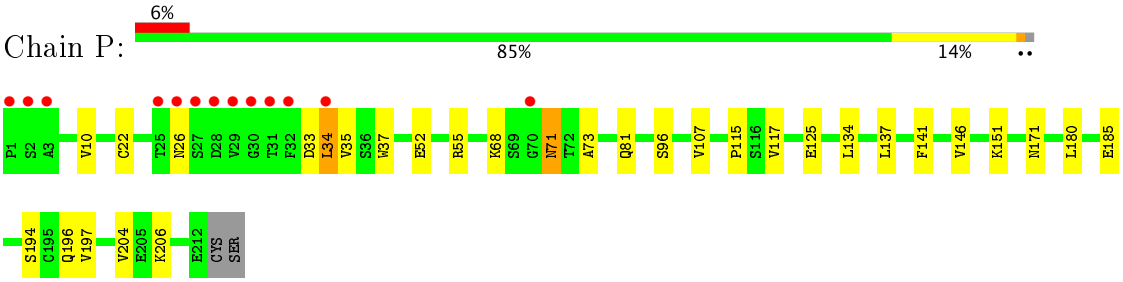


• Molecule 3: K03.12 antibody light chain



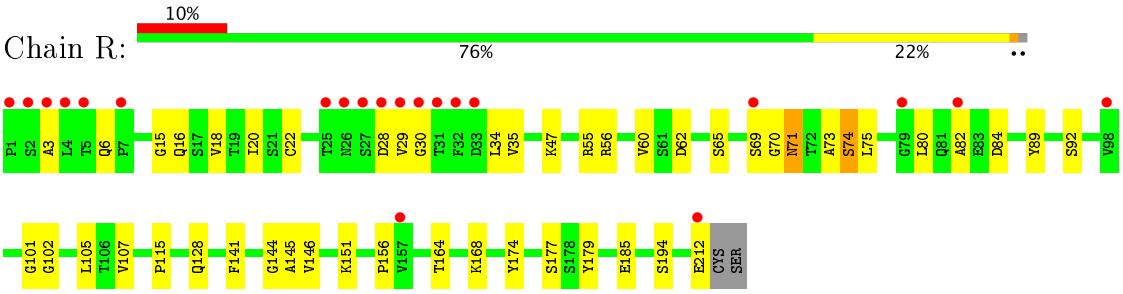
• Molecule 3: K03.12 antibody light chain

Chain P:



- Molecule 3: K03.12 antibody light chain

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.80Å 325.12Å 156.99Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	49.41 – 2.60 49.41 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.41-2.60) 99.2 (49.41-2.60)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.240 , 0.262 0.237 , 0.258	Depositor DCC
R_{free} test set	9071 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	34382	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: GOL, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.36	0/2213	0.50	0/3006
1	B	0.26	0/2225	0.48	0/3023
1	C	0.30	0/2213	0.50	0/3006
1	D	0.26	0/2220	0.47	0/3016
1	E	0.27	0/2220	0.50	0/3016
1	F	0.27	0/2225	0.52	0/3023
2	G	0.28	0/1837	0.52	0/2506
2	I	0.28	0/1854	0.52	0/2528
2	K	0.27	0/1831	0.50	0/2498
2	M	0.27	0/1831	0.51	0/2498
2	O	0.27	0/1831	0.50	0/2498
2	Q	0.27	0/1831	0.50	0/2498
3	H	0.33	0/1597	0.51	0/2178
3	J	0.27	0/1605	0.51	0/2189
3	L	0.33	0/1591	0.55	0/2170
3	N	0.27	0/1599	0.51	0/2181
3	P	0.28	0/1599	0.51	0/2181
3	R	0.30	0/1599	0.53	0/2181
All	All	0.29	0/33921	0.51	0/46196

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2159	0	2106	74	0
1	B	2171	0	2118	58	0
1	C	2159	0	2105	85	0
1	D	2166	0	2112	48	0
1	E	2166	0	2113	68	0
1	F	2171	0	2117	80	0
2	G	1790	0	1735	33	0
2	I	1807	0	1752	44	0
2	K	1784	0	1731	45	0
2	M	1784	0	1731	29	0
2	O	1784	0	1731	33	0
2	Q	1784	0	1731	36	0
3	H	1561	0	1505	31	0
3	J	1568	0	1515	37	0
3	L	1555	0	1501	51	0
3	N	1562	0	1511	40	0
3	P	1562	0	1511	27	0
3	R	1562	0	1511	48	0
4	A	98	0	88	38	0
4	B	98	0	87	13	0
4	C	70	0	63	3	0
4	D	98	0	89	19	0
4	E	70	0	63	5	0
4	F	70	0	63	1	0
5	A	11	0	10	0	0
5	B	11	0	10	0	0
5	C	11	0	10	1	0
5	E	11	0	10	0	0
5	F	11	0	10	0	0
6	I	6	0	8	0	0
7	A	58	0	0	30	0
7	B	79	0	0	35	0
7	C	48	0	0	24	0
7	D	49	0	0	11	0
7	E	46	0	0	33	0
7	F	37	0	0	29	0
7	G	45	0	0	11	1
7	H	41	0	0	13	1
7	I	55	0	0	12	0
7	J	43	0	0	15	0
7	K	29	0	0	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	23	0	0	20	0
7	M	28	0	0	11	0
7	N	40	0	0	14	0
7	O	30	0	0	8	0
7	P	22	0	0	10	0
7	Q	24	0	0	13	0
7	R	25	0	0	12	0
All	All	34382	0	32647	890	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (890) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:HD21	4:A:403:NAG:C2	1.17	1.52
1:A:144:ASN:HD21	4:A:406:NAG:C1	1.21	1.49
1:C:220:ARG:CB	1:C:229:ARG:HH12	1.31	1.44
1:A:63:ASN:HD21	4:A:403:NAG:C1	1.41	1.32
1:A:144:ASN:ND2	4:A:406:NAG:C1	1.91	1.28
1:A:63:ASN:ND2	4:A:403:NAG:C2	1.95	1.27
1:B:201:ARG:HG3	7:B:505:HOH:O	1.16	1.26
1:A:290:ASN:HB2	7:A:501:HOH:O	1.27	1.25
3:L:172:ASN:CA	7:L:301:HOH:O	1.82	1.24
1:C:90:ARG:HB3	7:C:506:HOH:O	1.32	1.24
1:C:220:ARG:CB	1:C:229:ARG:NH1	1.99	1.23
1:F:283:THR:HG22	1:F:286:GLY:O	1.35	1.23
1:F:201:ARG:HA	7:F:506:HOH:O	1.41	1.20
2:K:1:GLU:HA	7:K:304:HOH:O	1.05	1.20
2:O:101:THR:CB	7:O:301:HOH:O	1.88	1.19
1:A:63:ASN:ND2	4:A:403:NAG:H2	1.57	1.16
2:I:150:SER:HB3	7:I:404:HOH:O	1.46	1.16
1:C:220:ARG:HB3	1:C:229:ARG:NH1	1.54	1.15
3:J:33:ASP:OD2	3:J:68:LYS:HD2	1.43	1.14
2:K:10:GLU:N	7:K:302:HOH:O	1.81	1.13
2:K:10:GLU:CA	7:K:302:HOH:O	1.95	1.12
2:O:37:VAL:HG12	2:O:47:TRP:HA	1.31	1.12
3:R:145:ALA:N	7:R:303:HOH:O	1.82	1.12
3:N:91:SER:CB	7:N:303:HOH:O	1.94	1.11
1:B:207:LYS:C	7:B:502:HOH:O	1.89	1.11
3:R:145:ALA:C	7:R:303:HOH:O	1.88	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:33:ASP:OD2	3:J:68:LYS:CD	2.00	1.09
3:R:47:LYS:NZ	7:R:301:HOH:O	1.80	1.09
1:A:225:ASN:C	7:A:503:HOH:O	1.91	1.06
3:L:172:ASN:CB	7:L:301:HOH:O	1.96	1.06
1:A:63:ASN:ND2	4:A:403:NAG:C1	2.14	1.06
2:O:101:THR:HB	7:O:301:HOH:O	1.47	1.05
1:C:219:PHE:N	7:C:503:HOH:O	1.80	1.04
2:G:176:SER:C	7:G:303:HOH:O	1.93	1.04
3:L:25:THR:HG23	7:L:317:HOH:O	1.57	1.03
1:C:199:SER:O	7:C:502:HOH:O	1.73	1.03
1:A:290:ASN:CA	7:A:501:HOH:O	2.03	1.02
1:B:207:LYS:CA	7:B:502:HOH:O	2.06	1.02
1:F:142:ARG:N	7:F:505:HOH:O	1.90	1.02
1:B:202:ILE:N	7:B:505:HOH:O	1.91	1.02
3:N:158:LYS:N	7:N:301:HOH:O	1.83	1.01
1:C:220:ARG:HB3	1:C:229:ARG:HH12	0.88	1.01
2:K:224:ASN:ND2	7:K:303:HOH:O	1.82	1.01
1:E:242:ILE:HB	7:E:502:HOH:O	1.62	0.99
3:L:172:ASN:O	7:L:301:HOH:O	1.80	0.99
3:R:146:VAL:HG23	7:R:303:HOH:O	1.62	0.99
1:A:144:ASN:ND2	4:A:406:NAG:N2	2.09	0.99
1:F:201:ARG:CA	7:F:506:HOH:O	2.03	0.98
3:H:52:GLU:OE2	7:H:301:HOH:O	1.81	0.98
1:C:91:SER:N	7:C:506:HOH:O	1.94	0.98
2:K:216:CYS:O	7:K:301:HOH:O	1.80	0.97
1:A:279:SER:O	7:A:502:HOH:O	1.82	0.97
2:K:10:GLU:CB	7:K:302:HOH:O	2.11	0.97
1:F:132:GLN:O	7:F:501:HOH:O	1.81	0.97
2:I:33:TYR:OH	7:I:401:HOH:O	1.81	0.97
1:D:166:VAL:O	7:D:501:HOH:O	1.83	0.97
3:L:48:LEU:O	7:L:302:HOH:O	1.82	0.96
1:C:220:ARG:HB2	1:C:229:ARG:HH12	1.26	0.96
1:A:290:ASN:O	7:A:501:HOH:O	1.81	0.96
1:A:290:ASN:C	7:A:501:HOH:O	2.04	0.95
1:B:206:THR:O	7:B:502:HOH:O	1.85	0.95
1:D:224:ARG:NH1	7:D:503:HOH:O	2.00	0.95
1:F:77:ASP:OD1	7:F:503:HOH:O	1.84	0.95
2:K:216:CYS:C	7:K:301:HOH:O	2.04	0.95
3:L:188:LYS:NZ	7:L:307:HOH:O	2.00	0.94
1:D:103:PRO:O	7:D:502:HOH:O	1.83	0.94
1:F:145:ASN:O	7:F:502:HOH:O	1.83	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:172:ASN:HB3	7:L:301:HOH:O	1.58	0.94
1:B:279:SER:O	7:B:501:HOH:O	1.84	0.94
1:E:172:GLU:OE1	7:E:501:HOH:O	1.84	0.94
1:A:144:ASN:HD22	4:A:406:NAG:HN2	1.00	0.94
3:P:125:GLU:CD	7:P:305:HOH:O	2.04	0.93
1:A:225:ASN:O	7:A:503:HOH:O	1.85	0.93
1:A:63:ASN:HD21	4:A:403:NAG:H2	1.15	0.93
1:A:175:ASP:OD2	1:A:238:LYS:NZ	2.01	0.93
4:D:406:NAG:H5	4:D:406:NAG:C8	1.97	0.93
1:E:174:PHE:CE2	7:E:501:HOH:O	2.20	0.93
1:C:206:THR:HG23	1:C:208:ARG:H	1.32	0.93
3:L:5:THR:O	7:L:303:HOH:O	1.85	0.93
3:J:99:PHE:CE1	7:J:303:HOH:O	2.22	0.93
3:P:204:VAL:O	7:P:301:HOH:O	1.86	0.92
1:C:220:ARG:HB2	1:C:229:ARG:NH1	1.82	0.91
3:N:92:SER:N	7:N:303:HOH:O	2.02	0.91
1:A:144:ASN:ND2	4:A:406:NAG:HN2	1.67	0.91
1:F:283:THR:CG2	1:F:286:GLY:O	2.18	0.91
2:M:85:ARG:HA	7:M:303:HOH:O	1.70	0.91
4:A:403:NAG:H5	7:A:514:HOH:O	1.69	0.91
3:N:25:THR:HG22	3:N:26:ASN:H	1.35	0.91
1:F:108:LEU:O	7:F:504:HOH:O	1.89	0.91
2:K:1:GLU:OE1	7:K:304:HOH:O	1.87	0.91
2:M:85:ARG:N	7:M:303:HOH:O	1.99	0.90
2:M:149:LYS:O	7:M:301:HOH:O	1.90	0.90
3:J:112:LYS:O	7:J:301:HOH:O	1.89	0.90
1:E:283:THR:CB	7:E:510:HOH:O	2.21	0.89
2:O:99:ASP:OD1	7:O:301:HOH:O	1.88	0.89
2:G:44:GLY:O	7:G:301:HOH:O	1.89	0.89
1:D:165:ASN:HD22	4:D:403:NAG:H61	1.35	0.88
1:E:242:ILE:O	7:E:502:HOH:O	1.91	0.88
2:Q:39:GLN:OE1	7:Q:301:HOH:O	1.91	0.88
4:B:407:NAG:O3	7:B:504:HOH:O	1.91	0.88
2:K:103:MET:O	7:K:305:HOH:O	1.92	0.88
1:C:219:PHE:HB2	7:C:503:HOH:O	1.73	0.88
1:E:283:THR:HB	7:E:510:HOH:O	1.74	0.87
1:F:111:LEU:HB3	7:F:504:HOH:O	1.74	0.87
2:I:149:LYS:C	7:I:404:HOH:O	2.12	0.87
2:M:85:ARG:CA	7:M:303:HOH:O	2.20	0.87
3:H:32:PHE:HB3	3:H:34:LEU:HD13	1.54	0.87
1:C:191:GLN:NE2	1:C:195:TYR:HD2	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PHE:CB	7:C:503:HOH:O	2.23	0.86
1:F:200:GLY:O	7:F:506:HOH:O	1.93	0.86
2:G:100:LEU:O	7:G:302:HOH:O	1.91	0.86
3:H:162:GLU:OE2	7:H:302:HOH:O	1.92	0.86
3:R:101:GLY:O	7:R:305:HOH:O	1.91	0.86
3:R:6:GLN:HE22	3:R:102:GLY:N	1.73	0.86
1:E:172:GLU:HB3	7:E:501:HOH:O	1.76	0.85
1:A:233:TYR:HA	7:A:507:HOH:O	1.76	0.85
3:H:211:THR:CB	7:H:304:HOH:O	2.22	0.85
1:A:123:GLU:OE2	7:A:506:HOH:O	1.94	0.85
2:G:176:SER:O	7:G:303:HOH:O	1.92	0.85
1:E:242:ILE:O	7:E:504:HOH:O	1.94	0.84
1:E:199:SER:OG	7:E:503:HOH:O	1.94	0.84
1:E:243:LEU:HA	7:E:504:HOH:O	1.77	0.84
2:I:150:SER:CB	7:I:404:HOH:O	2.14	0.84
2:I:150:SER:N	7:I:404:HOH:O	2.10	0.84
3:L:32:PHE:O	7:L:304:HOH:O	1.95	0.84
1:A:234:TRP:N	7:A:507:HOH:O	1.98	0.84
1:C:118:LEU:O	7:C:505:HOH:O	1.94	0.83
3:L:34:LEU:O	7:L:305:HOH:O	1.96	0.83
1:A:144:ASN:ND2	4:A:406:NAG:C2	2.42	0.82
1:F:176:LYS:HB2	1:F:237:VAL:CG2	2.09	0.82
1:A:144:ASN:HD21	4:A:406:NAG:C2	1.93	0.81
1:E:144:ASN:ND2	4:E:405:NAG:O7	2.13	0.81
4:B:402:NAG:H4	7:B:515:HOH:O	1.79	0.81
1:C:41:GLU:HG2	1:C:42:LEU:H	1.43	0.81
2:I:83:LEU:HD23	2:I:86:LEU:CD2	2.11	0.81
4:D:406:NAG:H82	4:D:406:NAG:H5	1.62	0.80
3:L:175:ALA:O	7:L:306:HOH:O	1.99	0.80
3:N:104:LYS:NZ	7:N:306:HOH:O	2.14	0.80
3:P:52:GLU:OE1	7:P:303:HOH:O	2.00	0.80
2:K:10:GLU:OE1	2:K:12:LYS:NZ	2.15	0.80
2:O:44:GLY:O	7:O:302:HOH:O	1.99	0.80
1:B:202:ILE:CD1	1:B:247:SER:HB2	2.11	0.79
1:E:90:ARG:NH1	1:E:270:SER:O	2.14	0.79
1:B:201:ARG:CA	7:B:505:HOH:O	2.31	0.79
1:F:186:VAL:HG21	1:F:227:PRO:HG2	1.62	0.79
2:G:164:ASP:OD2	7:G:304:HOH:O	1.99	0.79
1:B:285:ASN:OD1	7:B:508:HOH:O	1.98	0.79
3:J:91:SER:CB	7:J:303:HOH:O	2.30	0.79
1:A:150:ARG:HH12	4:A:407:NAG:H5	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:67:ARG:CZ	2:G:87:ARG:HH12	1.94	0.79
1:F:114:SER:O	7:F:507:HOH:O	2.01	0.79
3:J:99:PHE:CZ	7:J:303:HOH:O	2.36	0.79
2:K:10:GLU:HB2	7:K:302:HOH:O	1.76	0.79
1:A:63:ASN:ND2	4:A:403:NAG:N2	2.29	0.78
3:N:91:SER:OG	7:N:303:HOH:O	1.91	0.78
1:B:208:ARG:N	7:B:502:HOH:O	2.09	0.78
1:B:109:ARG:NH1	7:B:510:HOH:O	2.05	0.78
3:N:25:THR:HG22	3:N:26:ASN:N	1.97	0.78
1:C:191:GLN:NE2	1:C:195:TYR:CD2	2.52	0.77
2:M:42:GLY:N	7:M:302:HOH:O	1.95	0.77
3:P:196:GLN:OE1	7:P:304:HOH:O	2.02	0.77
1:F:293:PRO:N	7:F:510:HOH:O	2.18	0.77
4:A:406:NAG:C6	7:A:513:HOH:O	2.33	0.77
1:A:47:SER:HB3	1:A:288:ILE:HG22	1.66	0.77
1:D:66:LEU:HD21	1:D:112:VAL:HG13	1.67	0.77
3:J:155:SER:CB	7:J:304:HOH:O	2.32	0.77
2:Q:118:TYR:O	7:Q:302:HOH:O	2.01	0.77
3:L:5:THR:N	7:L:303:HOH:O	2.07	0.76
1:F:142:ARG:CA	7:F:505:HOH:O	2.32	0.76
2:I:27:TYR:O	7:I:402:HOH:O	2.03	0.76
3:R:28:ASP:O	3:R:30:GLY:N	2.15	0.76
3:L:172:ASN:C	7:L:301:HOH:O	1.98	0.76
1:A:233:TYR:CA	7:A:507:HOH:O	2.33	0.76
1:C:77:ASP:OD2	7:C:507:HOH:O	2.01	0.76
1:E:262:SER:O	7:E:505:HOH:O	2.04	0.75
1:F:292:LYS:C	7:F:510:HOH:O	2.24	0.75
1:A:206:THR:HG23	1:A:208:ARG:H	1.51	0.75
3:R:151:LYS:NZ	3:R:156:PRO:HG3	2.02	0.75
3:N:91:SER:C	7:N:303:HOH:O	2.23	0.75
1:C:90:ARG:CB	7:C:506:HOH:O	2.07	0.74
3:R:145:ALA:CA	7:R:303:HOH:O	2.17	0.74
1:B:103:PRO:O	7:B:509:HOH:O	2.04	0.74
3:J:91:SER:OG	7:J:303:HOH:O	2.03	0.74
1:F:108:LEU:HA	7:F:504:HOH:O	1.86	0.74
1:F:201:ARG:CB	7:F:506:HOH:O	2.33	0.74
1:A:137:SER:OG	7:A:508:HOH:O	2.05	0.74
1:C:123:GLU:OE1	7:C:508:HOH:O	2.04	0.74
4:A:403:NAG:O7	4:A:403:NAG:O3	2.06	0.74
1:C:90:ARG:C	7:C:506:HOH:O	2.24	0.74
1:E:69:ALA:O	7:E:507:HOH:O	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:TRP:HE1	1:D:235:THR:HG23	1.52	0.74
1:E:68:ASP:OD2	7:E:506:HOH:O	2.05	0.74
4:B:401:NAG:O3	4:B:401:NAG:O7	2.06	0.73
3:L:209:ALA:HB3	3:L:212:GLU:OE2	1.87	0.73
1:F:115:SER:O	7:F:508:HOH:O	2.05	0.73
3:R:80:LEU:HD21	3:R:107:VAL:HG22	1.68	0.73
4:A:403:NAG:O5	7:A:509:HOH:O	2.06	0.73
2:O:101:THR:N	7:O:301:HOH:O	2.02	0.73
2:K:73:ASP:OD1	7:K:306:HOH:O	2.06	0.73
4:B:407:NAG:C3	7:B:504:HOH:O	2.36	0.73
3:H:211:THR:OG1	7:H:304:HOH:O	2.05	0.73
1:B:201:ARG:CG	7:B:505:HOH:O	1.93	0.72
1:F:120:PHE:HE2	1:F:122:ASN:OD1	1.71	0.72
3:J:151:LYS:HE2	7:J:324:HOH:O	1.89	0.72
2:K:217:ASN:CA	7:K:301:HOH:O	2.37	0.72
1:D:186:VAL:HG21	1:D:227:PRO:HG2	1.69	0.72
3:N:91:SER:HB2	7:N:303:HOH:O	1.70	0.72
3:P:125:GLU:OE2	7:P:305:HOH:O	2.04	0.72
2:Q:40:ALA:C	7:Q:304:HOH:O	2.26	0.72
1:A:121:ASN:HA	4:A:407:NAG:H82	1.70	0.72
2:I:83:LEU:HD23	2:I:86:LEU:HD21	1.71	0.72
1:D:263:GLY:O	7:D:504:HOH:O	2.07	0.72
1:E:158:ASN:OD1	7:E:508:HOH:O	2.07	0.72
2:M:147:SER:O	7:M:301:HOH:O	2.07	0.71
2:K:217:ASN:HA	7:K:301:HOH:O	1.89	0.71
1:B:141:ARG:NH2	1:B:147:PHE:O	2.23	0.71
1:E:242:ILE:CA	7:E:502:HOH:O	2.37	0.71
4:A:408:NAG:O4	7:A:510:HOH:O	2.07	0.71
2:M:42:GLY:CA	7:M:302:HOH:O	2.32	0.71
1:B:211:GLN:NE2	7:B:516:HOH:O	2.24	0.71
3:L:32:PHE:HB3	3:L:34:LEU:HD13	1.71	0.71
2:M:187:PRO:O	7:M:304:HOH:O	2.07	0.71
3:R:101:GLY:C	7:R:305:HOH:O	2.26	0.71
1:A:186:VAL:HG11	1:A:227:PRO:HG2	1.72	0.70
3:J:52:GLU:OE2	7:J:305:HOH:O	2.09	0.70
1:B:119:GLU:OE1	1:B:261:ARG:NH1	2.23	0.70
3:J:155:SER:N	7:J:304:HOH:O	2.08	0.70
3:J:91:SER:HB2	7:J:303:HOH:O	1.89	0.70
3:R:20:ILE:O	3:R:74:SER:HA	1.91	0.70
2:I:192:SER:OG	7:I:403:HOH:O	2.09	0.70
2:Q:102:LEU:N	7:Q:305:HOH:O	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:150:SER:CA	7:I:404:HOH:O	2.38	0.69
1:B:118:LEU:O	7:B:511:HOH:O	2.09	0.69
2:Q:41:PRO:N	7:Q:304:HOH:O	2.26	0.69
4:D:402:NAG:O5	7:D:505:HOH:O	2.08	0.69
1:E:62:GLU:O	7:E:509:HOH:O	2.09	0.69
1:B:202:ILE:HD13	1:B:247:SER:HB2	1.74	0.69
3:H:100:GLY:O	7:H:305:HOH:O	2.09	0.69
2:I:83:LEU:CD2	2:I:86:LEU:CD2	2.71	0.69
4:D:405:NAG:H82	4:D:405:NAG:H3	1.74	0.69
2:G:176:SER:CA	7:G:303:HOH:O	2.36	0.69
2:G:43:GLN:O	7:G:306:HOH:O	2.10	0.69
1:C:150:ARG:O	7:C:509:HOH:O	2.11	0.68
1:F:305:CYS:O	7:F:509:HOH:O	2.11	0.68
2:G:93:VAL:HG22	2:G:128:THR:HG22	1.73	0.68
1:F:201:ARG:HB2	7:F:506:HOH:O	1.92	0.68
4:A:407:NAG:O7	7:A:512:HOH:O	2.12	0.68
1:C:203:THR:HG22	1:C:246:ASN:HB2	1.75	0.68
4:D:406:NAG:C1	4:D:406:NAG:H82	2.24	0.68
2:G:60:TYR:HB2	2:G:65:GLN:HG2	1.76	0.68
3:H:5:THR:O	7:H:307:HOH:O	2.10	0.68
1:B:207:LYS:HA	7:B:502:HOH:O	1.80	0.68
1:F:44:GLN:NE2	7:F:511:HOH:O	2.23	0.67
2:Q:72:ARG:NH1	7:Q:308:HOH:O	2.26	0.67
3:L:172:ASN:HA	7:L:301:HOH:O	1.68	0.67
1:E:283:THR:OG1	7:E:510:HOH:O	2.10	0.67
1:E:242:ILE:CB	7:E:502:HOH:O	2.32	0.67
1:E:60:ASP:OD1	1:E:90:ARG:NE	2.27	0.67
2:O:72:ARG:NH1	7:O:304:HOH:O	2.28	0.67
3:R:6:GLN:NE2	3:R:102:GLY:N	2.43	0.67
1:D:52:CYS:O	7:D:507:HOH:O	2.12	0.67
4:D:406:NAG:H5	4:D:406:NAG:H83	1.77	0.66
1:E:206:THR:HG22	7:E:504:HOH:O	1.96	0.66
3:H:211:THR:HB	7:H:304:HOH:O	1.87	0.66
1:C:288:ILE:HG21	1:C:297:VAL:HG21	1.77	0.66
2:G:67:ARG:CZ	2:G:87:ARG:NH1	2.58	0.66
3:J:200:GLU:OE2	7:J:306:HOH:O	2.13	0.66
2:I:118:TYR:O	7:I:405:HOH:O	2.14	0.66
2:Q:2:VAL:CG1	2:Q:122:VAL:HG21	2.25	0.66
1:F:288:ILE:HG21	1:F:297:VAL:HG21	1.77	0.66
1:F:42:LEU:HD23	1:F:42:LEU:O	1.95	0.66
1:B:65:THR:HG23	7:B:518:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:151:LYS:HZ3	3:R:156:PRO:HG3	1.60	0.65
1:A:187:THR:OG1	7:A:504:HOH:O	1.93	0.65
1:A:62:GLU:HG2	4:A:403:NAG:C8	2.27	0.65
2:Q:101:THR:O	7:Q:303:HOH:O	2.13	0.65
1:B:202:ILE:HD12	1:B:251:LEU:HB2	1.79	0.65
2:I:73:ASP:OD1	7:I:406:HOH:O	2.14	0.65
2:M:88:SER:HA	2:M:131:VAL:HG13	1.78	0.65
3:H:33:ASP:HB3	3:H:68:LYS:NZ	2.12	0.65
1:E:199:SER:CB	7:E:503:HOH:O	2.43	0.65
1:B:70:LEU:O	7:B:512:HOH:O	2.14	0.65
3:J:155:SER:HB2	7:J:304:HOH:O	1.95	0.65
4:A:403:NAG:O6	7:A:514:HOH:O	2.13	0.64
1:C:63:ASN:OD1	1:C:92:LYS:HG3	1.97	0.64
1:C:154:LEU:O	7:C:512:HOH:O	2.15	0.64
1:A:290:ASN:CB	7:A:501:HOH:O	1.89	0.64
2:K:1:GLU:CA	7:K:304:HOH:O	1.88	0.64
1:B:177:LEU:HB2	1:B:260:ILE:HD11	1.79	0.64
3:R:71:ASN:ND2	3:R:71:ASN:O	2.31	0.64
1:C:90:ARG:CA	7:C:506:HOH:O	2.38	0.64
2:K:30:THR:HA	2:K:53:PRO:HB2	1.78	0.64
3:P:125:GLU:OE1	7:P:305:HOH:O	2.08	0.64
3:L:106:THR:HG21	3:L:143:PRO:HB3	1.81	0.63
1:A:63:ASN:HD22	4:A:403:NAG:H2	1.57	0.63
4:B:402:NAG:C5	7:B:515:HOH:O	2.46	0.63
1:B:185:PRO:HG2	1:B:217:ILE:HG12	1.80	0.63
1:E:167:THR:HG23	1:E:242:ILE:HG21	1.80	0.63
3:R:174:TYR:HE2	7:R:310:HOH:O	1.81	0.63
3:R:22:CYS:HB3	3:R:73:ALA:HB3	1.80	0.63
1:F:176:LYS:HB2	1:F:237:VAL:HG23	1.79	0.63
3:L:115:PRO:HB3	3:L:141:PHE:HB3	1.79	0.63
1:B:310:LYS:HB2	7:B:507:HOH:O	1.97	0.62
4:A:406:NAG:H61	7:A:513:HOH:O	1.95	0.62
1:F:186:VAL:HG12	1:F:187:THR:HG23	1.82	0.62
1:A:42:LEU:HA	1:A:292:LYS:HD2	1.81	0.62
1:A:150:ARG:NH1	4:A:407:NAG:H5	2.14	0.62
2:O:165:TYR:CE1	2:O:170:VAL:HG23	2.34	0.62
3:J:29:VAL:O	3:J:33:ASP:OD1	2.17	0.62
1:A:62:GLU:HG2	4:A:403:NAG:H83	1.81	0.62
4:D:403:NAG:O7	4:D:403:NAG:O3	2.18	0.62
3:P:151:LYS:HB2	3:P:194:SER:HB2	1.82	0.61
1:C:207:LYS:NZ	1:C:241:ASP:HA	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ILE:N	7:D:501:HOH:O	2.29	0.61
4:C:406:NAG:O7	4:C:406:NAG:H3	1.99	0.61
3:J:56:ARG:HG2	3:J:60:VAL:HB	1.82	0.61
1:D:186:VAL:HG23	1:D:228:SER:OG	2.00	0.61
1:F:138:ALA:CB	1:F:226:ILE:CD1	2.79	0.61
2:I:87:ARG:O	2:I:131:VAL:HG11	2.00	0.61
3:N:10:VAL:HG23	3:N:105:LEU:HD13	1.83	0.61
2:M:87:ARG:O	2:M:131:VAL:HG11	2.01	0.61
4:B:402:NAG:C4	7:B:515:HOH:O	2.45	0.61
1:B:80:GLN:O	7:B:514:HOH:O	2.16	0.61
4:D:406:NAG:H82	4:D:406:NAG:C5	2.30	0.61
2:M:42:GLY:HA2	7:M:302:HOH:O	1.98	0.61
1:F:120:PHE:CE2	1:F:122:ASN:OD1	2.53	0.61
3:J:152:ALA:O	7:J:304:HOH:O	2.16	0.61
1:E:165:ASN:HD22	4:E:406:NAG:H61	1.66	0.60
1:D:66:LEU:CD2	1:D:112:VAL:HG13	2.32	0.60
1:E:166:VAL:HG12	1:E:245:ILE:HB	1.84	0.60
3:N:185:GLU:OE1	3:N:185:GLU:N	2.33	0.60
3:H:159:ALA:O	7:H:308:HOH:O	2.16	0.60
3:L:169:GLN:N	7:L:311:HOH:O	2.34	0.60
3:N:10:VAL:HG23	3:N:105:LEU:CD1	2.31	0.60
2:Q:91:THR:HG23	2:Q:130:ALA:HA	1.83	0.60
1:F:177:LEU:HB2	1:F:260:ILE:HD11	1.83	0.60
2:G:83:LEU:HD23	2:G:86:LEU:CD2	2.31	0.59
2:O:2:VAL:HG12	2:O:122:VAL:HG11	1.84	0.59
2:Q:37:VAL:HG22	2:Q:47:TRP:HA	1.84	0.59
1:A:62:GLU:HB3	4:A:403:NAG:H82	1.85	0.59
1:D:165:ASN:ND2	4:D:403:NAG:H61	2.13	0.59
4:F:406:NAG:O7	4:F:406:NAG:O3	2.19	0.59
2:G:2:VAL:HG12	2:G:122:VAL:HG11	1.82	0.59
3:L:209:ALA:HB3	3:L:212:GLU:CD	2.22	0.59
3:P:134:LEU:HD12	3:P:180:LEU:HD23	1.84	0.59
1:C:220:ARG:CG	1:C:229:ARG:NH1	2.66	0.59
2:G:101:THR:O	7:G:307:HOH:O	2.17	0.59
2:G:103:MET:HE2	2:G:112:ARG:HB3	1.83	0.59
3:H:211:THR:N	7:H:304:HOH:O	2.34	0.59
3:P:71:ASN:O	3:P:71:ASN:ND2	2.34	0.59
2:Q:234:LYS:NZ	3:R:212:GLU:OE2	2.28	0.59
2:I:189:VAL:HG21	3:J:162:GLU:HG3	1.85	0.59
1:D:62:GLU:O	7:D:508:HOH:O	2.17	0.59
1:F:306:PRO:HA	7:F:509:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:33:ASP:OD2	3:J:68:LYS:CE	2.51	0.59
2:Q:53:PRO:HA	2:Q:72:ARG:HD2	1.83	0.59
1:C:47:SER:HB2	1:C:288:ILE:HG22	1.85	0.58
2:K:10:GLU:C	7:K:302:HOH:O	2.32	0.58
3:P:185:GLU:OE1	3:P:185:GLU:N	2.33	0.58
1:A:207:LYS:HZ2	1:A:242:ILE:HD12	1.69	0.58
1:A:63:ASN:CG	4:A:403:NAG:C1	2.71	0.58
2:Q:2:VAL:HG11	2:Q:122:VAL:HG21	1.85	0.58
4:D:405:NAG:C8	4:D:405:NAG:H3	2.29	0.58
1:F:138:ALA:CB	1:F:226:ILE:HD12	2.34	0.58
3:L:110:GLN:OE1	3:L:173:LYS:NZ	2.21	0.58
3:N:32:PHE:HB3	3:N:34:LEU:HD13	1.86	0.58
1:B:283:THR:OG1	1:B:286:GLY:O	2.19	0.57
4:D:405:NAG:C7	4:D:405:NAG:HO4	2.16	0.57
2:Q:2:VAL:HG23	2:Q:27:TYR:CD1	2.38	0.57
1:E:206:THR:HA	7:E:504:HOH:O	2.04	0.57
1:C:107:SER:OG	1:D:208:ARG:O	2.22	0.57
3:L:209:ALA:HB3	3:L:212:GLU:OE1	2.03	0.57
1:B:202:ILE:HD11	1:B:249:GLY:O	2.04	0.57
1:E:232:ILE:O	7:E:511:HOH:O	2.18	0.57
2:K:217:ASN:N	7:K:301:HOH:O	2.30	0.57
3:R:6:GLN:HE22	3:R:102:GLY:H	1.47	0.57
3:R:56:ARG:CZ	3:R:62:ASP:HA	2.33	0.57
2:I:53:PRO:O	2:I:72:ARG:NH1	2.37	0.57
3:N:33:ASP:O	3:N:35:VAL:N	2.29	0.57
3:N:71:ASN:ND2	3:N:71:ASN:O	2.36	0.57
1:B:201:ARG:HA	7:B:505:HOH:O	2.01	0.57
2:I:231:VAL:O	7:I:407:HOH:O	2.17	0.57
3:R:185:GLU:OE1	3:R:185:GLU:N	2.35	0.57
2:O:229:LYS:NZ	3:P:125:GLU:OE2	2.37	0.57
1:C:223:ILE:HD13	1:C:229:ARG:HH21	1.70	0.57
2:K:131:VAL:HG13	2:K:131:VAL:O	2.05	0.57
3:L:18:VAL:HG21	3:L:105:LEU:HD11	1.85	0.57
3:R:164:THR:HG22	3:R:177:SER:H	1.69	0.57
1:E:142:ARG:NH1	7:E:515:HOH:O	2.36	0.57
3:P:37:TRP:NE1	7:P:302:HOH:O	1.94	0.57
1:A:45:ASN:HA	1:A:296:ASN:OD1	2.05	0.56
1:D:206:THR:HG23	1:D:208:ARG:H	1.70	0.56
1:A:291:ASP:OD2	7:A:516:HOH:O	2.18	0.56
1:A:144:ASN:CG	4:A:406:NAG:C1	2.71	0.56
1:C:219:PHE:CD2	7:C:503:HOH:O	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PHE:HD2	7:C:503:HOH:O	1.88	0.56
1:F:138:ALA:HB2	1:F:226:ILE:CD1	2.35	0.56
3:J:81:GLN:O	3:J:107:VAL:HG21	2.05	0.56
2:O:91:THR:HG23	2:O:130:ALA:HA	1.88	0.56
2:K:88:SER:HA	2:K:131:VAL:HG13	1.86	0.56
1:D:81:ASN:HD21	4:D:405:NAG:C8	2.18	0.56
3:H:81:GLN:O	3:H:107:VAL:HG21	2.06	0.56
3:J:33:ASP:CG	3:J:68:LYS:CD	2.74	0.56
1:A:234:TRP:NE1	7:A:505:HOH:O	1.94	0.56
3:R:6:GLN:HE22	3:R:102:GLY:C	2.09	0.56
7:Q:301:HOH:O	3:R:89:TYR:OH	2.14	0.56
1:D:81:ASN:HD21	4:D:405:NAG:C7	2.19	0.56
4:D:405:NAG:O7	4:D:405:NAG:O4	2.24	0.56
3:H:33:ASP:HB3	3:H:68:LYS:HZ3	1.70	0.56
3:N:110:GLN:NE2	7:N:304:HOH:O	1.97	0.55
1:A:289:PRO:HB3	1:C:199:SER:HB3	1.87	0.55
1:C:206:THR:HG23	1:C:208:ARG:N	2.12	0.55
3:R:115:PRO:HB3	3:R:141:PHE:HB3	1.87	0.55
4:A:408:NAG:O7	7:A:517:HOH:O	2.18	0.55
3:H:56:ARG:HG2	3:H:60:VAL:HB	1.88	0.55
2:I:131:VAL:HG13	2:I:131:VAL:O	2.05	0.55
2:K:91:THR:HG23	2:K:130:ALA:HA	1.87	0.55
3:L:151:LYS:HB2	3:L:194:SER:HB2	1.87	0.55
1:C:87:PHE:HB3	1:C:267:ILE:HD12	1.88	0.55
2:O:83:LEU:HD23	2:O:86:LEU:CD2	2.37	0.55
1:E:174:PHE:CZ	7:E:501:HOH:O	2.52	0.55
1:F:238:LYS:HG3	1:F:239:PRO:HD2	1.88	0.55
2:I:148:SER:OG	3:J:213:CYS:HB3	2.07	0.55
3:L:85:GLU:HG3	3:L:105:LEU:O	2.07	0.55
1:A:269:ARG:NE	7:A:515:HOH:O	2.16	0.55
2:Q:44:GLY:HA2	3:R:89:TYR:HE2	1.72	0.55
1:A:43:VAL:HG22	1:A:294:PHE:HB2	1.88	0.55
2:I:2:VAL:HG13	2:I:27:TYR:CD1	2.42	0.55
2:M:2:VAL:HG12	2:M:122:VAL:HG11	1.89	0.55
3:H:173:LYS:NZ	7:H:309:HOH:O	2.16	0.54
2:I:91:THR:HG23	2:I:130:ALA:HA	1.90	0.54
1:A:259:LYS:HB3	1:A:259:LYS:NZ	2.22	0.54
2:Q:2:VAL:HG23	2:Q:27:TYR:HD1	1.73	0.54
1:C:42:LEU:O	1:C:292:LYS:HB3	2.07	0.54
1:B:311:GLN:N	7:B:507:HOH:O	1.93	0.54
1:E:242:ILE:N	7:E:502:HOH:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HD3	7:A:503:HOH:O	2.06	0.54
1:C:94:TYR:HE1	4:C:402:NAG:HN2	1.55	0.54
1:E:299:ARG:NH2	7:E:516:HOH:O	2.37	0.54
1:E:97:CYS:SG	1:E:98:TYR:N	2.79	0.54
2:M:131:VAL:O	2:M:131:VAL:HG13	2.07	0.54
1:F:176:LYS:HB2	1:F:237:VAL:HG22	1.88	0.54
3:H:28:ASP:OD2	3:H:29:VAL:HG13	2.08	0.54
1:A:207:LYS:NZ	1:A:242:ILE:HD12	2.23	0.53
1:C:237:VAL:HG21	1:C:243:LEU:HB2	1.90	0.53
1:C:283:THR:HG22	1:C:301:THR:HG22	1.88	0.53
1:F:241:ASP:OD1	1:F:242:ILE:N	2.40	0.53
3:J:151:LYS:HB2	3:J:194:SER:HB2	1.89	0.53
1:B:74:PRO:HB3	1:B:141:ARG:HB2	1.89	0.53
1:E:45:ASN:HA	1:E:296:ASN:OD1	2.09	0.53
3:R:168:LYS:HA	3:R:174:TYR:HD1	1.74	0.53
1:E:67:ILE:HG13	1:E:105:TYR:HE1	1.73	0.53
7:K:311:HOH:O	3:L:44:LYS:C	2.46	0.53
1:E:288:ILE:HG21	1:E:297:VAL:HG21	1.90	0.53
1:F:108:LEU:CA	7:F:504:HOH:O	2.52	0.53
1:C:283:THR:OG1	1:C:286:GLY:O	2.22	0.53
1:D:47:SER:HB3	1:D:288:ILE:HG22	1.89	0.53
3:N:32:PHE:HB3	3:N:34:LEU:CD1	2.39	0.53
1:A:173:GLN:NE2	1:F:307:ARG:NH1	2.57	0.53
1:B:186:VAL:HG21	1:B:227:PRO:HG2	1.91	0.53
2:K:218:VAL:HB	2:K:227:VAL:HG22	1.91	0.53
3:P:146:VAL:CG2	3:P:197:VAL:HG13	2.39	0.53
1:B:241:ASP:OD1	1:B:242:ILE:N	2.38	0.52
1:E:169:PRO:HB3	1:E:242:ILE:HD12	1.91	0.52
3:R:128:GLN:NE2	7:R:304:HOH:O	1.88	0.52
1:C:291:ASP:N	7:C:521:HOH:O	2.41	0.52
3:N:159:ALA:N	7:N:301:HOH:O	2.03	0.52
3:P:115:PRO:HB3	3:P:141:PHE:HB3	1.91	0.52
1:C:221:PRO:O	1:C:229:ARG:NH2	2.42	0.52
2:G:139:PRO:HB3	2:G:165:TYR:HB3	1.91	0.52
3:L:82:ALA:HA	3:L:107:VAL:HG11	1.90	0.52
1:F:138:ALA:CB	1:F:226:ILE:HD11	2.40	0.52
4:A:406:NAG:O6	7:A:513:HOH:O	2.13	0.52
1:A:68:ASP:OD1	1:A:100:TYR:OH	2.21	0.52
1:C:186:VAL:HG21	1:C:227:PRO:HG2	1.90	0.52
2:K:228:ASP:HA	7:K:301:HOH:O	2.08	0.52
1:E:158:ASN:ND2	3:P:52:GLU:OE1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:THR:C	7:B:502:HOH:O	2.37	0.52
2:M:87:ARG:HD2	7:M:311:HOH:O	2.10	0.52
3:N:134:LEU:HD12	3:N:180:LEU:HD23	1.92	0.52
1:E:42:LEU:HA	1:E:292:LYS:HD2	1.92	0.52
1:E:182:VAL:HG11	1:E:213:VAL:HG11	1.92	0.52
1:F:87:PHE:HB3	1:F:267:ILE:HD12	1.92	0.52
1:C:175:ASP:OD2	1:C:238:LYS:NZ	2.41	0.52
2:K:218:VAL:HB	2:K:227:VAL:CG2	2.40	0.52
2:K:117:TYR:O	3:L:34:LEU:HD23	2.10	0.52
3:P:52:GLU:HB3	3:P:55:ARG:HH21	1.73	0.52
3:R:6:GLN:HE22	3:R:102:GLY:CA	2.22	0.52
1:B:202:ILE:CD1	1:B:251:LEU:HB2	2.38	0.52
1:A:189:LYS:O	1:A:193:PHE:HD2	1.93	0.51
4:D:406:NAG:C1	4:D:406:NAG:C8	2.85	0.51
1:E:40:THR:OG1	1:E:41:GLU:N	2.44	0.51
2:K:87:ARG:O	2:K:131:VAL:HG11	2.10	0.51
3:H:194:SER:OG	7:H:310:HOH:O	2.19	0.51
3:R:28:ASP:C	3:R:30:GLY:H	2.11	0.51
1:A:283:THR:HG22	1:A:301:THR:HG22	1.92	0.51
1:C:182:VAL:HG22	1:C:202:ILE:HD12	1.92	0.51
3:J:168:LYS:HD3	3:J:172:ASN:OD1	2.09	0.51
1:E:310:LYS:O	1:E:311:GLN:HG3	2.11	0.51
2:M:4:LEU:HD22	2:M:24:THR:HG22	1.93	0.51
3:P:22:CYS:HB3	3:P:73:ALA:HB3	1.92	0.51
2:G:57:ASP:OD1	2:G:58:THR:N	2.44	0.51
2:M:37:VAL:HG22	2:M:47:TRP:HA	1.92	0.51
1:F:138:ALA:HB2	1:F:226:ILE:HD11	1.91	0.51
1:F:109:ARG:HH12	1:F:269:ARG:NE	2.08	0.51
3:J:33:ASP:CG	3:J:68:LYS:HD2	2.25	0.51
1:D:177:LEU:HB2	1:D:260:ILE:HD11	1.92	0.51
2:Q:40:ALA:CB	7:Q:304:HOH:O	2.59	0.51
1:C:138:ALA:HB2	1:C:226:ILE:CD1	2.40	0.50
1:F:114:SER:C	7:F:507:HOH:O	2.43	0.50
1:F:97:CYS:SG	1:F:98:TYR:N	2.80	0.50
2:Q:4:LEU:HD22	2:Q:24:THR:HG22	1.93	0.50
3:L:23:THR:O	7:L:303:HOH:O	2.19	0.50
2:Q:139:PRO:HB3	2:Q:165:TYR:HB3	1.92	0.50
1:D:204:VAL:HG13	1:D:245:ILE:HG12	1.92	0.50
1:F:59:LEU:HD22	1:F:87:PHE:CE2	2.47	0.50
1:C:222:ARG:HH21	1:C:225:ASN:CG	2.15	0.50
1:D:222:ARG:NH1	1:D:227:PRO:HD3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:151:LYS:NZ	3:N:156:PRO:HG3	2.27	0.50
2:K:158:LEU:HB2	2:K:231:VAL:HG11	1.93	0.50
3:L:56:ARG:CZ	3:L:62:ASP:HA	2.42	0.50
2:M:1:GLU:O	2:M:1:GLU:HG2	2.11	0.50
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.92	0.50
1:C:207:LYS:HZ1	1:C:241:ASP:HA	1.76	0.50
1:E:199:SER:HB3	7:E:503:HOH:O	2.10	0.50
3:L:58:SER:O	7:L:310:HOH:O	2.20	0.50
4:B:407:NAG:C4	7:B:503:HOH:O	2.49	0.50
1:D:97:CYS:SG	1:D:98:TYR:N	2.83	0.50
2:K:37:VAL:HG21	2:K:123:TRP:CZ3	2.46	0.50
3:L:30:GLY:HA3	3:L:71:ASN:HA	1.94	0.50
1:C:283:THR:CB	7:C:513:HOH:O	2.60	0.50
4:A:403:NAG:C5	7:A:509:HOH:O	2.58	0.49
1:B:79:PHE:HA	1:B:82:LYS:HD2	1.95	0.49
1:E:118:LEU:O	7:E:512:HOH:O	2.19	0.49
1:E:167:THR:HG23	1:E:242:ILE:CG2	2.42	0.49
3:L:29:VAL:HG23	3:L:35:VAL:HG21	1.92	0.49
1:B:259:LYS:NZ	1:B:259:LYS:HB3	2.27	0.49
1:B:47:SER:HB3	1:B:288:ILE:HG22	1.93	0.49
3:H:37:TRP:HB2	3:H:50:ILE:HB	1.93	0.49
2:K:210:GLY:HA2	7:K:307:HOH:O	2.11	0.49
3:P:117:VAL:O	3:P:206:LYS:NZ	2.43	0.49
4:B:402:NAG:O5	7:B:515:HOH:O	2.20	0.49
4:E:401:NAG:H3	4:E:401:NAG:O7	2.11	0.49
3:H:33:ASP:CB	3:H:68:LYS:HZ1	2.25	0.49
3:H:33:ASP:C	3:H:35:VAL:H	2.13	0.49
1:E:125:PHE:O	7:E:513:HOH:O	2.20	0.49
2:K:10:GLU:O	7:K:302:HOH:O	2.20	0.49
2:Q:41:PRO:O	7:Q:304:HOH:O	2.19	0.49
4:A:403:NAG:C7	4:A:403:NAG:HO3	2.18	0.49
1:B:43:VAL:HG22	1:B:294:PHE:HB2	1.94	0.49
4:B:401:NAG:C7	4:B:401:NAG:HO3	2.17	0.49
1:E:283:THR:OG1	1:E:286:GLY:O	2.28	0.49
2:I:189:VAL:HB	3:J:164:THR:HG22	1.93	0.49
2:K:139:PRO:HB3	2:K:165:TYR:HB3	1.94	0.49
2:M:139:PRO:HB3	2:M:165:TYR:HB3	1.94	0.49
1:C:203:THR:CG2	1:C:246:ASN:HB2	2.42	0.49
1:F:261:ARG:HB2	7:F:508:HOH:O	2.12	0.49
1:A:301:THR:HB	1:A:305:CYS:SG	2.53	0.49
3:R:179:TYR:O	7:R:306:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:PHE:HA	1:C:82:LYS:HD2	1.95	0.49
1:E:261:ARG:NH1	7:E:521:HOH:O	2.45	0.49
1:F:306:PRO:CA	7:F:509:HOH:O	2.59	0.49
1:A:97:CYS:SG	1:A:98:TYR:N	2.84	0.48
1:D:241:ASP:OD1	1:D:242:ILE:N	2.43	0.48
3:R:15:GLY:N	3:R:80:LEU:O	2.37	0.48
1:F:201:ARG:O	1:F:247:SER:HA	2.12	0.48
7:Q:301:HOH:O	3:R:89:TYR:CE2	2.66	0.48
3:N:117:VAL:O	3:N:206:LYS:NZ	2.46	0.48
2:O:37:VAL:HG12	2:O:47:TRP:CA	2.23	0.48
2:O:67:ARG:NH2	2:O:90:ASP:OD2	2.45	0.48
1:D:168:MET:HE2	1:D:169:PRO:HD2	1.95	0.48
3:N:23:THR:HG22	3:N:72:THR:HG23	1.95	0.48
1:C:301:THR:HB	1:C:305:CYS:SG	2.54	0.48
3:H:69:SER:OG	3:H:70:GLY:N	2.45	0.48
2:Q:40:ALA:HB1	7:Q:304:HOH:O	2.13	0.48
1:C:138:ALA:HB2	1:C:226:ILE:HD11	1.95	0.48
1:F:109:ARG:HH12	1:F:269:ARG:HE	1.60	0.48
3:P:81:GLN:O	3:P:107:VAL:HG21	2.13	0.48
1:B:295:GLN:HG2	1:B:297:VAL:H	1.79	0.48
1:C:97:CYS:SG	1:C:98:TYR:N	2.84	0.48
2:I:12:LYS:O	2:I:131:VAL:HA	2.14	0.48
2:I:4:LEU:HD22	2:I:24:THR:HG22	1.95	0.48
3:R:18:VAL:HG21	3:R:105:LEU:HD11	1.95	0.48
1:C:92:LYS:HG2	7:C:506:HOH:O	2.12	0.48
1:E:299:ARG:NE	7:E:516:HOH:O	2.44	0.48
2:I:36:TRP:CE3	2:I:81:MET:HE2	2.48	0.48
2:O:83:LEU:HD23	2:O:86:LEU:HD21	1.95	0.48
1:B:214:ILE:O	1:B:214:ILE:HG13	2.12	0.48
2:K:209:LEU:O	7:K:307:HOH:O	2.20	0.48
3:R:6:GLN:NE2	3:R:102:GLY:H	2.09	0.48
4:D:406:NAG:O6	7:D:506:HOH:O	2.20	0.47
2:G:126:GLY:O	7:G:308:HOH:O	2.20	0.47
2:G:189:VAL:HB	3:H:164:THR:HG22	1.95	0.47
2:O:201:VAL:HG21	3:P:137:LEU:HD13	1.95	0.47
2:Q:234:LYS:HG2	2:Q:235:SER:H	1.79	0.47
1:D:108:LEU:O	1:D:112:VAL:HG12	2.14	0.47
3:J:27:SER:HA	3:J:31:THR:OG1	2.14	0.47
2:K:47:TRP:CG	3:L:97:VAL:HB	2.48	0.47
2:Q:12:LYS:O	2:Q:131:VAL:HA	2.15	0.47
3:R:151:LYS:HZ2	3:R:156:PRO:HG3	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:56:ARG:HD3	3:R:60:VAL:O	2.14	0.47
2:G:10:GLU:HB2	2:G:129:VAL:HG12	1.95	0.47
3:H:85:GLU:CD	7:H:316:HOH:O	2.53	0.47
1:D:84:TRP:CE2	1:D:116:GLY:HA2	2.49	0.47
1:F:47:SER:HB3	1:F:288:ILE:HG22	1.96	0.47
2:I:139:PRO:HB3	2:I:165:TYR:HB3	1.97	0.47
2:I:46:GLU:OE2	2:I:63:LYS:HE2	2.14	0.47
2:M:234:LYS:HG2	2:M:235:SER:N	2.29	0.47
1:B:176:LYS:HD3	1:B:257:TYR:CD1	2.50	0.47
1:D:79:PHE:HA	1:D:82:LYS:HD2	1.96	0.47
1:F:75:GLN:NE2	1:F:94:TYR:O	2.43	0.47
2:G:4:LEU:HD22	2:G:24:THR:HG22	1.97	0.47
3:P:33:ASP:C	3:P:35:VAL:H	2.18	0.47
1:B:280:GLU:O	1:B:280:GLU:HG3	2.14	0.47
1:B:97:CYS:SG	1:B:98:TYR:N	2.84	0.47
1:D:202:ILE:HD13	1:D:247:SER:HB2	1.96	0.47
3:L:89:TYR:OH	7:L:308:HOH:O	2.03	0.47
2:Q:10:GLU:HB2	2:Q:129:VAL:HG23	1.97	0.47
1:D:134:GLY:HA3	1:D:153:TRP:HB3	1.97	0.47
1:D:254:PRO:O	7:D:509:HOH:O	2.20	0.47
1:F:114:SER:HA	1:F:265:SER:O	2.15	0.47
1:F:79:PHE:HA	1:F:82:LYS:HG3	1.96	0.47
2:I:171:THR:OG1	2:I:219:ASN:HB3	2.15	0.47
1:D:206:THR:OG1	1:D:207:LYS:N	2.48	0.47
3:N:25:THR:CG2	3:N:26:ASN:N	2.68	0.47
4:A:403:NAG:C5	7:A:514:HOH:O	2.44	0.47
1:F:176:LYS:HD3	1:F:257:TYR:CD1	2.50	0.47
3:H:23:THR:N	7:H:307:HOH:O	2.47	0.47
2:I:60:TYR:HB2	2:I:65:GLN:HG2	1.96	0.47
3:J:33:ASP:OD2	3:J:68:LYS:HD3	2.08	0.47
2:K:141:VAL:HG21	2:K:227:VAL:HG21	1.96	0.47
1:C:304:ALA:N	7:C:520:HOH:O	2.39	0.47
3:L:191:ARG:O	3:L:209:ALA:HB1	2.15	0.47
1:E:295:GLN:HB3	1:E:306:PRO:HG2	1.96	0.46
2:O:101:THR:OG1	7:O:301:HOH:O	2.14	0.46
2:O:229:LYS:NZ	7:P:305:HOH:O	2.47	0.46
2:O:4:LEU:HD22	2:O:24:THR:HG22	1.96	0.46
3:P:33:ASP:O	3:P:35:VAL:N	2.41	0.46
1:E:167:THR:CG2	1:E:242:ILE:HG21	2.45	0.46
2:I:47:TRP:O	7:I:408:HOH:O	2.20	0.46
2:O:64:PHE:O	2:O:68:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:VAL:HG12	1:C:245:ILE:HB	1.97	0.46
1:D:203:THR:CG2	1:D:246:ASN:HB2	2.45	0.46
1:D:206:THR:HG23	1:D:209:SER:H	1.80	0.46
2:Q:41:PRO:C	7:Q:304:HOH:O	2.54	0.46
3:N:165:THR:O	7:N:307:HOH:O	2.21	0.46
1:E:165:ASN:ND2	4:E:406:NAG:H61	2.31	0.46
1:F:108:LEU:HD12	7:F:504:HOH:O	2.15	0.46
2:O:117:TYR:O	3:P:34:LEU:HD23	2.14	0.46
1:B:189:LYS:NZ	7:B:529:HOH:O	2.48	0.46
1:A:42:LEU:O	1:A:292:LYS:HB3	2.16	0.46
1:E:268:MET:HE2	1:E:284:PRO:HD3	1.97	0.46
1:F:138:ALA:HB3	1:F:226:ILE:CD1	2.44	0.46
1:E:176:LYS:HD3	1:E:257:TYR:CD1	2.50	0.46
1:F:306:PRO:C	7:F:509:HOH:O	2.53	0.46
2:Q:103:MET:HE3	2:Q:112:ARG:HB3	1.98	0.46
1:C:185:PRO:HG3	1:C:191:GLN:OE1	2.15	0.46
1:F:291:ASP:HA	7:F:513:HOH:O	2.15	0.46
2:I:54:ASN:ND2	2:I:106:PHE:HE1	2.14	0.46
2:M:91:THR:HG23	2:M:130:ALA:HA	1.97	0.46
1:C:292:LYS:H	1:C:292:LYS:HD2	1.81	0.45
1:E:242:ILE:C	7:E:502:HOH:O	2.38	0.45
2:I:48:MET:HG2	2:I:64:PHE:CE2	2.50	0.45
3:L:209:ALA:CB	3:L:212:GLU:OE2	2.62	0.45
3:R:89:TYR:HA	7:R:309:HOH:O	2.15	0.45
1:A:63:ASN:OD1	4:A:403:NAG:C1	2.64	0.45
1:B:176:LYS:HB2	1:B:237:VAL:HG22	1.98	0.45
2:G:158:LEU:HB2	2:G:231:VAL:HG11	1.98	0.45
2:G:117:TYR:O	3:H:34:LEU:HD23	2.17	0.45
3:J:4:LEU:HD21	3:J:28:ASP:OD2	2.17	0.45
2:M:45:PHE:CZ	3:N:46:PRO:HG3	2.51	0.45
3:R:35:VAL:HG22	3:R:92:SER:OG	2.16	0.45
4:D:405:NAG:O3	4:D:405:NAG:H62	2.16	0.45
1:D:295:GLN:OE1	1:D:297:VAL:N	2.50	0.45
1:E:262:SER:N	7:E:505:HOH:O	2.36	0.45
1:F:109:ARG:NH1	1:F:269:ARG:NH2	2.65	0.45
2:I:67:ARG:NH2	2:I:83:LEU:HD11	2.30	0.45
3:J:165:THR:HG22	7:J:328:HOH:O	2.17	0.45
3:N:69:SER:HA	7:N:313:HOH:O	2.16	0.45
3:R:55:ARG:NH2	7:R:311:HOH:O	2.49	0.45
1:B:141:ARG:HD3	7:B:520:HOH:O	2.16	0.45
1:F:182:VAL:HG22	1:F:202:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:91:THR:HG23	2:G:130:ALA:HA	1.99	0.45
3:H:115:PRO:HB3	3:H:141:PHE:HB3	1.98	0.45
1:F:83:LYS:HB2	1:F:83:LYS:NZ	2.31	0.45
2:M:30:THR:HA	2:M:53:PRO:HB2	1.99	0.45
1:C:207:LYS:HZ3	1:C:241:ASP:HA	1.79	0.45
1:F:178:TYR:HE2	1:F:237:VAL:HG21	1.82	0.45
1:F:99:PRO:HB2	1:F:229:ARG:HD3	1.98	0.45
2:O:158:LEU:HB2	2:O:231:VAL:HG11	1.98	0.45
3:P:52:GLU:OE2	3:P:55:ARG:NH2	2.49	0.45
2:Q:2:VAL:CG2	2:Q:27:TYR:CD1	2.99	0.45
1:C:168:MET:HG2	7:C:508:HOH:O	2.17	0.45
1:C:158:ASN:ND2	3:L:52:GLU:OE2	2.35	0.45
2:Q:166:PHE:HA	2:Q:167:PRO:HA	1.78	0.45
4:B:402:NAG:C6	7:B:515:HOH:O	2.65	0.45
2:G:30:THR:HA	2:G:53:PRO:HB2	1.99	0.45
2:K:45:PHE:CZ	3:L:46:PRO:HG3	2.52	0.45
1:D:81:ASN:ND2	4:D:405:NAG:C8	2.80	0.45
2:I:83:LEU:CD2	2:I:86:LEU:HD23	2.47	0.45
2:G:193:SER:OG	7:G:305:HOH:O	2.04	0.44
2:I:37:VAL:HG21	2:I:123:TRP:CZ3	2.52	0.44
2:I:61:ALA:O	2:I:65:GLN:HG3	2.15	0.44
3:L:212:GLU:N	3:L:212:GLU:OE1	2.49	0.44
2:Q:112:ARG:NH1	2:Q:114:ALA:O	2.49	0.44
1:B:298:ASN:OD1	1:B:300:ILE:N	2.47	0.44
1:C:167:THR:HG23	1:C:242:ILE:HG21	2.00	0.44
4:C:403:NAG:H3	5:C:404:BMA:O2	2.17	0.44
1:C:236:ILE:HD12	1:C:260:ILE:HD11	1.98	0.44
1:F:176:LYS:HD3	1:F:257:TYR:CG	2.52	0.44
3:J:115:PRO:HB3	3:J:141:PHE:HB3	1.99	0.44
3:J:62:ASP:CG	7:J:302:HOH:O	2.56	0.44
3:H:85:GLU:HG3	3:H:105:LEU:O	2.16	0.44
2:I:45:PHE:CZ	3:J:46:PRO:HG3	2.52	0.44
3:L:85:GLU:HG3	3:L:106:THR:HA	1.99	0.44
2:O:49:ALA:HB2	2:O:60:TYR:HA	1.99	0.44
1:A:75:GLN:NE2	1:A:94:TYR:O	2.44	0.44
1:E:176:LYS:HD3	1:E:257:TYR:CG	2.52	0.44
3:H:168:LYS:HB3	3:H:168:LYS:HE3	1.73	0.44
1:C:165:ASN:OD1	1:C:165:ASN:O	2.35	0.44
1:F:67:ILE:HG13	1:F:105:TYR:CE1	2.52	0.44
3:N:81:GLN:O	3:N:107:VAL:HG21	2.17	0.44
3:P:96:SER:HA	7:P:312:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:THR:HG21	1:B:237:VAL:HG12	1.98	0.44
4:B:407:NAG:C5	7:B:503:HOH:O	2.66	0.44
1:F:150:ARG:HG2	1:F:258:PHE:CZ	2.52	0.44
1:F:59:LEU:HD21	1:F:79:PHE:CD1	2.53	0.44
2:I:40:ALA:HB3	2:I:43:GLN:HG3	1.99	0.44
2:K:2:VAL:HG12	2:K:122:VAL:HG11	2.00	0.44
3:N:33:ASP:C	3:N:35:VAL:H	2.16	0.44
2:O:101:THR:CA	7:O:301:HOH:O	2.29	0.44
2:Q:151:THR:HG22	2:Q:152:SER:H	1.83	0.44
1:D:45:ASN:HA	1:D:296:ASN:OD1	2.17	0.43
4:E:406:NAG:O4	4:E:406:NAG:O6	2.26	0.43
1:F:150:ARG:HG2	1:F:258:PHE:HZ	1.82	0.43
2:M:12:LYS:O	2:M:131:VAL:HA	2.18	0.43
3:N:51:TYR:OH	7:N:305:HOH:O	2.10	0.43
3:H:80:LEU:HG	3:H:107:VAL:HG22	2.00	0.43
2:K:188:ALA:HA	2:K:198:LEU:HB3	1.99	0.43
3:L:37:TRP:HB2	3:L:50:ILE:HB	1.99	0.43
2:M:164:ASP:HB3	2:M:195:LEU:HD13	1.99	0.43
2:O:112:ARG:NH1	2:O:114:ALA:O	2.47	0.43
1:A:176:LYS:HD3	1:A:257:TYR:CG	2.52	0.43
1:D:167:THR:HG23	1:D:242:ILE:CG2	2.48	0.43
1:E:67:ILE:HG13	1:E:105:TYR:CE1	2.53	0.43
1:F:67:ILE:HG13	1:F:105:TYR:HE1	1.83	0.43
1:F:45:ASN:HA	1:F:296:ASN:OD1	2.19	0.43
3:R:65:SER:O	3:R:75:LEU:HD12	2.17	0.43
1:A:176:LYS:HD3	1:A:257:TYR:CD1	2.53	0.43
1:D:160:LYS:HD3	1:D:162:PRO:HD3	2.00	0.43
2:K:48:MET:HG2	2:K:64:PHE:CE2	2.53	0.43
2:M:147:SER:HB3	7:M:301:HOH:O	2.19	0.43
1:C:206:THR:CG2	1:C:209:SER:H	2.30	0.43
1:D:150:ARG:HG3	1:D:258:PHE:HZ	1.83	0.43
2:M:10:GLU:HB2	2:M:129:VAL:HG23	2.00	0.43
3:N:85:GLU:HG3	3:N:105:LEU:O	2.18	0.43
1:D:157:LEU:HD11	2:Q:118:TYR:CZ	2.54	0.43
1:A:270:SER:HB2	1:A:284:PRO:HA	2.01	0.43
1:F:134:GLY:HA3	1:F:153:TRP:HB3	2.00	0.43
1:F:168:MET:HE2	1:F:169:PRO:HD2	2.01	0.43
1:E:141:ARG:NH1	1:E:146:SER:OG	2.52	0.43
2:O:103:MET:HE3	2:O:112:ARG:HB3	2.00	0.43
1:C:283:THR:HB	7:C:513:HOH:O	2.18	0.43
1:D:131:THR:HG1	1:D:155:THR:HG1	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:SER:N	7:F:505:HOH:O	2.48	0.43
2:K:36:TRP:CE3	2:K:81:MET:HE2	2.53	0.43
2:Q:155:THR:HB	2:Q:203:THR:HG22	2.01	0.43
1:E:311:GLN:HB3	1:E:312:SER:H	1.59	0.43
1:F:48:ILE:HG13	1:F:50:GLU:H	1.83	0.43
2:Q:83:LEU:HD23	2:Q:86:LEU:HD23	2.00	0.43
1:A:90:ARG:NH2	1:A:272:ALA:O	2.51	0.43
1:C:237:VAL:HA	7:C:504:HOH:O	2.18	0.43
1:E:42:LEU:O	1:E:292:LYS:HB3	2.18	0.43
2:K:4:LEU:HD22	2:K:24:THR:HG22	2.01	0.43
4:B:408:NAG:H83	4:B:408:NAG:O4	2.18	0.42
2:G:176:SER:HA	7:G:303:HOH:O	2.08	0.42
2:K:1:GLU:C	7:K:304:HOH:O	2.40	0.42
2:M:53:PRO:O	2:M:72:ARG:NH1	2.52	0.42
3:N:28:ASP:HB3	3:N:94:ALA:HB2	2.01	0.42
3:R:16:GLN:O	3:R:80:LEU:N	2.46	0.42
1:C:298:ASN:OD1	1:C:300:ILE:N	2.51	0.42
1:C:190:ASP:OD2	2:K:107:ASP:HB2	2.19	0.42
2:M:103:MET:HE3	2:M:112:ARG:HB3	2.00	0.42
1:B:295:GLN:HE21	1:B:295:GLN:HB3	1.58	0.42
1:C:283:THR:CG2	1:C:301:THR:HG22	2.49	0.42
2:G:83:LEU:CD2	2:G:86:LEU:CD2	2.97	0.42
3:L:191:ARG:O	3:L:191:ARG:NH1	2.52	0.42
3:N:10:VAL:HG23	3:N:105:LEU:HD12	2.01	0.42
3:R:6:GLN:NE2	3:R:102:GLY:C	2.73	0.42
1:E:138:ALA:HB2	1:E:226:ILE:HD13	2.01	0.42
3:N:68:LYS:HE3	7:N:331:HOH:O	2.19	0.42
2:G:54:ASN:ND2	2:G:106:PHE:HE1	2.17	0.42
3:L:23:THR:N	7:L:303:HOH:O	2.45	0.42
2:M:166:PHE:HA	2:M:167:PRO:HA	1.78	0.42
1:B:310:LYS:CA	7:B:507:HOH:O	2.67	0.42
1:B:75:GLN:NE2	1:B:94:TYR:O	2.48	0.42
1:C:194:LEU:CD1	2:K:105:VAL:HG11	2.50	0.42
2:O:27:TYR:CZ	2:O:98:LYS:HD2	2.55	0.42
2:Q:61:ALA:O	2:Q:65:GLN:N	2.53	0.42
1:A:75:GLN:HG3	1:A:76:CYS:SG	2.59	0.42
1:B:108:LEU:HB2	1:B:234:TRP:CZ3	2.55	0.42
1:D:114:SER:HA	1:D:265:SER:O	2.19	0.42
1:F:109:ARG:HE	1:F:267:ILE:HG12	1.85	0.42
2:G:61:ALA:O	2:G:65:GLN:HG3	2.20	0.42
3:L:142:TYR:HB2	3:L:173:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:197:VAL:HB	7:P:301:HOH:O	2.20	0.42
1:C:178:TYR:CD2	1:C:243:LEU:HD22	2.55	0.42
2:K:54:ASN:ND2	2:K:106:PHE:HE1	2.18	0.42
2:I:236:CYS:SG	2:I:237:ASP:N	2.93	0.42
3:L:11:SER:HA	3:L:106:THR:O	2.19	0.42
4:A:403:NAG:C2	4:A:403:NAG:C6	2.94	0.42
1:B:75:GLN:HG3	1:B:76:CYS:SG	2.60	0.42
1:C:295:GLN:N	1:C:307:ARG:O	2.52	0.42
1:D:202:ILE:HD11	1:D:245:ILE:HG23	2.02	0.42
1:E:178:TYR:CD2	1:E:243:LEU:HD22	2.55	0.42
1:E:51:ILE:HB	1:E:274:ILE:HD13	2.01	0.42
2:O:213:THR:HG22	2:O:230:ARG:HH12	1.85	0.42
3:R:144:GLY:CA	3:R:174:TYR:HD2	2.33	0.42
1:C:295:GLN:HG3	1:C:307:ARG:O	2.20	0.41
3:N:80:LEU:HG	3:N:107:VAL:HG22	2.02	0.41
2:Q:161:LEU:HG	2:Q:163:LYS:HG3	2.02	0.41
3:R:144:GLY:HA3	3:R:174:TYR:CD2	2.54	0.41
1:B:176:LYS:HD3	1:B:257:TYR:CG	2.55	0.41
1:D:67:ILE:HG12	7:D:524:HOH:O	2.19	0.41
1:E:186:VAL:HG22	1:E:187:THR:HG23	2.02	0.41
3:J:37:TRP:HB2	3:J:50:ILE:HB	2.02	0.41
2:K:38:ARG:HH21	2:K:63:LYS:NZ	2.19	0.41
2:O:165:TYR:CE1	2:O:170:VAL:CG2	3.01	0.41
1:B:202:ILE:HD12	1:B:247:SER:HB2	1.99	0.41
1:C:262:SER:HA	7:C:515:HOH:O	2.20	0.41
1:F:168:MET:CE	1:F:169:PRO:HD2	2.50	0.41
1:F:307:ARG:N	7:F:509:HOH:O	2.52	0.41
2:I:88:SER:HA	2:I:131:VAL:HG13	2.02	0.41
1:A:202:ILE:HD11	1:A:251:LEU:HA	2.01	0.41
4:B:407:NAG:H2	7:B:504:HOH:O	2.20	0.41
1:C:241:ASP:OD1	1:C:242:ILE:N	2.52	0.41
1:D:222:ARG:HB3	1:D:225:ASN:HA	2.03	0.41
2:Q:2:VAL:HG13	2:Q:122:VAL:HG21	2.00	0.41
1:E:191:GLN:HG3	1:E:197:GLN:O	2.21	0.41
1:E:42:LEU:HA	1:E:42:LEU:HD23	1.88	0.41
1:F:73:ASP:OD1	1:F:75:GLN:HG2	2.20	0.41
2:G:166:PHE:HA	2:G:167:PRO:HA	1.80	0.41
3:L:23:THR:HG22	3:L:72:THR:HG23	2.02	0.41
3:N:10:VAL:CG2	3:N:105:LEU:HD13	2.49	0.41
2:O:81:MET:HE3	2:O:81:MET:HB3	1.95	0.41
1:C:113:ALA:HB1	1:C:267:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:GLU:HG2	1:C:42:LEU:N	2.24	0.41
3:H:33:ASP:CB	3:H:68:LYS:NZ	2.80	0.41
2:I:148:SER:HB2	2:I:237:ASP:HB3	2.02	0.41
3:L:117:VAL:O	3:L:206:LYS:NZ	2.53	0.41
3:N:46:PRO:O	7:N:308:HOH:O	2.22	0.41
2:O:36:TRP:CE3	2:O:81:MET:HE2	2.55	0.41
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.56	0.41
1:E:79:PHE:HA	1:E:82:LYS:HD2	2.01	0.41
2:I:83:LEU:HG	2:I:86:LEU:HD23	2.03	0.41
3:L:24:GLY:C	7:L:317:HOH:O	2.58	0.41
1:A:73:ASP:OD1	1:A:75:GLN:HG2	2.20	0.41
2:I:166:PHE:HA	2:I:167:PRO:HA	1.83	0.41
1:B:176:LYS:HB2	1:B:237:VAL:CG2	2.51	0.41
2:G:64:PHE:O	2:G:68:VAL:HG12	2.21	0.41
3:H:33:ASP:O	3:H:35:VAL:N	2.43	0.41
3:L:29:VAL:HG23	3:L:35:VAL:CG2	2.51	0.41
3:R:151:LYS:HB2	3:R:194:SER:HB3	2.03	0.41
1:A:175:ASP:CG	1:A:238:LYS:NZ	2.71	0.41
1:C:90:ARG:HB3	1:C:92:LYS:HG2	2.03	0.41
1:A:206:THR:HG23	1:A:208:ARG:N	2.28	0.41
1:D:176:LYS:HD3	1:D:257:TYR:CD1	2.56	0.41
3:J:35:VAL:HA	3:J:91:SER:O	2.20	0.41
3:L:147:THR:OG1	3:L:198:THR:HB	2.21	0.41
2:O:162:VAL:HG11	2:O:170:VAL:HG11	2.03	0.41
3:R:164:THR:CG2	3:R:177:SER:H	2.33	0.41
1:A:168:MET:HE2	1:A:169:PRO:HD2	2.03	0.40
1:D:180:TRP:HB3	1:D:254:PRO:HD3	2.02	0.40
3:N:151:LYS:HD3	3:N:156:PRO:HA	2.03	0.40
3:P:146:VAL:HG21	3:P:197:VAL:HG13	2.02	0.40
3:R:82:ALA:C	3:R:84:ASP:H	2.24	0.40
1:A:178:TYR:HA	7:A:526:HOH:O	2.21	0.40
1:A:89:GLU:HG3	1:A:267:ILE:HD11	2.02	0.40
1:C:206:THR:HG22	1:C:209:SER:H	1.86	0.40
1:C:184:HIS:HD1	1:C:216:ASN:H	1.69	0.40
2:O:38:ARG:NH2	2:O:63:LYS:NZ	2.68	0.40
3:J:209:ALA:O	3:J:212:GLU:HG3	2.21	0.40
3:N:115:PRO:HB3	3:N:141:PHE:HB3	2.04	0.40
3:N:25:THR:CG2	3:N:26:ASN:H	2.10	0.40
1:B:207:LYS:NZ	1:B:241:ASP:HA	2.35	0.40
2:G:11:VAL:O	2:G:11:VAL:HG23	2.22	0.40
2:I:34:LEU:HA	2:I:34:LEU:HD23	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:151:LYS:HD2	3:J:196:GLN:NE2	2.37	0.40
1:F:184:HIS:HB3	1:F:220:ARG:HH22	1.86	0.40
3:N:37:TRP:HB2	3:N:50:ILE:HB	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:334:HOH:O	7:H:338:HOH:O[1_455]	1.91	0.29

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	270/291 (93%)	255 (94%)	14 (5%)	1 (0%)	38 63
1	B	272/291 (94%)	259 (95%)	12 (4%)	1 (0%)	38 63
1	C	270/291 (93%)	257 (95%)	13 (5%)	0	100 100
1	D	271/291 (93%)	258 (95%)	13 (5%)	0	100 100
1	E	271/291 (93%)	256 (94%)	13 (5%)	2 (1%)	25 49
1	F	272/291 (94%)	257 (94%)	15 (6%)	0	100 100
2	G	234/244 (96%)	228 (97%)	6 (3%)	0	100 100
2	I	236/244 (97%)	228 (97%)	8 (3%)	0	100 100
2	K	233/244 (96%)	227 (97%)	5 (2%)	1 (0%)	38 63
2	M	233/244 (96%)	227 (97%)	6 (3%)	0	100 100
2	O	233/244 (96%)	227 (97%)	6 (3%)	0	100 100
2	Q	233/244 (96%)	225 (97%)	6 (3%)	2 (1%)	20 40
3	H	210/214 (98%)	199 (95%)	10 (5%)	1 (0%)	32 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	J	211/214 (99%)	196 (93%)	14 (7%)	1 (0%)	32 58
3	L	209/214 (98%)	194 (93%)	11 (5%)	4 (2%)	9 18
3	N	210/214 (98%)	194 (92%)	15 (7%)	1 (0%)	32 58
3	P	210/214 (98%)	197 (94%)	11 (5%)	2 (1%)	18 37
3	R	210/214 (98%)	188 (90%)	16 (8%)	6 (3%)	5 8
All	All	4288/4494 (95%)	4072 (95%)	194 (4%)	22 (0%)	32 58

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	LYS
3	H	34	LEU
3	L	26	ASN
3	N	34	LEU
2	Q	154	GLY
3	R	29	VAL
1	E	310	LYS
1	E	311	GLN
3	P	34	LEU
2	Q	234	LYS
3	R	3	ALA
3	R	74	SER
3	R	69	SER
2	K	2	VAL
3	L	71	ASN
3	R	34	LEU
3	R	70	GLY
3	J	83	GLU
3	L	83	GLU
3	L	112	LYS
1	B	311	GLN
3	P	26	ASN

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	244/258 (95%)	242 (99%)	2 (1%)	85 94
1	B	245/258 (95%)	243 (99%)	2 (1%)	85 94
1	C	244/258 (95%)	244 (100%)	0	100 100
1	D	245/258 (95%)	244 (100%)	1 (0%)	93 98
1	E	245/258 (95%)	244 (100%)	1 (0%)	93 98
1	F	245/258 (95%)	245 (100%)	0	100 100
2	G	197/205 (96%)	195 (99%)	2 (1%)	80 93
2	I	199/205 (97%)	196 (98%)	3 (2%)	70 88
2	K	196/205 (96%)	193 (98%)	3 (2%)	70 88
2	M	196/205 (96%)	192 (98%)	4 (2%)	60 83
2	O	196/205 (96%)	194 (99%)	2 (1%)	80 93
2	Q	196/205 (96%)	195 (100%)	1 (0%)	91 97
3	H	176/178 (99%)	175 (99%)	1 (1%)	89 96
3	J	177/178 (99%)	176 (99%)	1 (1%)	89 96
3	L	175/178 (98%)	174 (99%)	1 (1%)	89 96
3	N	176/178 (99%)	173 (98%)	3 (2%)	66 86
3	P	176/178 (99%)	172 (98%)	4 (2%)	56 81
3	R	176/178 (99%)	175 (99%)	1 (1%)	89 96
All	All	3704/3846 (96%)	3672 (99%)	32 (1%)	82 93

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	186	VAL
1	B	295	GLN
1	B	307	ARG
1	D	295	GLN
1	E	90	ARG
2	G	72	ARG
2	G	236	CYS
3	H	87	ASP
2	I	72	ARG
2	I	81	MET
2	I	234	LYS

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Mol	Chain	Res	Type
3	J	87	ASP
2	K	67	ARG
2	K	81	MET
2	K	83	LEU
3	L	87	ASP
2	M	13	LYS
2	M	72	ARG
2	M	83	LEU
2	M	98	LYS
3	N	68	LYS
3	N	71	ASN
3	N	87	ASP
2	O	72	ARG
2	O	81	MET
3	P	10	VAL
3	P	68	LYS
3	P	71	ASN
3	P	171	ASN
2	Q	72	ARG
3	R	71	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	144	ASN
1	C	165	ASN
1	D	165	ASN
1	E	158	ASN
3	L	196	GLN
2	O	191	GLN
3	R	6	GLN
3	R	71	ASN
3	R	169	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	401	1,4	14,14,15	0.28	0	15,19,21	0.57	0
4	NAG	A	402	4	14,14,15	0.28	0	15,19,21	0.58	0
4	NAG	A	403	4	14,14,15	0.30	0	15,19,21	0.46	0
4	NAG	A	404	5,4	14,14,15	0.28	0	15,19,21	0.58	0
5	BMA	A	405	4	11,11,12	0.28	0	13,15,17	0.54	0
4	NAG	A	406	-	14,14,15	0.28	0	15,19,21	0.58	0
4	NAG	A	407	1	14,14,15	0.32	0	15,19,21	0.67	0
4	NAG	A	408	1	14,14,15	0.36	0	15,19,21	0.71	0
4	NAG	B	401	1,4	14,14,15	0.29	0	15,19,21	0.56	0
4	NAG	B	402	5,4	14,14,15	0.29	0	15,19,21	0.58	0
5	BMA	B	403	4	11,11,12	0.26	0	13,15,17	0.54	0
4	NAG	B	404	1,4	14,14,15	0.91	1 (7%)	15,19,21	1.39	1 (6%)
4	NAG	B	405	4	14,14,15	0.40	0	15,19,21	0.57	0
4	NAG	B	406	1,4	14,14,15	0.34	0	15,19,21	0.50	0
4	NAG	B	407	4	14,14,15	0.50	0	15,19,21	0.49	0
4	NAG	B	408	1	14,14,15	1.22	2 (14%)	15,19,21	1.87	5 (33%)
4	NAG	C	401	1	14,14,15	0.29	0	15,19,21	0.48	0
4	NAG	C	402	1,4	14,14,15	0.34	0	15,19,21	0.71	1 (6%)
4	NAG	C	403	5,4	14,14,15	0.43	0	15,19,21	0.99	1 (6%)
5	BMA	C	404	4	11,11,12	0.89	1 (9%)	13,15,17	0.84	1 (7%)
4	NAG	C	405	1	14,14,15	0.69	1 (7%)	15,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	406	1	14,14,15	0.31	0	15,19,21	0.57	0
4	NAG	D	401	1,4	14,14,15	0.37	0	15,19,21	0.54	0
4	NAG	D	402	4	14,14,15	0.22	0	15,19,21	0.46	0
4	NAG	D	403	1,4	14,14,15	0.43	0	15,19,21	0.65	0
4	NAG	D	404	4	14,14,15	0.27	0	15,19,21	0.37	0
4	NAG	D	405	1	14,14,15	0.41	0	15,19,21	1.25	3 (20%)
4	NAG	D	406	1	14,14,15	0.23	0	15,19,21	0.97	1 (6%)
4	NAG	D	407	1	14,14,15	0.34	0	15,19,21	0.93	0
4	NAG	E	401	1,4	14,14,15	0.39	0	15,19,21	0.92	1 (6%)
4	NAG	E	402	5,4	14,14,15	0.42	0	15,19,21	0.98	1 (6%)
5	BMA	E	403	4	11,11,12	0.32	0	13,15,17	1.16	1 (7%)
4	NAG	E	404	1	14,14,15	0.60	1 (7%)	15,19,21	0.43	0
4	NAG	E	405	1	14,14,15	0.88	1 (7%)	15,19,21	1.50	3 (20%)
4	NAG	E	406	1	14,14,15	0.28	0	15,19,21	0.79	1 (6%)
4	NAG	F	401	1,4	14,14,15	0.39	0	15,19,21	0.55	0
4	NAG	F	402	5,4	14,14,15	0.29	0	15,19,21	0.46	0
5	BMA	F	403	4	11,11,12	0.70	0	13,15,17	0.72	0
4	NAG	F	404	1	14,14,15	0.36	0	15,19,21	0.78	0
4	NAG	F	405	1	14,14,15	0.41	0	15,19,21	1.46	1 (6%)
4	NAG	F	406	1	14,14,15	0.34	0	15,19,21	0.63	0
6	GOL	I	301	-	5,5,5	0.36	0	5,5,5	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	402	4	-	0/6/23/26	0/1/1/1
4	NAG	A	403	4	-	0/6/23/26	0/1/1/1
4	NAG	A	404	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	405	4	-	0/2/19/22	0/1/1/1
4	NAG	A	406	-	-	0/6/23/26	0/1/1/1
4	NAG	A	407	1	-	0/6/23/26	0/1/1/1
4	NAG	A	408	1	-	0/6/23/26	0/1/1/1
4	NAG	B	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	402	5,4	-	0/6/23/26	0/1/1/1
5	BMA	B	403	4	-	0/2/19/22	0/1/1/1
4	NAG	B	404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	405	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	407	4	-	0/6/23/26	0/1/1/1
4	NAG	B	408	1	-	0/6/23/26	0/1/1/1
4	NAG	C	401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	403	5,4	-	0/6/23/26	0/1/1/1
5	BMA	C	404	4	-	0/2/19/22	0/1/1/1
4	NAG	C	405	1	-	0/6/23/26	0/1/1/1
4	NAG	C	406	1	-	0/6/23/26	0/1/1/1
4	NAG	D	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	402	4	-	0/6/23/26	0/1/1/1
4	NAG	D	403	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	404	4	-	0/6/23/26	0/1/1/1
4	NAG	D	405	1	-	1/6/23/26	0/1/1/1
4	NAG	D	406	1	-	1/6/23/26	0/1/1/1
4	NAG	D	407	1	-	0/6/23/26	0/1/1/1
4	NAG	E	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	402	5,4	-	0/6/23/26	0/1/1/1
5	BMA	E	403	4	-	0/2/19/22	0/1/1/1
4	NAG	E	404	1	-	0/6/23/26	0/1/1/1
4	NAG	E	405	1	-	0/6/23/26	0/1/1/1
4	NAG	E	406	1	-	0/6/23/26	0/1/1/1
4	NAG	F	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	402	5,4	-	0/6/23/26	0/1/1/1
5	BMA	F	403	4	-	0/2/19/22	0/1/1/1
4	NAG	F	404	1	-	0/6/23/26	0/1/1/1
4	NAG	F	405	1	-	0/6/23/26	0/1/1/1
4	NAG	F	406	1	-	0/6/23/26	0/1/1/1
6	GOL	I	301	-	-	0/4/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	408	NAG	O5-C1	-3.54	1.37	1.43
4	E	404	NAG	C1-C2	2.04	1.55	1.52
4	B	408	NAG	C1-C2	2.28	1.55	1.52
4	C	405	NAG	C1-C2	2.32	1.55	1.52
5	C	404	BMA	C1-C2	2.46	1.58	1.52
4	E	405	NAG	O5-C1	2.60	1.48	1.43
4	B	404	NAG	O5-C1	3.28	1.49	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	401	NAG	O5-C1-C2	-2.42	108.11	111.47
4	B	408	NAG	C1-O5-C5	-2.21	109.12	112.17
4	D	406	NAG	C1-C2-N2	-2.18	106.77	110.49
4	E	402	NAG	O5-C1-C2	-2.11	108.54	111.47
4	E	406	NAG	C4-C3-C2	-2.07	107.98	111.02
4	D	405	NAG	C2-N2-C7	-2.03	119.99	122.94
5	C	404	BMA	O2-C2-C3	-2.02	106.20	110.17
4	B	408	NAG	C3-C4-C5	2.06	113.85	110.22
4	E	405	NAG	C1-O5-C5	2.08	115.03	112.17
4	C	402	NAG	C1-O5-C5	2.14	115.12	112.17
5	E	403	BMA	C3-C4-C5	2.24	114.17	110.22
4	C	403	NAG	C2-N2-C7	2.41	126.46	122.94
4	B	408	NAG	C1-C2-N2	2.76	115.21	110.49
4	D	405	NAG	C1-O5-C5	2.84	116.08	112.17
4	D	405	NAG	O5-C1-C2	3.09	115.77	111.47
4	E	405	NAG	C1-C2-N2	3.09	115.76	110.49
4	B	408	NAG	C4-C3-C2	3.25	115.79	111.02
4	E	405	NAG	C2-N2-C7	4.05	128.85	122.94
4	B	408	NAG	C2-N2-C7	4.67	129.75	122.94
4	F	405	NAG	C1-O5-C5	5.11	119.21	112.17
4	B	404	NAG	C1-O5-C5	5.17	119.30	112.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	405	NAG	O7-C7-N2-C2
4	D	406	NAG	O7-C7-N2-C2

There are no ring outliers.

20 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	NAG	21	0
4	A	406	NAG	11	0
4	A	407	NAG	4	0
4	A	408	NAG	2	0
4	B	401	NAG	2	0
4	B	402	NAG	5	0
4	B	407	NAG	5	0
4	B	408	NAG	1	0
4	C	402	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	NAG	1	0
5	C	404	BMA	1	0
4	C	406	NAG	1	0
4	D	402	NAG	1	0
4	D	403	NAG	3	0
4	D	405	NAG	8	0
4	D	406	NAG	7	0
4	E	401	NAG	1	0
4	E	405	NAG	1	0
4	E	406	NAG	3	0
4	F	406	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	272/291 (93%)	0.35	9 (3%) 47 39	23, 49, 83, 116	0
1	B	274/291 (94%)	0.25	6 (2%) 62 56	26, 45, 82, 134	0
1	C	272/291 (93%)	0.39	11 (4%) 39 31	28, 62, 97, 136	0
1	D	273/291 (93%)	0.40	10 (3%) 42 34	35, 57, 95, 156	0
1	E	273/291 (93%)	0.30	6 (2%) 62 56	29, 59, 96, 141	0
1	F	274/291 (94%)	0.64	23 (8%) 12 8	39, 73, 111, 206	0
2	G	236/244 (96%)	0.25	2 (0%) 86 83	26, 44, 72, 139	0
2	I	238/244 (97%)	0.23	4 (1%) 70 65	25, 44, 72, 156	0
2	K	235/244 (96%)	0.35	3 (1%) 77 73	35, 57, 85, 110	0
2	M	235/244 (96%)	0.37	12 (5%) 29 22	33, 49, 90, 158	0
2	O	235/244 (96%)	0.49	15 (6%) 20 15	34, 52, 87, 159	0
2	Q	235/244 (96%)	0.62	17 (7%) 16 12	41, 63, 108, 153	0
3	H	212/214 (99%)	0.42	12 (5%) 24 18	29, 47, 112, 200	0
3	J	213/214 (99%)	0.48	15 (7%) 17 12	22, 44, 121, 182	0
3	L	211/214 (98%)	0.68	17 (8%) 13 8	40, 66, 119, 156	0
3	N	212/214 (99%)	0.47	17 (8%) 13 9	33, 54, 133, 167	0
3	P	212/214 (99%)	0.51	13 (6%) 22 16	38, 62, 116, 160	0
3	R	212/214 (99%)	0.82	21 (9%) 8 5	45, 81, 143, 166	0
All	All	4324/4494 (96%)	0.44	213 (4%) 30 24	22, 56, 105, 206	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	1	PRO	10.1
3	J	31	THR	9.9
3	R	1	PRO	9.7

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Mol	Chain	Res	Type	RSRZ
3	R	29	VAL	9.5
3	R	2	SER	8.8
3	L	30	GLY	8.3
1	F	312	SER	8.3
3	P	30	GLY	8.1
2	O	153	GLY	8.0
3	N	1	PRO	8.0
2	M	152	SER	7.8
3	J	30	GLY	7.8
1	D	312	SER	7.7
3	N	27	SER	6.9
2	M	151	THR	6.8
3	J	1	PRO	6.6
3	H	31	THR	6.6
2	O	152	SER	6.5
3	J	32	PHE	6.5
3	J	28	ASP	6.5
3	N	32	PHE	6.4
1	E	312	SER	6.3
3	H	32	PHE	6.2
2	O	150	SER	6.1
3	P	28	ASP	6.1
3	H	28	ASP	6.0
3	N	29	VAL	6.0
3	N	28	ASP	6.0
2	M	153	GLY	5.9
3	L	31	THR	5.8
3	L	29	VAL	5.8
1	B	310	LYS	5.7
3	P	29	VAL	5.6
2	Q	150	SER	5.5
3	L	26	ASN	5.5
2	O	151	THR	5.5
3	P	2	SER	5.4
2	Q	154	GLY	5.4
3	R	28	ASP	5.3
3	R	27	SER	5.3
1	A	312	SER	5.3
3	R	31	THR	5.2
1	D	310	LYS	5.0
2	Q	209	LEU	4.8
2	Q	151	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	39	ALA	4.8
2	Q	211	THR	4.7
3	R	82	ALA	4.7
3	N	34	LEU	4.7
3	L	212	GLU	4.7
3	N	31	THR	4.6
2	Q	153	GLY	4.6
3	R	5	THR	4.5
3	R	32	PHE	4.5
3	N	25	THR	4.5
3	J	2	SER	4.4
3	R	30	GLY	4.4
3	J	158	LYS	4.4
3	P	32	PHE	4.3
2	M	150	SER	4.2
1	D	40	THR	4.2
3	N	26	ASN	4.1
2	M	149	LYS	4.0
3	H	29	VAL	3.9
3	L	28	ASP	3.9
1	C	312	SER	3.9
3	R	3	ALA	3.9
2	O	154	GLY	3.9
3	L	27	SER	3.9
3	P	70	GLY	3.8
1	C	310	LYS	3.8
2	M	209	LEU	3.7
1	F	294	PHE	3.6
2	M	1	GLU	3.6
1	D	43	VAL	3.6
2	Q	206	SER	3.6
3	L	32	PHE	3.5
2	Q	152	SER	3.5
1	F	304	ALA	3.5
3	J	213	CYS	3.4
1	F	297	VAL	3.4
2	G	1	GLU	3.4
3	J	29	VAL	3.4
3	P	31	THR	3.4
1	E	310	LYS	3.4
2	O	155	THR	3.3
2	Q	148	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	42	LEU	3.2
3	H	71	ASN	3.2
3	R	26	ASN	3.2
2	M	204	VAL	3.2
3	H	33	ASP	3.1
2	O	209	LEU	3.0
3	L	2	SER	3.0
3	N	33	ASP	3.0
3	H	30	GLY	3.0
1	C	311	GLN	3.0
1	B	40	THR	3.0
3	P	26	ASN	3.0
3	N	82	ALA	3.0
1	A	310	LYS	2.9
2	Q	210	GLY	2.9
1	C	299	ARG	2.9
2	Q	1	GLU	2.9
3	H	2	SER	2.9
2	O	149	LYS	2.9
2	O	178	ALA	2.9
3	H	27	SER	2.8
1	F	309	VAL	2.8
1	F	310	LYS	2.8
3	J	27	SER	2.8
3	R	7	PRO	2.8
1	F	43	VAL	2.8
3	H	157	VAL	2.7
1	C	307	ARG	2.7
3	P	25	THR	2.7
3	L	25	THR	2.7
2	M	154	GLY	2.7
3	L	156	PRO	2.7
1	E	299	ARG	2.7
3	L	158	LYS	2.7
2	I	1	GLU	2.7
3	R	25	THR	2.7
1	F	305	CYS	2.7
3	J	33	ASP	2.6
3	L	111	PRO	2.6
3	R	212	GLU	2.6
1	C	208	ARG	2.6
1	D	294	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	312	SER	2.6
2	Q	149	LYS	2.6
1	F	311	GLN	2.6
3	L	34	LEU	2.6
1	F	39	ALA	2.6
2	Q	62	GLN	2.6
3	R	79	GLY	2.5
3	N	30	GLY	2.5
1	A	294	PHE	2.5
1	A	299	ARG	2.5
1	E	208	ARG	2.5
2	M	210	GLY	2.5
2	O	204	VAL	2.5
1	E	294	PHE	2.5
3	R	33	ASP	2.5
3	H	34	LEU	2.4
3	H	213	CYS	2.4
3	L	33	ASP	2.4
1	C	264	LYS	2.4
2	Q	70	LEU	2.4
1	F	291	ASP	2.4
3	N	3	ALA	2.4
3	P	34	LEU	2.4
1	B	210	GLN	2.4
2	K	177	GLY	2.4
3	L	95	GLY	2.4
2	M	148	SER	2.4
2	O	211	THR	2.4
3	R	4	LEU	2.4
1	D	303	GLY	2.4
1	D	305	CYS	2.4
3	N	71	ASN	2.4
2	K	207	SER	2.3
3	L	211	THR	2.3
1	F	171	ASN	2.3
2	O	1	GLU	2.3
3	R	69	SER	2.3
3	N	94	ALA	2.3
2	I	237	ASP	2.3
2	O	210	GLY	2.3
3	J	26	ASN	2.3
1	A	175	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	291	ASP	2.3
3	P	3	ALA	2.3
3	N	157	VAL	2.3
2	O	205	PRO	2.2
1	F	306	PRO	2.2
1	C	240	GLY	2.2
1	E	300	ILE	2.2
2	I	65	GLN	2.2
3	N	152	ALA	2.2
2	K	62	GLN	2.2
1	F	261	ARG	2.2
2	Q	207	SER	2.2
1	F	85	ASP	2.2
3	J	159	ALA	2.2
2	Q	208	SER	2.2
1	A	42	LEU	2.2
1	A	279	SER	2.2
3	J	3	ALA	2.2
2	G	65	GLN	2.1
1	F	200	GLY	2.1
2	Q	49	ALA	2.1
1	A	41	GLU	2.1
1	F	41	GLU	2.1
1	C	173	GLN	2.1
1	D	128	ASN	2.1
1	F	260	ILE	2.1
1	C	188	ASP	2.1
1	D	169	PRO	2.1
1	F	188	ASP	2.1
1	F	237	VAL	2.1
2	I	238	LYS	2.1
1	B	262	SER	2.1
3	P	27	SER	2.1
2	M	205	PRO	2.1
1	D	126	ASN	2.1
1	C	143	SER	2.1
3	J	185	GLU	2.1
1	F	125	PHE	2.1
2	O	135	SER	2.1
3	R	157	VAL	2.0
3	R	98	VAL	2.0
1	F	172	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	A	407	14/15	0.79	0.55	26.34	45,50,53,54	0
4	NAG	E	404	14/15	0.83	0.30	3.59	40,44,48,51	0
6	GOL	I	301	6/6	0.89	0.24	0.83	53,53,53,53	0
4	NAG	F	401	14/15	0.89	0.23	-	46,48,51,56	0
4	NAG	A	401	14/15	0.86	0.31	-	44,49,53,58	0
4	NAG	C	405	14/15	0.76	0.39	-	50,52,54,55	0
4	NAG	B	401	14/15	0.79	0.28	-	46,47,50,55	0
4	NAG	E	402	14/15	0.82	0.33	-	63,67,69,72	0
4	NAG	E	406	14/15	0.86	0.40	-	41,47,48,49	0
4	NAG	E	401	14/15	0.84	0.21	-	44,49,52,57	0
4	NAG	C	402	14/15	0.64	0.38	-	50,52,55,60	0
4	NAG	C	403	14/15	0.86	0.40	-	65,70,71,73	0
4	NAG	A	404	14/15	0.80	0.40	-	63,68,70,73	0
4	NAG	D	406	14/15	0.74	0.47	-	43,47,52,53	0
4	NAG	E	405	14/15	0.76	0.32	-	46,50,52,52	0
4	NAG	F	405	14/15	0.63	0.33	-	46,46,49,49	0
4	NAG	B	406	14/15	0.71	0.35	-	47,52,54,58	0
4	NAG	C	401	14/15	0.73	0.42	-	46,50,53,53	0
4	NAG	D	403	14/15	0.87	0.31	-	58,64,65,67	0
4	NAG	B	407	14/15	0.84	0.37	-	61,65,66,66	0
4	NAG	B	408	14/15	0.84	0.35	-	48,52,55,56	0
4	NAG	B	402	14/15	0.81	0.36	-	60,64,66,68	0
5	BMA	A	405	11/12	0.56	0.46	-	75,77,77,78	0
5	BMA	B	403	11/12	0.62	0.41	-	71,73,74,74	0
4	NAG	D	401	14/15	0.90	0.23	-	45,47,49,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	BMA	F	403	11/12	0.68	0.45	-	72,73,74,74	0
4	NAG	F	402	14/15	0.72	0.30	-	61,66,68,70	0
4	NAG	D	405	14/15	0.57	0.62	-	43,47,49,50	0
4	NAG	D	404	14/15	0.66	0.43	-	69,71,72,73	0
4	NAG	C	406	14/15	0.80	0.29	-	38,43,45,46	0
4	NAG	B	404	14/15	0.90	0.18	-	38,44,46,51	0
4	NAG	D	407	14/15	0.80	0.33	-	42,46,48,48	0
4	NAG	A	408	14/15	0.63	0.33	-	41,46,47,47	0
4	NAG	A	403	14/15	0.86	0.26	-	45,46,51,57	0
4	NAG	F	406	14/15	0.85	0.40	-	37,39,40,41	0
4	NAG	D	402	14/15	0.85	0.35	-	58,61,62,62	0
4	NAG	B	405	14/15	0.87	0.27	-	54,57,58,59	0
5	BMA	E	403	11/12	0.71	0.44	-	75,76,77,77	0
4	NAG	A	406	14/15	0.85	0.29	-	43,46,48,49	0
4	NAG	A	402	14/15	0.73	0.31	-	63,67,68,68	0
5	BMA	C	404	11/12	0.81	0.43	-	75,77,77,77	0
4	NAG	F	404	14/15	0.86	0.32	-	41,45,47,49	0

6.5 Other polymers

There are no such residues in this entry.