Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:20 AM GMT

PDB ID	:	2WIN
Title	:	C3 CONVERTASE (C3BBB) STABILIZED BY SCIN
Authors	:	Wu, J.; Janssen, B.J.; Gros, P.
Deposited on	:	2009-05-13
Resolution	:	3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

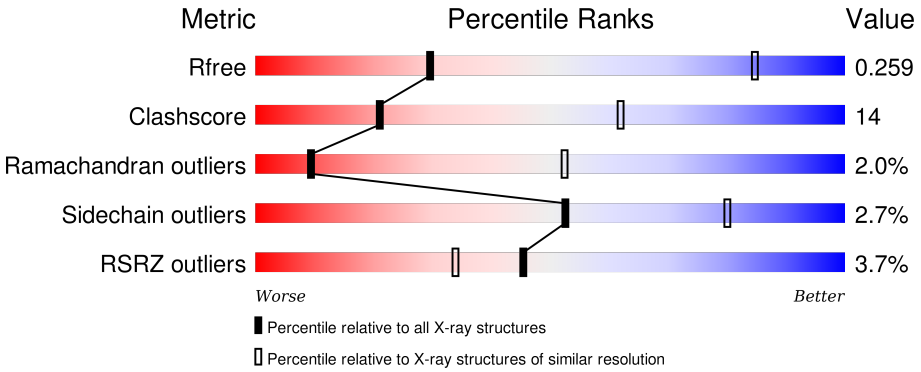
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	645	3% 72% 25%
1	C	645	2% 72% 26%
1	E	645	2% 72% 26%
1	G	645	9% 71% 27%
2	B	915	3% 69% 26%

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Mol	Chain	Length	Quality of chain
2	D	915	3% 70% 25%
2	F	915	6% 68% 27%
2	H	915	4% 75% 20%
3	I	507	% 67% 30%
3	J	507	3% 68% 29%
3	K	507	5% 68% 29%
3	L	507	% 68% 29%
4	M	92	% 57% 30% 9%
4	N	92	2% 58% 29% 9%
4	P	92	2% 58% 29% 9%
4	Q	92	2% 57% 30% 9%

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
10	NDG	H	2642	X	-	-	-
10	MAN	H	2644	X	-	-	-
10	MAN	H	2645	X	-	-	-
12	NDG	I	1743	X	-	-	-
12	MAN	I	1745	X	-	-	-
12	NDG	J	1743	X	-	-	-
12	MAN	J	1745	X	-	-	-
13	NDG	I	1746	X	-	-	-
14	NDG	K	1743	X	-	-	-
14	MAN	K	1745	X	-	-	-
14	MAN	K	1746	X	-	-	-
14	MAN	K	1748	X	-	-	-
15	NDG	L	1746	X	-	-	-
16	NDG	L	1743	X	-	-	-
5	NDG	B	2642	X	-	-	-
5	NDG	D	2642	X	-	-	-
5	NDG	E	1646	X	-	-	-
7	NDG	C	1646	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NDG	G	1646	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 67989 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 COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	C	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	E	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	G	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7177	4545	1209	1386	37			
2	D	901	Total	C	N	O	S	0	0	0
			7166	4537	1208	1384	37			
2	F	900	Total	C	N	O	S	0	0	0
			7172	4545	1206	1384	37			
2	H	900	Total	C	N	O	S	2313	0	0
			7175	4547	1209	1382	37			

- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	J	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	K	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	L	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			

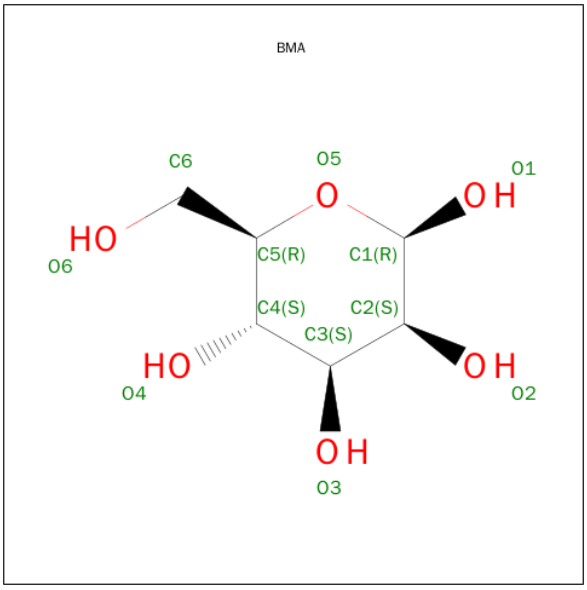
- Molecule 4 is a protein called STAPHYLOCOCCAL COMPLEMENT INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	N	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	P	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	Q	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			50	28	2	20		
5	B	4	Total	C	N	O	0	0
			50	28	2	20		
5	D	4	Total	C	N	O	0	0
			50	28	2	20		
5	E	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	K	1	Total C O 11 6 5	0	0

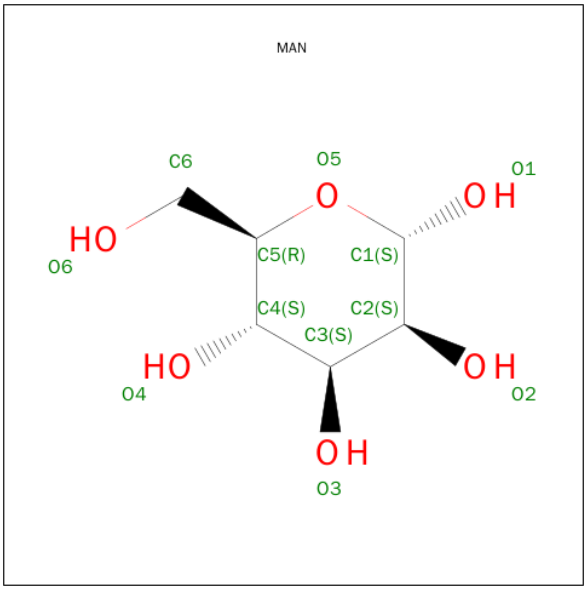
- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	5	Total C N O 61 34 2 25	0	0
7	G	5	Total C N O 61 34 2 25	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	6	Total C N O 72 40 2 30	0	0

- Molecule 9 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	1	Total C O 11 6 5	0	0

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

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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total	Mg	0	0
			1	1		
11	I	1	Total	Mg	0	0
			1	1		
11	L	1	Total	Mg	0	0
			1	1		
11	K	1	Total	Mg	0	0
			1	1		

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	I	3	Total	C	N	O	0	0
			39	22	2	15		
12	J	3	Total	C	N	O	0	0
			39	22	2	15		

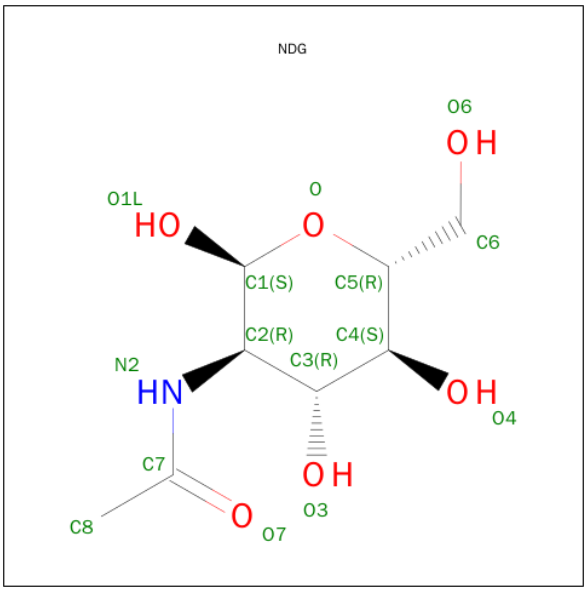
- Molecule 13 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 14 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	K	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 15 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total C N O 14 8 1 5	0	0
15	L	1	Total C N O 14 8 1 5	0	0

- Molecule 16 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 17 is water.

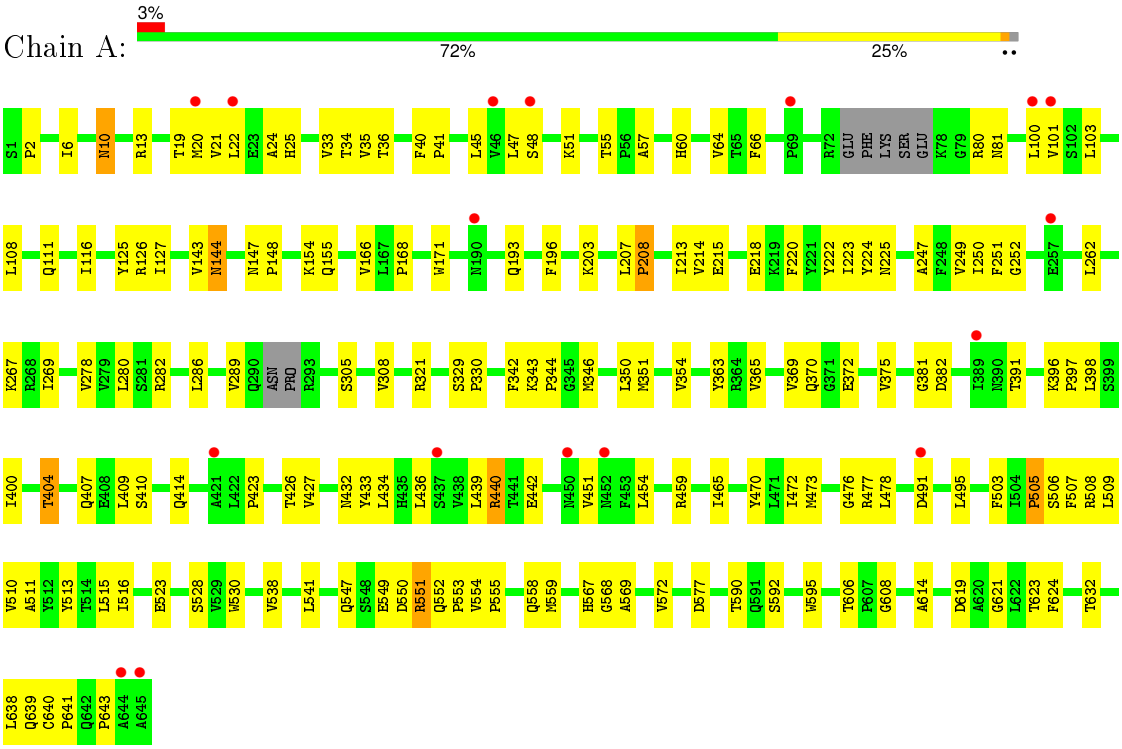
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total O 1 1	0	0
17	I	2	Total O 2 2	0	0
17	J	2	Total O 2 2	0	0
17	K	2	Total O 2 2	0	0
17	L	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

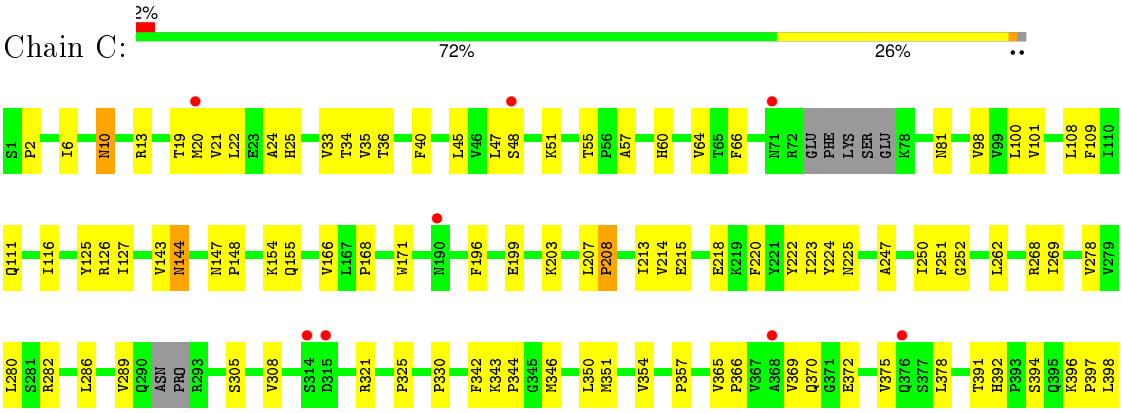
- Molecule 1: COMPLEMENT C3 BETA CHAIN

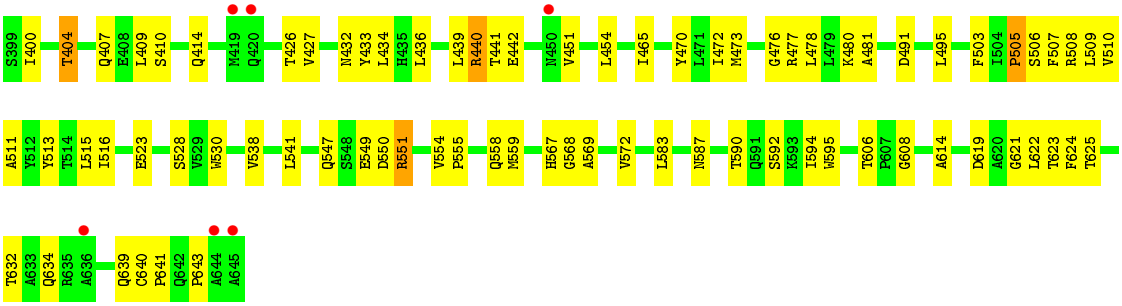
Chain A:



- Molecule 1: COMPLEMENT C3 BETA CHAIN

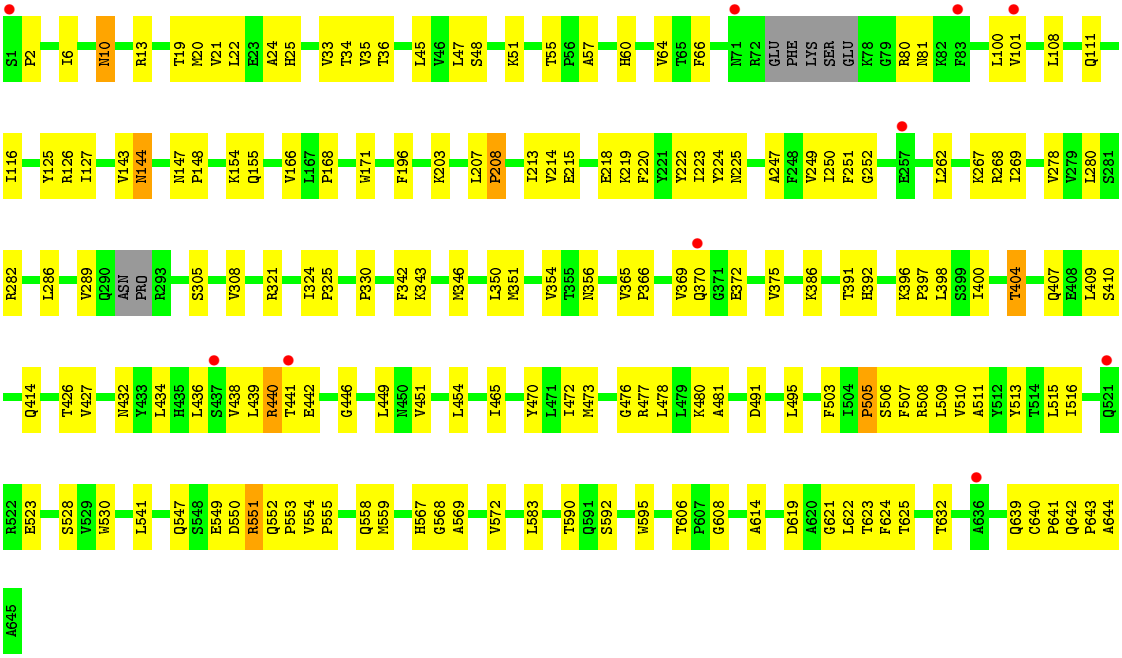
Chain C:





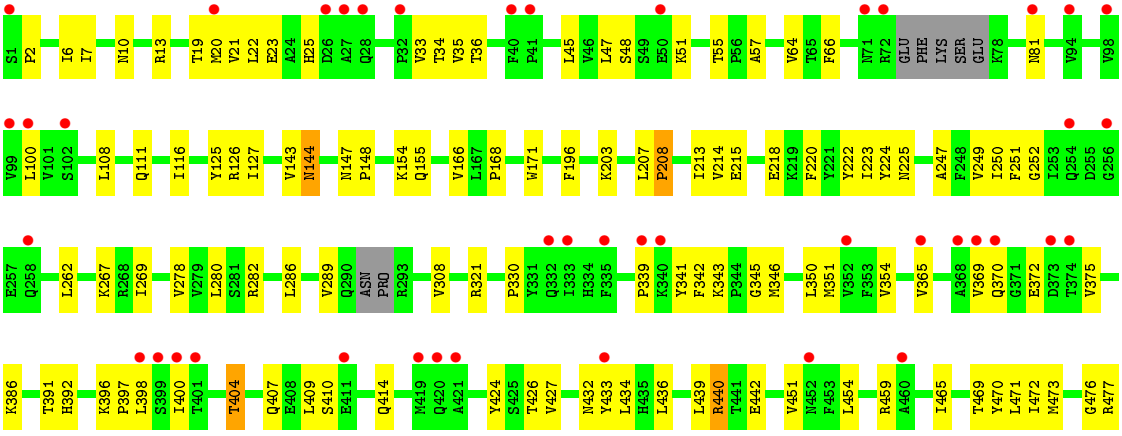
- Molecule 1: COMPLEMENT C3 BETA CHAIN

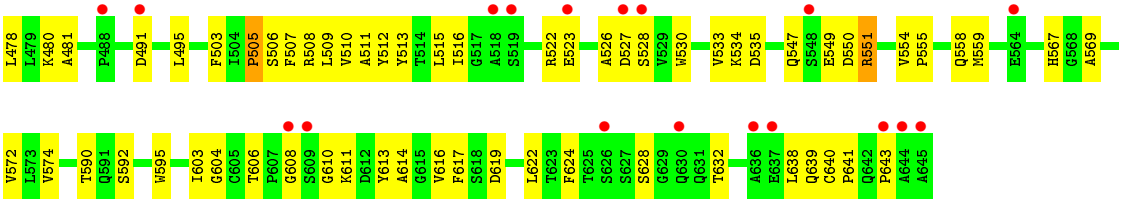
Chain E:



- Molecule 1: COMPLEMENT C3 BETA CHAIN

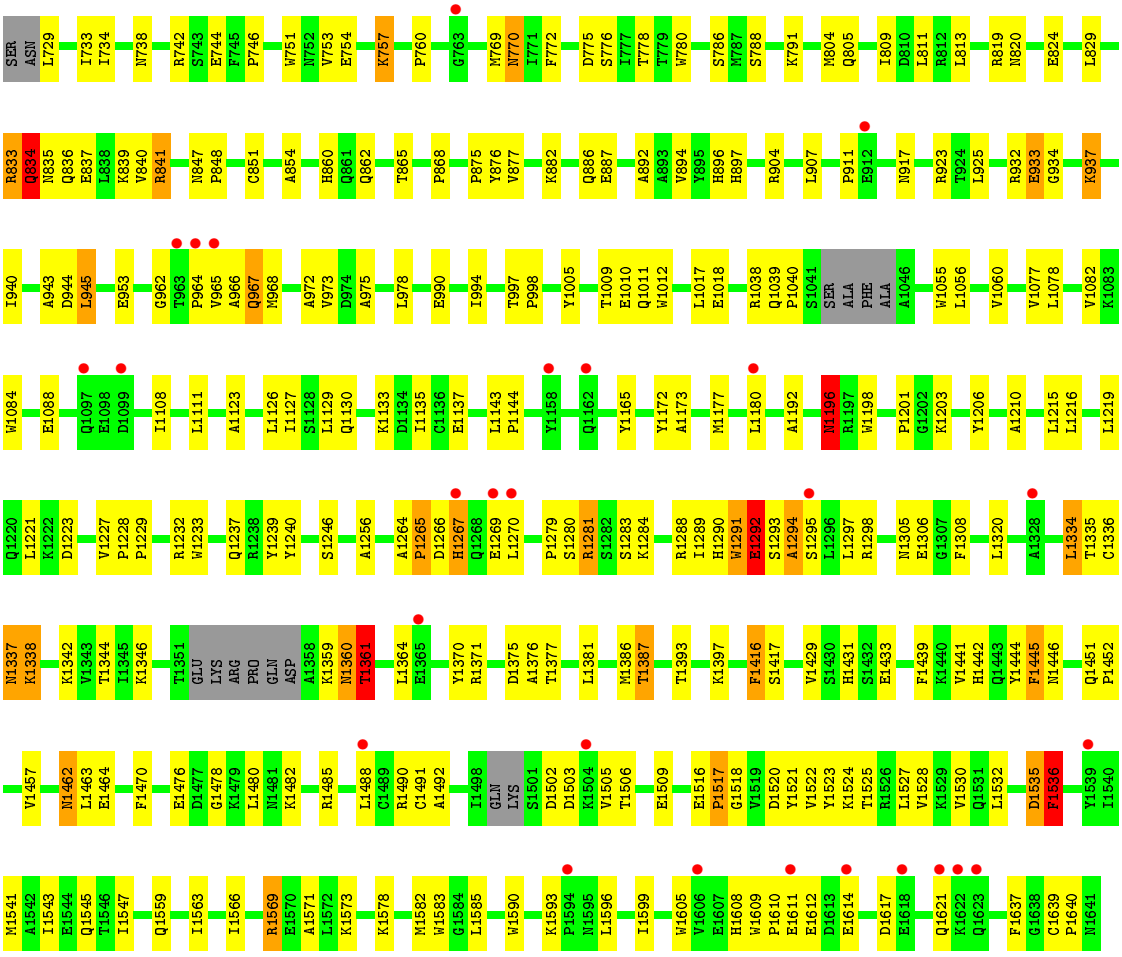
Chain G:





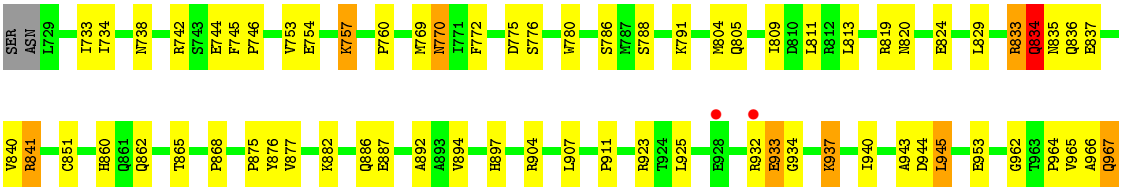
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

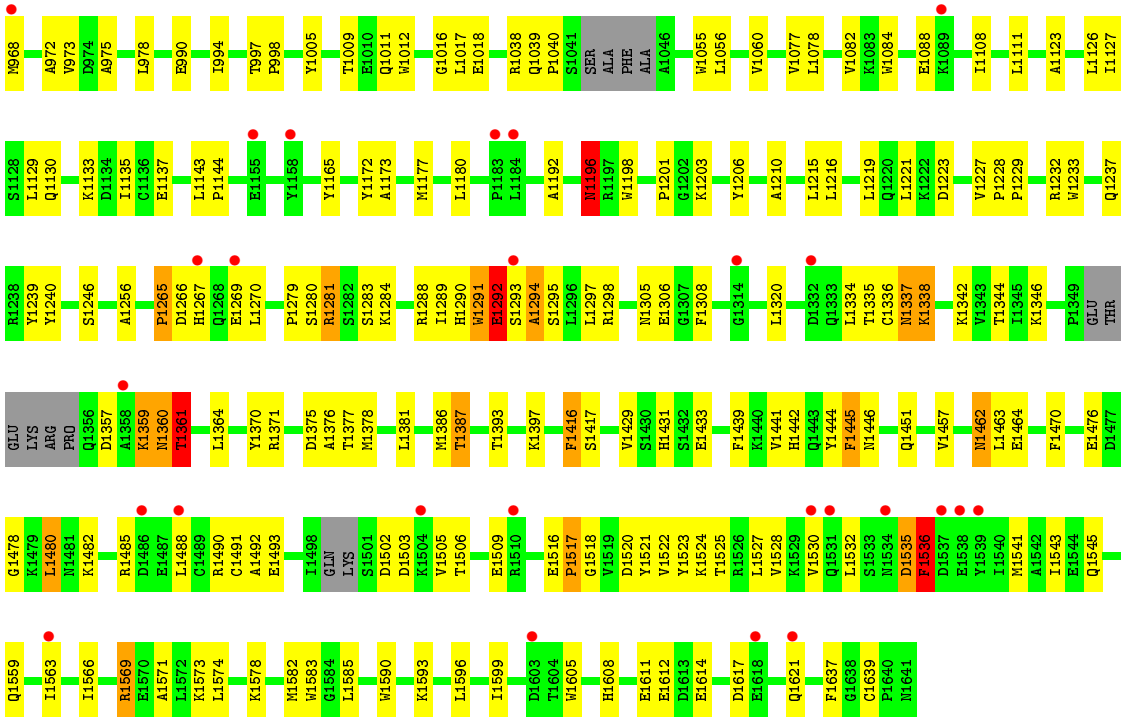
Chain B:



• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

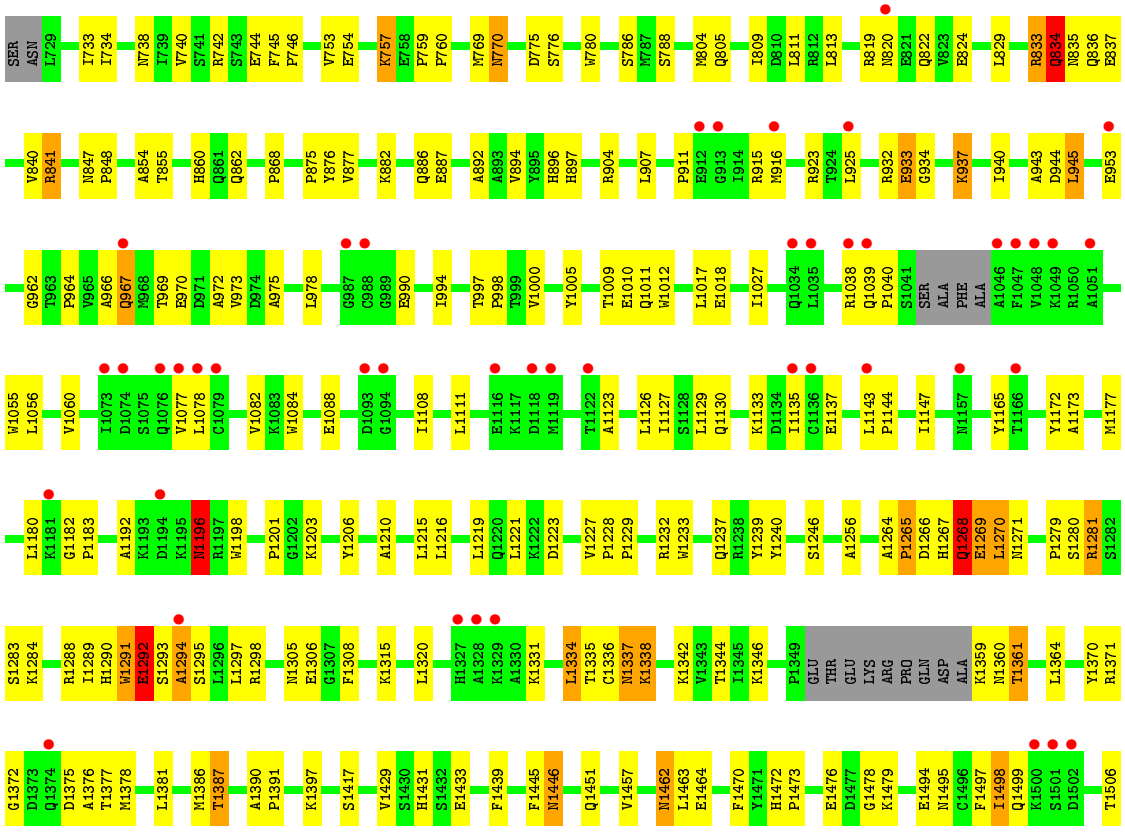
Chain D:

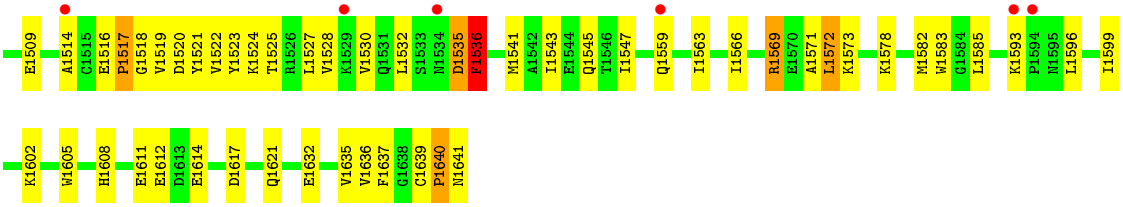




• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

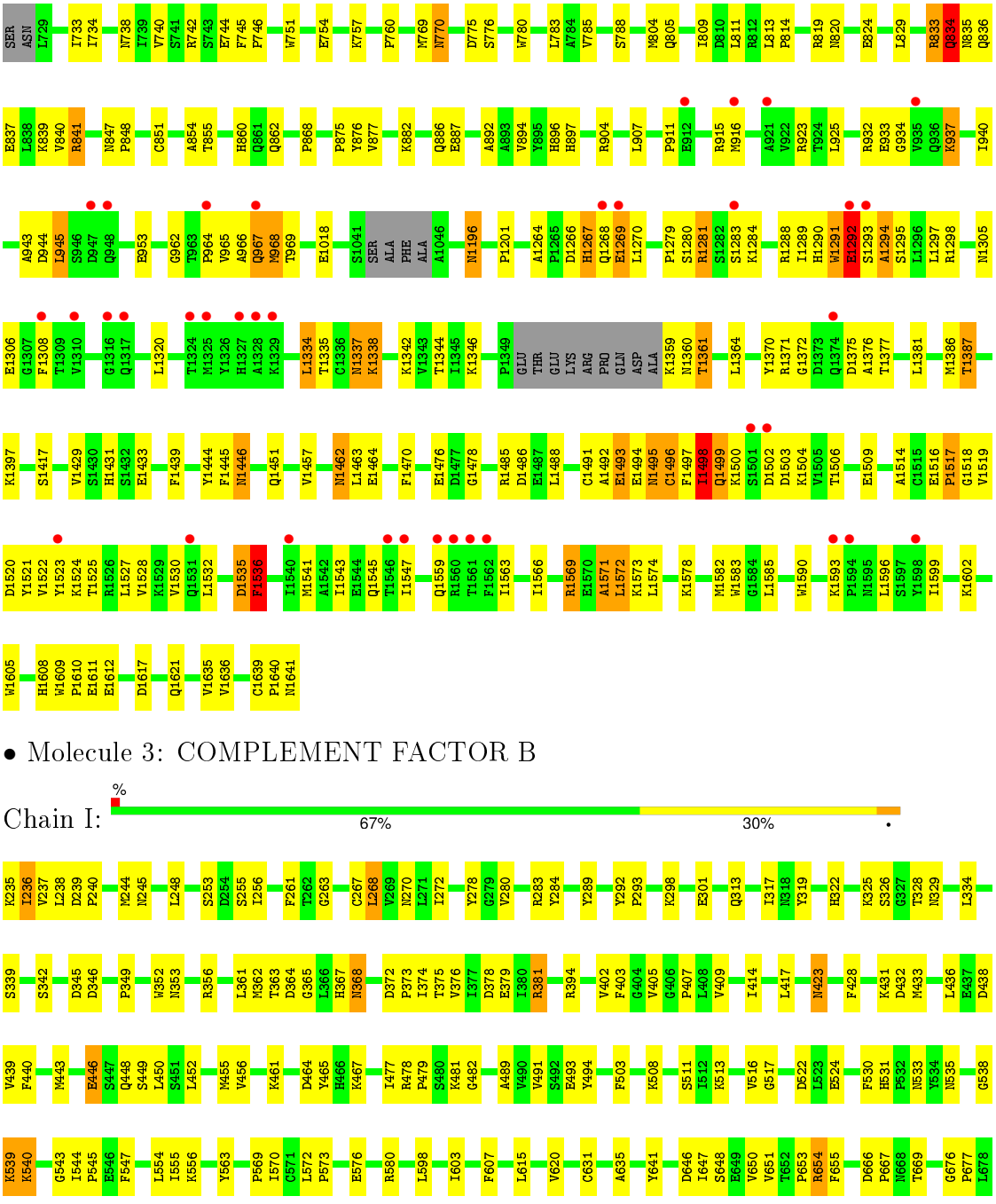
Chain F:





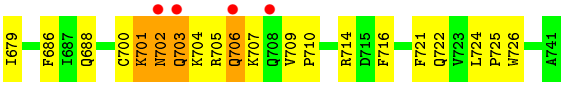
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

Chain H:

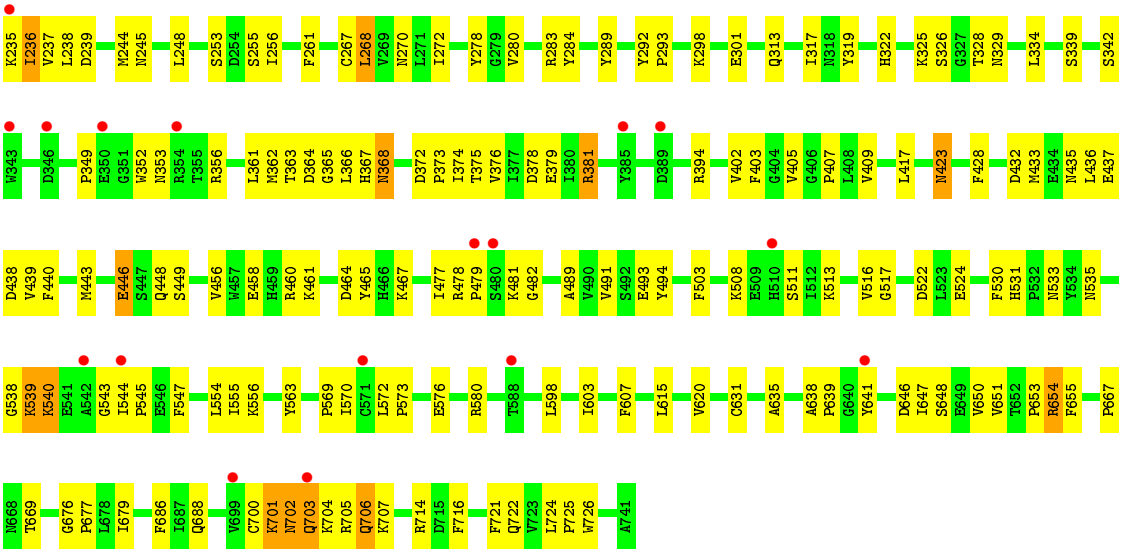


• Molecule 3: COMPLEMENT FACTOR B

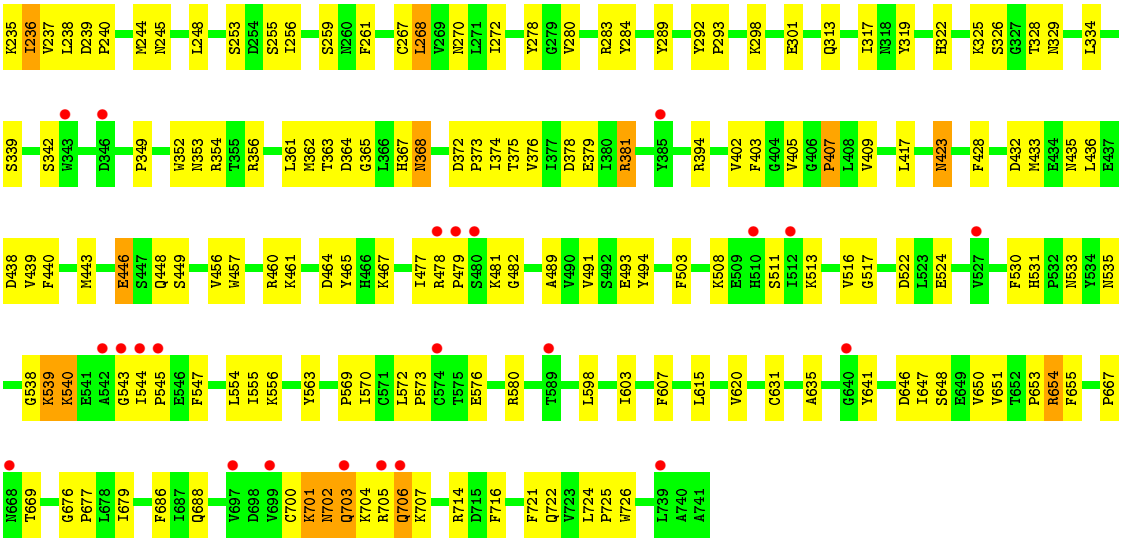
Chain I:



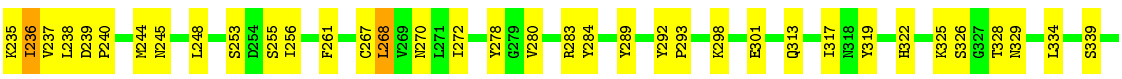
• Molecule 3: COMPLEMENT FACTOR B

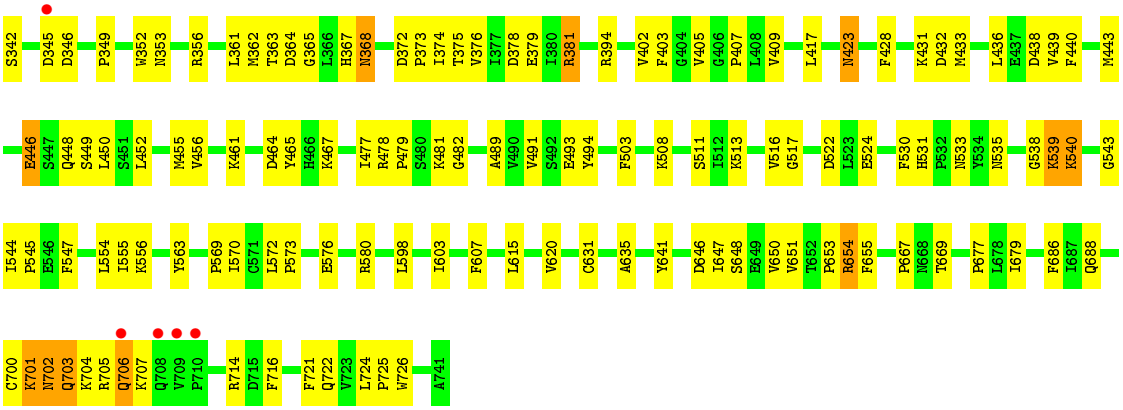


• Molecule 3: COMPLEMENT FACTOR B



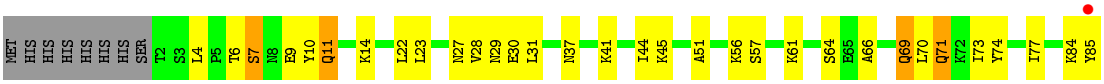
• Molecule 3: COMPLEMENT FACTOR B





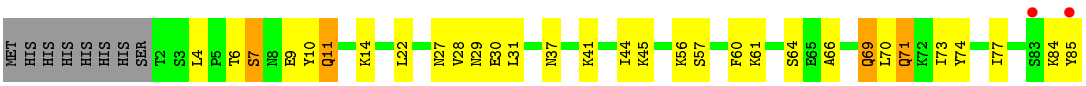
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

Chain M:



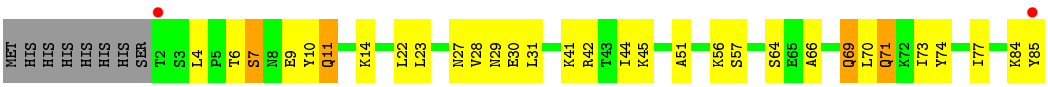
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

Chain N:



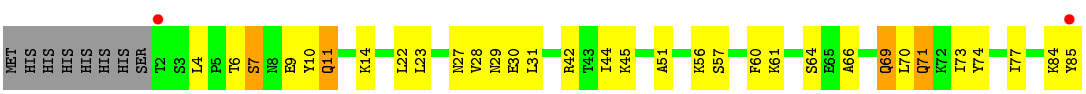
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

Chain P:



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	228.63Å 121.49Å 280.78Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	39.67 – 3.90 39.68 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.67-3.90) 97.6 (39.68-3.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 3.87Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.253 , 0.268 0.244 , 0.259	Depositor DCC
R_{free} test set	2089 reflections (1.52%)	DCC
Wilson B-factor (Å^2)	125.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 71.6	EDS
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 137471 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	67989	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, NDG, 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	0.20	0/5056	0.37	0/6870
1	C	0.20	0/5056	0.37	0/6870
1	E	0.20	0/5056	0.37	0/6870
1	G	0.21	0/5056	0.38	0/6870
2	B	0.21	0/7317	0.36	0/9907
2	D	0.21	0/7306	0.36	0/9894
2	F	0.21	0/7314	0.36	0/9905
2	H	0.22	0/7315	0.36	0/9902
3	I	0.20	0/4092	0.37	0/5543
3	J	0.20	0/4092	0.37	0/5543
3	K	0.20	0/4092	0.37	0/5543
3	L	0.20	0/4092	0.37	0/5543
4	M	0.21	0/690	0.33	0/923
4	N	0.21	0/690	0.32	0/923
4	P	0.21	0/690	0.33	0/923
4	Q	0.21	0/690	0.33	0/923
All	All	0.21	0/68604	0.36	0/92952

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
5	B	1	0
5	D	1	0
5	E	1	0
7	C	1	0
7	G	1	0
10	H	3	0
12	I	2	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	J	2	0
13	I	1	0
14	K	4	0
16	L	1	0
All	All	18	0

There are no bond length outliers.

There are no bond angle outliers.

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	2642	NDG	C1
7	C	1646	NDG	C1
5	D	2642	NDG	C1
5	E	1646	NDG	C1
7	G	1646	NDG	C1
10	H	2642	NDG	C1
10	H	2644	MAN	C1
10	H	2645	MAN	C1
12	I	1743	NDG	C1
12	I	1745	MAN	C1
13	I	1746	NDG	C1
12	J	1743	NDG	C1
12	J	1745	MAN	C1
14	K	1743	NDG	C1
14	K	1745	MAN	C1
14	K	1746	MAN	C1
14	K	1748	MAN	C1
16	L	1743	NDG	C1

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	4958	0	5017	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4958	0	5017	129	0
1	E	4958	0	5017	132	0
1	G	4958	0	5016	145	0
2	B	7177	0	7085	201	0
2	D	7166	0	7062	193	0
2	F	7172	0	7080	220	0
2	H	7175	0	7087	195	0
3	I	4004	0	3966	129	0
3	J	4004	0	3967	129	0
3	K	4004	0	3965	128	0
3	L	4004	0	3966	126	0
4	M	682	0	697	35	0
4	N	682	0	697	38	0
4	P	682	0	697	33	0
4	Q	682	0	697	38	0
5	A	50	0	43	1	0
5	B	50	0	42	1	0
5	D	50	0	43	1	0
5	E	50	0	43	5	0
6	B	11	0	10	0	0
6	K	11	0	10	0	0
7	C	61	0	52	2	0
7	G	61	0	52	6	0
8	F	72	0	61	2	0
9	G	11	0	10	1	0
10	H	50	0	43	2	0
11	I	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
12	I	39	0	34	3	0
12	J	39	0	34	2	0
13	I	28	0	25	0	0
14	K	61	0	52	6	0
15	K	14	0	13	3	0
15	L	14	0	13	0	0
16	L	39	0	34	0	0
17	B	1	0	0	0	0
17	I	2	0	0	0	0
17	J	2	0	0	1	0
17	K	2	0	0	0	0
17	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	67989	0	67647	1876	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 (1876) 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:G:426:THR:HG21	1:G:432:ASN:H	1.20	1.07
2:H:1494:GLU:HB3	2:H:1602:LYS:HB3	1.36	1.04
2:D:1569:ARG:HB2	2:D:1569:ARG:HH11	1.32	0.94
2:F:1569:ARG:HB2	2:F:1569:ARG:HH11	1.32	0.94
2:H:1569:ARG:HB2	2:H:1569:ARG:HH11	1.32	0.94
2:B:1569:ARG:HH11	2:B:1569:ARG:HB2	1.32	0.94
2:H:1268:GLN:HG3	2:H:1269:GLU:H	1.34	0.92
1:G:505:PRO:HG3	1:G:595:TRP:CE3	2.08	0.88
3:L:267:CYS:HB2	3:L:433:MET:HE1	1.54	0.87
2:F:1359:LYS:HD2	4:M:4:LEU:HD11	1.58	0.86
1:A:549:GLU:HG2	1:A:550:ASP:H	1.44	0.83
1:G:477:ARG:HH11	1:G:477:ARG:HG2	1.44	0.83
1:C:549:GLU:HG2	1:C:550:ASP:H	1.44	0.82
2:H:1497:PHE:HE2	2:H:1571:ALA:HB1	1.43	0.82
1:E:477:ARG:HH11	1:E:477:ARG:HG2	1.44	0.82
1:E:547:GLN:HE22	1:E:559:MET:HA	1.44	0.82
3:J:381:ARG:HH21	3:J:381:ARG:HG2	1.45	0.82
1:G:549:GLU:HG2	1:G:550:ASP:H	1.44	0.82
1:E:549:GLU:HG2	1:E:550:ASP:H	1.44	0.82
4:Q:6:THR:H	4:Q:9:GLU:HB3	1.45	0.82
4:N:6:THR:H	4:N:9:GLU:HB3	1.45	0.81
4:P:6:THR:H	4:P:9:GLU:HB3	1.45	0.81
2:H:1485:ARG:HD3	2:H:1536:PHE:CZ	2.16	0.81
1:A:547:GLN:HE22	1:A:559:MET:HA	1.44	0.81
3:K:381:ARG:HG2	3:K:381:ARG:HH21	1.45	0.81
1:G:547:GLN:HE22	1:G:559:MET:HA	1.44	0.81
1:C:547:GLN:HE22	1:C:559:MET:HA	1.44	0.81
4:M:6:THR:H	4:M:9:GLU:HB3	1.45	0.81
1:C:477:ARG:HH11	1:C:477:ARG:HG2	1.44	0.80
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.44	0.80
1:G:508:ARG:CZ	1:G:604:GLY:HA3	2.12	0.80
3:L:381:ARG:HG2	3:L:381:ARG:HH21	1.45	0.80
2:B:819:ARG:HG2	2:B:819:ARG:HH11	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:481:ALA:H	7:G:1646:NDG:H8C3	1.46	0.80
3:I:381:ARG:HH21	3:I:381:ARG:HG2	1.45	0.80
2:D:819:ARG:HG2	2:D:819:ARG:HH11	1.46	0.80
1:C:45:LEU:HD11	1:C:48:SER:HB3	1.64	0.79
2:H:833:ARG:HH11	2:H:833:ARG:HG2	1.48	0.79
2:H:1488:LEU:HG	2:H:1590:TRP:HH2	1.47	0.79
2:D:833:ARG:HG2	2:D:833:ARG:HH11	1.48	0.79
2:F:819:ARG:HH11	2:F:819:ARG:HG2	1.46	0.79
2:H:819:ARG:HG2	2:H:819:ARG:HH11	1.46	0.79
2:D:1532:LEU:HD11	2:D:1569:ARG:HD3	1.65	0.78
3:I:244:MET:HG3	3:I:356:ARG:HB2	1.65	0.78
1:G:45:LEU:HD11	1:G:48:SER:HB3	1.64	0.78
2:H:1532:LEU:HD11	2:H:1569:ARG:HD3	1.65	0.78
2:F:1532:LEU:HD11	2:F:1569:ARG:HD3	1.65	0.78
1:E:45:LEU:HD11	1:E:48:SER:HB3	1.64	0.78
2:B:1532:LEU:HD11	2:B:1569:ARG:HD3	1.65	0.78
2:F:738:ASN:HD22	4:P:45:LYS:HE2	1.47	0.78
2:H:966:ALA:O	2:H:967:GLN:HB2	1.83	0.78
1:A:45:LEU:HD11	1:A:48:SER:HB3	1.64	0.78
2:F:833:ARG:HG2	2:F:833:ARG:HH11	1.48	0.78
2:B:833:ARG:HH11	2:B:833:ARG:HG2	1.48	0.77
2:F:932:ARG:NH1	3:L:339:SER:HB2	1.99	0.77
2:H:738:ASN:HD22	4:Q:45:LYS:HE2	1.49	0.77
2:F:841:ARG:HH11	2:F:841:ARG:HG2	1.50	0.77
3:J:244:MET:HG3	3:J:356:ARG:HB2	1.65	0.77
3:L:244:MET:HG3	3:L:356:ARG:HB2	1.65	0.77
3:K:244:MET:HG3	3:K:356:ARG:HB2	1.65	0.77
1:G:506:SER:HB2	1:G:530:TRP:HE1	1.50	0.77
2:F:742:ARG:HB3	2:F:775:ASP:HB3	1.67	0.77
2:B:841:ARG:HG2	2:B:841:ARG:HH11	1.50	0.76
2:F:740:VAL:HB	4:P:42:ARG:HB2	1.68	0.76
1:A:506:SER:HB2	1:A:530:TRP:HE1	1.50	0.76
1:E:506:SER:HB2	1:E:530:TRP:HE1	1.50	0.76
3:L:705:ARG:O	3:L:706:GLN:HB2	1.86	0.75
3:I:705:ARG:O	3:I:706:GLN:HB2	1.86	0.75
2:D:841:ARG:HH11	2:D:841:ARG:HG2	1.50	0.75
2:H:1498:ILE:HD12	2:H:1605:TRP:HA	1.65	0.75
3:J:705:ARG:O	3:J:706:GLN:HB2	1.86	0.75
2:F:1569:ARG:CB	2:F:1569:ARG:HH11	2.00	0.75
2:H:841:ARG:HG2	2:H:841:ARG:HH11	1.50	0.75
1:C:506:SER:HB2	1:C:530:TRP:HE1	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:ARG:HG3	1:C:440:ARG:O	1.85	0.75
3:L:446:GLU:O	3:L:450:LEU:HG	1.86	0.74
2:B:1569:ARG:HH11	2:B:1569:ARG:CB	2.00	0.74
1:C:404:THR:HG23	1:C:414:GLN:HE21	1.53	0.74
3:L:489:ALA:HB2	3:L:677:PRO:HG3	1.70	0.74
1:E:440:ARG:HG3	1:E:440:ARG:O	1.85	0.74
3:K:705:ARG:O	3:K:706:GLN:HB2	1.86	0.74
2:H:1569:ARG:HH11	2:H:1569:ARG:CB	2.00	0.74
3:I:464:ASP:HB3	3:I:615:LEU:HB2	1.70	0.74
2:H:877:VAL:HG22	2:H:1451:GLN:HE21	1.53	0.74
3:K:464:ASP:HB3	3:K:615:LEU:HB2	1.70	0.74
1:G:440:ARG:O	1:G:440:ARG:HG3	1.85	0.74
1:A:440:ARG:O	1:A:440:ARG:HG3	1.86	0.74
1:A:404:THR:HG23	1:A:414:GLN:HE21	1.53	0.74
1:E:223:ILE:HD12	1:E:223:ILE:H	1.53	0.74
2:H:740:VAL:HB	4:Q:42:ARG:HB2	1.69	0.74
2:F:834:GLN:NE2	2:F:835:ASN:H	1.86	0.73
2:D:1569:ARG:CB	2:D:1569:ARG:HH11	2.00	0.73
3:I:248:LEU:HD22	3:I:268:LEU:HD22	1.71	0.73
1:G:223:ILE:H	1:G:223:ILE:HD12	1.53	0.73
2:H:742:ARG:HB3	2:H:775:ASP:HB3	1.71	0.73
1:E:404:THR:HG23	1:E:414:GLN:HE21	1.53	0.73
2:B:834:GLN:NE2	2:B:835:ASN:H	1.86	0.73
1:G:404:THR:HG23	1:G:414:GLN:HE21	1.52	0.73
1:C:223:ILE:H	1:C:223:ILE:HD12	1.53	0.73
3:L:248:LEU:HD22	3:L:268:LEU:HD22	1.71	0.73
1:A:223:ILE:H	1:A:223:ILE:HD12	1.53	0.73
3:I:489:ALA:HB2	3:I:677:PRO:HG3	1.70	0.73
2:B:966:ALA:O	2:B:967:GLN:HB2	1.88	0.73
2:D:834:GLN:NE2	2:D:835:ASN:H	1.86	0.73
2:F:966:ALA:O	2:F:967:GLN:HB2	1.89	0.73
2:D:966:ALA:O	2:D:967:GLN:HB2	1.88	0.73
2:D:742:ARG:HB3	2:D:775:ASP:HB3	1.71	0.72
3:L:464:ASP:HB3	3:L:615:LEU:HB2	1.70	0.72
1:G:424:TYR:O	1:G:433:TYR:HE1	1.73	0.72
3:K:407:PRO:HD3	14:K:1743:NDG:H8C1	1.71	0.72
2:F:1269:GLU:HG3	2:F:1315:LYS:HB3	1.70	0.72
2:H:1497:PHE:CE2	2:H:1571:ALA:HB1	2.24	0.72
2:F:937:LYS:HG2	3:L:345:ASP:OD1	1.88	0.72
3:K:489:ALA:HB2	3:K:677:PRO:HG3	1.70	0.72
3:J:489:ALA:HB2	3:J:677:PRO:HG3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:426:THR:HG21	1:G:432:ASN:N	2.02	0.72
3:K:635:ALA:HB3	3:K:647:ILE:HD11	1.71	0.72
3:J:464:ASP:HB3	3:J:615:LEU:HB2	1.70	0.72
3:J:653:PRO:HD2	3:J:654:ARG:HH12	1.55	0.72
3:J:248:LEU:HD22	3:J:268:LEU:HD22	1.70	0.72
2:H:834:GLN:NE2	2:H:835:ASN:H	1.86	0.72
1:C:6:ILE:HD13	1:C:22:LEU:HD23	1.72	0.71
1:G:6:ILE:HD13	1:G:22:LEU:HD23	1.72	0.71
3:L:461:LYS:HE2	3:L:461:LYS:HA	1.73	0.71
3:J:576:GLU:HB3	3:J:580:ARG:HH22	1.55	0.71
3:K:539:LYS:HG2	3:K:544:ILE:HD12	1.73	0.71
3:J:539:LYS:HG2	3:J:544:ILE:HD12	1.73	0.71
3:J:635:ALA:HB3	3:J:647:ILE:HD11	1.71	0.71
1:C:13:ARG:HH22	1:C:476:GLY:HA3	1.54	0.71
3:K:461:LYS:HE2	3:K:461:LYS:HA	1.73	0.71
3:J:461:LYS:HA	3:J:461:LYS:HE2	1.73	0.71
3:I:461:LYS:HE2	3:I:461:LYS:HA	1.73	0.71
3:K:576:GLU:HB3	3:K:580:ARG:HH22	1.55	0.71
3:I:653:PRO:HD2	3:I:654:ARG:HH12	1.55	0.71
3:K:248:LEU:HD22	3:K:268:LEU:HD22	1.70	0.71
1:C:439:LEU:HG	1:E:439:LEU:HG	1.71	0.71
3:I:635:ALA:HB3	3:I:647:ILE:HD11	1.71	0.71
3:L:635:ALA:HB3	3:L:647:ILE:HD11	1.71	0.70
1:E:6:ILE:HD13	1:E:22:LEU:HD23	1.72	0.70
1:C:98:VAL:HG11	2:D:1017:LEU:HD13	1.73	0.70
3:K:653:PRO:HD2	3:K:654:ARG:HH12	1.55	0.70
4:Q:71:GLN:HE21	4:Q:71:GLN:HA	1.57	0.70
3:L:576:GLU:HB3	3:L:580:ARG:HH22	1.55	0.70
3:I:539:LYS:HG2	3:I:544:ILE:HD12	1.73	0.70
2:H:1446:ASN:HB2	4:N:4:LEU:HD13	1.74	0.70
4:P:71:GLN:HE21	4:P:71:GLN:HA	1.57	0.70
3:I:576:GLU:HB3	3:I:580:ARG:HH22	1.55	0.70
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.74	0.70
3:L:539:LYS:HG2	3:L:544:ILE:HD12	1.73	0.69
3:I:381:ARG:HH21	3:I:381:ARG:CG	2.05	0.69
3:L:373:PRO:HB2	3:L:417:LEU:HD21	1.75	0.69
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.72	0.69
3:J:238:LEU:HD11	3:J:278:TYR:HB3	1.74	0.69
2:D:1416:PHE:HZ	2:D:1442:HIS:HB2	1.57	0.69
3:K:381:ARG:HH21	3:K:381:ARG:CG	2.06	0.69
3:L:653:PRO:HD2	3:L:654:ARG:HH12	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:238:LEU:HD11	3:I:278:TYR:HB3	1.74	0.69
2:H:962:GLY:O	2:H:964:PRO:HD3	1.92	0.69
2:F:1387:THR:HG22	2:F:1451:GLN:H	1.58	0.69
1:E:426:THR:HG21	1:E:432:ASN:H	1.57	0.69
2:H:1446:ASN:HB2	4:N:4:LEU:CD1	2.21	0.69
3:L:238:LEU:HD11	3:L:278:TYR:HB3	1.74	0.69
2:H:855:THR:HB	2:H:1602:LYS:HZ3	1.56	0.69
1:G:505:PRO:HG3	1:G:595:TRP:HE3	1.55	0.69
4:N:71:GLN:HE21	4:N:71:GLN:HA	1.56	0.69
3:J:381:ARG:HH21	3:J:381:ARG:CG	2.05	0.69
2:H:1387:THR:HG22	2:H:1451:GLN:H	1.58	0.69
3:L:381:ARG:CG	3:L:381:ARG:HH21	2.05	0.69
2:D:962:GLY:O	2:D:964:PRO:HD3	1.93	0.69
3:J:705:ARG:HG3	3:J:705:ARG:O	1.93	0.68
2:B:1416:PHE:HZ	2:B:1442:HIS:HB2	1.57	0.68
2:B:841:ARG:NH1	2:B:841:ARG:HG2	2.08	0.68
2:B:1488:LEU:HG	2:B:1590:TRP:CZ2	2.27	0.68
2:F:841:ARG:NH1	2:F:841:ARG:HG2	2.08	0.68
2:D:1488:LEU:HG	2:D:1590:TRP:CZ2	2.27	0.68
4:M:71:GLN:HA	4:M:71:GLN:HE21	1.56	0.68
2:F:733:ILE:HG12	2:F:734:ILE:H	1.58	0.68
3:K:373:PRO:HB2	3:K:417:LEU:HD21	1.75	0.68
3:J:373:PRO:HB2	3:J:417:LEU:HD21	1.75	0.68
3:I:373:PRO:HB2	3:I:417:LEU:HD21	1.75	0.68
3:J:435:ASN:ND2	3:J:460:ARG:HH21	1.90	0.68
1:G:567:HIS:ND1	2:H:760:PRO:HG3	2.09	0.68
1:G:100:LEU:HD21	1:G:638:LEU:HD23	1.76	0.68
2:H:733:ILE:HG12	2:H:734:ILE:H	1.58	0.68
2:D:1445:PHE:CZ	4:P:7:SER:HA	2.28	0.68
1:C:606:THR:HG22	1:C:608:GLY:H	1.59	0.68
3:J:432:ASP:HA	4:Q:27:ASN:HD21	1.57	0.67
3:K:446:GLU:HB3	3:K:449:SER:HB2	1.77	0.67
3:K:354:ARG:HB2	15:K:1749:NDG:H8C2	1.74	0.67
1:C:372:GLU:O	1:C:375:VAL:HG12	1.95	0.67
2:D:733:ILE:HG12	2:D:734:ILE:H	1.58	0.67
3:K:705:ARG:HG3	3:K:705:ARG:O	1.93	0.67
2:D:1518:GLY:HA3	2:D:1585:LEU:HD22	1.77	0.67
2:H:841:ARG:HG2	2:H:841:ARG:NH1	2.08	0.67
3:K:238:LEU:HD11	3:K:278:TYR:HB3	1.74	0.67
2:B:733:ILE:HG12	2:B:734:ILE:H	1.58	0.67
3:I:705:ARG:HG3	3:I:705:ARG:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1268:GLN:CG	2:H:1269:GLU:H	2.00	0.67
1:G:351:MET:SD	1:G:440:ARG:HD2	2.35	0.67
2:B:1518:GLY:HA3	2:B:1585:LEU:HD22	1.77	0.67
3:L:705:ARG:O	3:L:705:ARG:HG3	1.94	0.67
2:H:1359:LYS:HD2	4:N:4:LEU:HD11	1.75	0.67
2:H:1518:GLY:HA3	2:H:1585:LEU:HD22	1.77	0.66
2:F:962:GLY:O	2:F:964:PRO:HD3	1.95	0.66
2:D:876:TYR:HA	2:D:1451:GLN:HE22	1.60	0.66
2:H:1499:GLN:HG2	2:H:1500:LYS:HG3	1.77	0.66
2:D:1337:ASN:O	2:D:1338:LYS:HB2	1.95	0.66
1:G:606:THR:HG22	1:G:608:GLY:H	1.59	0.66
1:G:55:THR:HG22	1:G:57:ALA:H	1.61	0.66
2:H:1498:ILE:HG12	2:H:1499:GLN:H	1.60	0.66
2:D:841:ARG:NH1	2:D:841:ARG:HG2	2.08	0.66
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.78	0.66
1:A:606:THR:HG22	1:A:608:GLY:H	1.59	0.66
2:B:877:VAL:HG22	2:B:1451:GLN:HE21	1.59	0.66
1:E:606:THR:HG22	1:E:608:GLY:H	1.59	0.66
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.60	0.66
3:J:446:GLU:HB3	3:J:449:SER:HB2	1.77	0.66
1:G:510:VAL:HG21	1:G:622:LEU:CD1	2.26	0.65
2:H:896:HIS:HB3	4:N:61:LYS:HD3	1.78	0.65
2:B:962:GLY:O	2:B:964:PRO:HD3	1.96	0.65
1:E:473:MET:HB2	1:E:508:ARG:HB2	1.78	0.65
3:I:478:ARG:HG3	3:I:479:PRO:HD2	1.79	0.65
2:B:1417:SER:HB2	4:Q:14:LYS:NZ	2.11	0.65
1:A:55:THR:HG22	1:A:57:ALA:H	1.61	0.65
3:I:446:GLU:HB3	3:I:449:SER:HB2	1.79	0.65
2:F:1518:GLY:HA3	2:F:1585:LEU:HD22	1.77	0.65
1:C:473:MET:HB2	1:C:508:ARG:HB2	1.78	0.65
2:F:829:LEU:HD23	2:F:840:VAL:HG11	1.78	0.65
2:F:1126:LEU:HG	2:F:1130:GLN:HE21	1.61	0.65
2:B:829:LEU:HD23	2:B:840:VAL:HG11	1.78	0.65
2:H:829:LEU:HD23	2:H:840:VAL:HG11	1.78	0.65
1:G:549:GLU:HG2	1:G:550:ASP:N	2.12	0.65
2:B:1337:ASN:O	2:B:1338:LYS:HB2	1.94	0.65
2:D:829:LEU:HD23	2:D:840:VAL:HG11	1.78	0.64
2:B:1126:LEU:HG	2:B:1130:GLN:HE21	1.61	0.64
1:C:55:THR:HG22	1:C:57:ALA:H	1.61	0.64
2:F:1265:PRO:O	2:F:1266:ASP:HB2	1.96	0.64
3:I:446:GLU:O	3:I:450:LEU:HG	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1387:THR:HG22	2:D:1451:GLN:H	1.60	0.64
1:E:55:THR:HG22	1:E:57:ALA:H	1.61	0.64
2:B:1265:PRO:O	2:B:1266:ASP:HB2	1.97	0.64
1:G:473:MET:HB2	1:G:508:ARG:HB2	1.78	0.64
3:J:478:ARG:HG3	3:J:479:PRO:HD2	1.79	0.64
2:D:1126:LEU:HG	2:D:1130:GLN:HE21	1.61	0.64
2:F:1268:GLN:O	2:F:1269:GLU:HG2	1.97	0.64
3:K:478:ARG:HG3	3:K:479:PRO:HD2	1.79	0.64
3:L:446:GLU:HB3	3:L:449:SER:HB2	1.79	0.64
2:B:837:GLU:HG2	4:Q:64:SER:OG	1.97	0.64
2:H:1338:LYS:HA	2:H:1371:ARG:HB2	1.80	0.64
2:F:1337:ASN:O	2:F:1338:LYS:HB2	1.97	0.64
2:D:1265:PRO:O	2:D:1266:ASP:HB2	1.98	0.64
1:C:549:GLU:HG2	1:C:550:ASP:N	2.12	0.63
2:D:1527:LEU:HD13	2:D:1541:MET:HG2	1.80	0.63
1:A:551:ARG:N	1:A:551:ARG:HD2	2.13	0.63
2:D:1416:PHE:CZ	2:D:1442:HIS:HB2	2.34	0.63
2:H:837:GLU:HG2	4:N:64:SER:OG	1.98	0.63
3:K:460:ARG:HE	4:P:28:VAL:HG21	1.63	0.63
3:K:513:LYS:HB3	3:K:522:ASP:HB3	1.81	0.63
2:H:1498:ILE:HG12	2:H:1499:GLN:N	2.13	0.63
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.81	0.63
1:C:551:ARG:N	1:C:551:ARG:HD2	2.13	0.63
3:L:478:ARG:HG3	3:L:479:PRO:HD2	1.79	0.63
2:F:1498:ILE:HG22	2:F:1499:GLN:N	2.13	0.63
2:H:876:TYR:HA	2:H:1451:GLN:HE22	1.64	0.63
7:C:1646:NDG:H6C1	7:C:1647:NAG:C7	2.29	0.63
2:H:1337:ASN:O	2:H:1338:LYS:HB2	1.97	0.63
1:E:567:HIS:ND1	2:F:760:PRO:HG3	2.13	0.63
1:E:551:ARG:HD2	1:E:551:ARG:N	2.13	0.63
1:G:551:ARG:HD2	1:G:551:ARG:N	2.13	0.63
1:C:634:GLN:HE22	2:D:1016:GLY:HA2	1.64	0.63
1:C:147:ASN:HB2	1:C:148:PRO:HD2	1.80	0.63
2:B:1527:LEU:HD13	2:B:1541:MET:HG2	1.80	0.63
1:A:351:MET:SD	1:A:440:ARG:HD2	2.39	0.63
2:B:1416:PHE:CZ	2:B:1442:HIS:HB2	2.34	0.63
3:J:460:ARG:HE	4:Q:28:VAL:HG21	1.64	0.62
3:L:513:LYS:HB3	3:L:522:ASP:HB3	1.81	0.62
1:G:512:TYR:CZ	1:G:624:PHE:HE1	2.16	0.62
2:H:1527:LEU:HD13	2:H:1541:MET:HG2	1.80	0.62
1:E:147:ASN:HB2	1:E:148:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:432:ASP:HA	4:P:27:ASN:HD21	1.63	0.62
2:D:1295:SER:O	2:D:1297:LEU:HD12	2.00	0.62
2:B:1295:SER:O	2:B:1297:LEU:HD12	2.00	0.62
2:B:876:TYR:HA	2:B:1451:GLN:HE22	1.63	0.62
3:K:433:MET:HE3	3:K:436:LEU:HD21	1.81	0.62
3:I:513:LYS:HB3	3:I:522:ASP:HB3	1.81	0.62
1:G:147:ASN:HB2	1:G:148:PRO:HD2	1.81	0.62
2:F:877:VAL:HG22	2:F:1451:GLN:HE21	1.65	0.62
2:H:1498:ILE:HG13	2:H:1605:TRP:CE3	2.34	0.62
2:B:1446:ASN:HB2	4:Q:4:LEU:HB2	1.81	0.62
1:A:549:GLU:HG2	1:A:550:ASP:N	2.12	0.62
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.81	0.62
2:H:855:THR:HB	2:H:1602:LYS:NZ	2.14	0.62
2:H:834:GLN:HE21	2:H:835:ASN:H	1.47	0.62
1:C:19:THR:HG21	7:C:1646:NDG:H8C2	1.80	0.62
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.35	0.62
2:F:1527:LEU:HD13	2:F:1541:MET:HG2	1.80	0.62
3:J:513:LYS:HB3	3:J:522:ASP:HB3	1.81	0.62
3:I:423:ASN:HD22	3:I:423:ASN:N	1.98	0.61
1:G:19:THR:HB	1:G:478:LEU:HB2	1.81	0.61
2:B:834:GLN:HE21	2:B:835:ASN:H	1.47	0.61
3:I:650:VAL:HG23	3:I:651:VAL:HG23	1.83	0.61
2:H:1611:GLU:HG3	2:H:1612:GLU:H	1.66	0.61
2:F:1295:SER:O	2:F:1297:LEU:HD12	2.00	0.61
1:E:222:TYR:CE2	1:E:224:TYR:HB2	2.35	0.61
2:H:1497:PHE:HB2	2:H:1498:ILE:HD13	1.82	0.61
3:L:461:LYS:HG2	4:N:28:VAL:HG12	1.81	0.61
1:C:13:ARG:NH2	1:C:476:GLY:HA3	2.15	0.61
3:K:423:ASN:N	3:K:423:ASN:HD22	1.98	0.61
3:I:267:CYS:HB2	3:I:433:MET:HE1	1.82	0.61
2:B:1490:ARG:HB3	2:B:1590:TRP:CH2	2.36	0.61
1:E:372:GLU:O	1:E:375:VAL:HG12	1.99	0.61
1:G:372:GLU:O	1:G:375:VAL:HG12	2.01	0.61
3:I:461:LYS:HG2	4:M:28:VAL:HG12	1.82	0.61
3:K:478:ARG:HE	3:K:481:LYS:HD2	1.65	0.61
1:G:222:TYR:CE2	1:G:224:TYR:HB2	2.35	0.61
3:L:650:VAL:HG23	3:L:651:VAL:HG23	1.83	0.61
2:B:1291:TRP:CG	2:B:1292:GLU:N	2.69	0.61
2:H:1498:ILE:CG1	2:H:1499:GLN:H	2.12	0.61
1:C:20:MET:HB3	1:C:64:VAL:HG23	1.83	0.61
2:D:1490:ARG:HB3	2:D:1590:TRP:CH2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:423:ASN:HD22	3:J:423:ASN:N	1.98	0.61
1:C:222:TYR:CE2	1:C:224:TYR:HB2	2.35	0.61
2:H:923:ARG:HH22	2:H:940:ILE:HG12	1.66	0.61
2:F:834:GLN:HE21	2:F:835:ASN:H	1.47	0.61
3:K:650:VAL:HG23	3:K:651:VAL:HG23	1.83	0.61
2:F:1338:LYS:HA	2:F:1371:ARG:HB2	1.81	0.61
2:F:1527:LEU:HD21	2:F:1530:VAL:HG22	1.83	0.61
3:I:478:ARG:HE	3:I:481:LYS:HD2	1.65	0.60
2:B:1527:LEU:HD21	2:B:1530:VAL:HG22	1.83	0.60
2:F:1611:GLU:HG3	2:F:1612:GLU:H	1.66	0.60
3:J:478:ARG:HE	3:J:481:LYS:HD2	1.65	0.60
1:A:372:GLU:O	1:A:375:VAL:HG12	2.01	0.60
2:F:923:ARG:HH22	2:F:940:ILE:HG12	1.66	0.60
2:D:1611:GLU:HG3	2:D:1612:GLU:H	1.66	0.60
1:G:20:MET:HB3	1:G:64:VAL:HG23	1.83	0.60
2:D:1291:TRP:CG	2:D:1292:GLU:N	2.69	0.60
2:F:837:GLU:HG2	4:M:64:SER:OG	2.00	0.60
3:L:449:SER:HA	3:L:452:LEU:HD13	1.84	0.60
3:L:478:ARG:HE	3:L:481:LYS:HD2	1.65	0.60
4:P:84:LYS:O	4:P:85:TYR:HB2	2.02	0.60
1:C:426:THR:HG21	1:C:432:ASN:H	1.65	0.60
2:H:1295:SER:O	2:H:1297:LEU:HD12	2.00	0.60
1:C:572:VAL:HG12	2:D:753:VAL:HG22	1.82	0.60
2:B:973:VAL:HG11	2:B:978:LEU:HD12	1.83	0.60
2:D:772:PHE:HD1	4:M:37:ASN:ND2	1.99	0.60
2:D:973:VAL:HG11	2:D:978:LEU:HD12	1.83	0.60
1:A:20:MET:HB3	1:A:64:VAL:HG23	1.83	0.60
2:B:1532:LEU:HD11	2:B:1569:ARG:CD	2.32	0.60
4:M:84:LYS:O	4:M:85:TYR:HB2	2.02	0.60
1:C:10:ASN:HB2	1:C:621:GLY:C	2.21	0.60
3:J:650:VAL:HG23	3:J:651:VAL:HG23	1.83	0.60
3:L:374:ILE:HD13	3:L:417:LEU:HD23	1.84	0.60
2:B:1039:GLN:HB3	2:B:1040:PRO:HD2	1.83	0.60
2:F:1446:ASN:HB2	4:M:4:LEU:CD1	2.32	0.60
2:D:834:GLN:HE21	2:D:835:ASN:H	1.47	0.60
3:J:460:ARG:NE	4:Q:28:VAL:HG21	2.16	0.60
1:E:20:MET:HB3	1:E:64:VAL:HG23	1.83	0.60
2:F:1291:TRP:CD1	2:F:1292:GLU:N	2.70	0.60
2:D:1532:LEU:HD11	2:D:1569:ARG:CD	2.32	0.59
2:F:876:TYR:HA	2:F:1451:GLN:HE22	1.67	0.59
1:E:220:PHE:CZ	1:E:330:PRO:HB3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1039:GLN:HB3	2:F:1040:PRO:HD2	1.83	0.59
2:D:877:VAL:HG22	2:D:1451:GLN:HE21	1.67	0.59
3:K:436:LEU:HB3	3:K:440:PHE:CE2	2.37	0.59
3:J:570:ILE:HD13	3:J:688:GLN:HB2	1.84	0.59
2:D:1039:GLN:HB3	2:D:1040:PRO:HD2	1.83	0.59
3:L:423:ASN:HD22	3:L:423:ASN:N	1.98	0.59
2:B:1611:GLU:HG3	2:B:1612:GLU:H	1.66	0.59
1:E:549:GLU:HG2	1:E:550:ASP:N	2.12	0.59
2:H:833:ARG:CG	2:H:833:ARG:HH11	2.15	0.59
2:D:1527:LEU:HD21	2:D:1530:VAL:HG22	1.83	0.59
3:I:570:ILE:HD13	3:I:688:GLN:HB2	1.84	0.59
1:G:13:ARG:NH2	1:G:476:GLY:HA3	2.18	0.59
3:I:563:TYR:CE2	3:I:569:PRO:HG3	2.38	0.59
1:G:555:PRO:HB3	2:H:775:ASP:HA	1.83	0.59
2:D:1337:ASN:O	2:D:1338:LYS:CB	2.51	0.59
2:H:1527:LEU:HD21	2:H:1530:VAL:HG22	1.83	0.59
4:N:84:LYS:O	4:N:85:TYR:HB2	2.02	0.59
3:L:570:ILE:HD13	3:L:688:GLN:HB2	1.84	0.59
3:K:563:TYR:CE2	3:K:569:PRO:HG3	2.38	0.59
1:G:350:LEU:HD21	1:G:400:ILE:HG21	1.83	0.59
4:N:22:LEU:HB3	4:N:74:TYR:HE2	1.68	0.59
3:J:563:TYR:CE2	3:J:569:PRO:HG3	2.38	0.59
1:C:558:GLN:HB3	2:D:770:ASN:HD21	1.68	0.59
4:Q:84:LYS:O	4:Q:85:TYR:HB2	2.02	0.59
3:J:436:LEU:HB3	3:J:440:PHE:CE2	2.37	0.59
3:L:508:LYS:HE2	3:L:508:LYS:HA	1.85	0.59
3:L:563:TYR:CE2	3:L:569:PRO:HG3	2.38	0.59
3:I:374:ILE:HD13	3:I:417:LEU:HD23	1.84	0.58
2:F:973:VAL:HG11	2:F:978:LEU:HD12	1.84	0.58
1:E:477:ARG:HH11	1:E:477:ARG:CG	2.16	0.58
2:D:833:ARG:CG	2:D:833:ARG:HH11	2.15	0.58
3:L:436:LEU:HB3	3:L:440:PHE:CE2	2.37	0.58
2:F:1215:LEU:HD23	2:F:1256:ALA:HB1	1.85	0.58
3:K:374:ILE:HD13	3:K:417:LEU:HD23	1.84	0.58
3:I:436:LEU:HB3	3:I:440:PHE:CE2	2.37	0.58
2:F:1532:LEU:HD11	2:F:1569:ARG:CD	2.34	0.58
1:C:40:PHE:CE2	2:D:1017:LEU:HD22	2.38	0.58
2:F:1291:TRP:CG	2:F:1292:GLU:N	2.70	0.58
3:J:374:ILE:HD13	3:J:417:LEU:HD23	1.84	0.58
4:P:22:LEU:HB3	4:P:74:TYR:HE2	1.68	0.58
2:H:1535:ASP:O	2:H:1536:PHE:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:22:LEU:HB3	4:M:74:TYR:HE2	1.68	0.58
3:I:508:LYS:HE2	3:I:508:LYS:HA	1.85	0.58
3:J:508:LYS:HA	3:J:508:LYS:HE2	1.85	0.58
3:K:570:ILE:HD13	3:K:688:GLN:HB2	1.84	0.58
2:H:877:VAL:H	2:H:1451:GLN:NE2	2.01	0.58
3:L:477:ILE:O	3:L:511:SER:HB2	2.04	0.58
2:H:1532:LEU:HD11	2:H:1569:ARG:CD	2.34	0.58
2:F:1359:LYS:HD2	4:M:4:LEU:CD1	2.32	0.58
2:B:833:ARG:HH11	2:B:833:ARG:CG	2.15	0.58
2:B:1215:LEU:HD23	2:B:1256:ALA:HB1	1.85	0.58
3:J:477:ILE:O	3:J:511:SER:HB2	2.04	0.58
4:Q:6:THR:H	4:Q:9:GLU:CB	2.16	0.57
1:G:527:ASP:N	1:G:616:VAL:HG11	2.19	0.57
2:D:1470:PHE:HB2	2:D:1478:GLY:HA3	1.86	0.57
2:H:1497:PHE:CZ	2:H:1572:LEU:HD23	2.39	0.57
2:H:1291:TRP:CD1	2:H:1292:GLU:N	2.70	0.57
1:G:510:VAL:HG11	1:G:622:LEU:HD12	1.86	0.57
3:I:477:ILE:O	3:I:511:SER:HB2	2.04	0.57
1:E:350:LEU:HD21	1:E:400:ILE:HG21	1.86	0.57
3:K:477:ILE:O	3:K:511:SER:HB2	2.04	0.57
2:H:1291:TRP:CG	2:H:1292:GLU:N	2.70	0.57
2:B:1445:PHE:CZ	4:Q:7:SER:HA	2.40	0.57
2:F:1133:LYS:O	2:F:1137:GLU:HG3	2.04	0.57
1:G:13:ARG:HH22	1:G:476:GLY:HA3	1.69	0.57
1:A:614:ALA:HB1	1:A:632:THR:HA	1.86	0.57
2:D:1215:LEU:HD23	2:D:1256:ALA:HB1	1.85	0.57
4:Q:22:LEU:HB3	4:Q:74:TYR:HE2	1.68	0.57
2:D:809:ILE:HD11	2:D:892:ALA:HB3	1.87	0.57
2:B:1337:ASN:O	2:B:1338:LYS:CB	2.51	0.57
2:B:1133:LYS:O	2:B:1137:GLU:HG3	2.04	0.57
2:F:1535:ASP:O	2:F:1536:PHE:HB3	2.03	0.57
2:F:1446:ASN:HB2	4:M:4:LEU:HD13	1.85	0.57
2:F:1269:GLU:HG3	2:F:1315:LYS:CB	2.35	0.57
2:D:962:GLY:C	2:D:964:PRO:HD3	2.24	0.57
2:B:809:ILE:HD11	2:B:892:ALA:HB3	1.87	0.57
3:K:460:ARG:NE	4:P:28:VAL:HG21	2.19	0.57
1:C:567:HIS:ND1	2:D:760:PRO:HG3	2.19	0.57
3:K:508:LYS:HA	3:K:508:LYS:HE2	1.85	0.57
1:E:614:ALA:HB1	1:E:632:THR:HA	1.86	0.57
2:B:836:GLN:HG2	2:B:897:HIS:HE1	1.70	0.57
2:H:1582:MET:HA	2:H:1605:TRP:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:923:ARG:NH2	2:H:940:ILE:HG12	2.19	0.57
2:D:1462:ASN:HD22	2:D:1463:LEU:N	2.03	0.57
2:B:1470:PHE:HB2	2:B:1478:GLY:HA3	1.86	0.57
2:H:819:ARG:HG2	2:H:819:ARG:NH1	2.19	0.57
2:F:1055:TRP:CZ2	2:F:1108:ILE:HA	2.40	0.57
2:H:1462:ASN:HD22	2:H:1463:LEU:N	2.03	0.57
3:L:253:SER:HB2	3:L:326:SER:O	2.05	0.56
2:B:965:VAL:O	2:B:1267:HIS:HD2	1.88	0.56
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.86	0.56
2:D:1055:TRP:CZ2	2:D:1108:ILE:HA	2.40	0.56
2:D:1143:LEU:HB3	2:D:1144:PRO:HD3	1.86	0.56
1:C:268:ARG:HD3	2:D:1378:MET:SD	2.44	0.56
2:H:1494:GLU:HG2	2:H:1602:LYS:HD3	1.87	0.56
1:G:481:ALA:N	7:G:1646:NDG:H8C3	2.17	0.56
2:F:833:ARG:CG	2:F:833:ARG:HH11	2.15	0.56
3:L:461:LYS:HD2	4:N:29:ASN:OD1	2.05	0.56
1:G:614:ALA:HB1	1:G:632:THR:HA	1.86	0.56
12:J:1743:NDG:H6C1	12:J:1744:NAG:C7	2.35	0.56
2:F:809:ILE:HD11	2:F:892:ALA:HB3	1.87	0.56
2:F:1582:MET:HA	2:F:1605:TRP:O	2.05	0.56
2:H:1566:ILE:O	2:H:1569:ARG:HG3	2.06	0.56
2:H:1337:ASN:O	2:H:1338:LYS:CB	2.53	0.56
2:B:923:ARG:HH22	2:B:940:ILE:HG12	1.70	0.56
2:D:925:LEU:HD11	2:D:1320:LEU:HD22	1.86	0.56
2:B:1462:ASN:HD22	2:B:1463:LEU:N	2.03	0.56
2:D:1535:ASP:O	2:D:1536:PHE:HB3	2.05	0.56
3:K:364:ASP:O	3:K:409:VAL:HG23	2.06	0.56
2:B:1516:GLU:HB3	2:B:1517:PRO:HD2	1.88	0.56
2:F:1462:ASN:HD22	2:F:1463:LEU:N	2.03	0.56
2:D:1133:LYS:O	2:D:1137:GLU:HG3	2.05	0.56
1:A:558:GLN:HB3	2:B:770:ASN:HD21	1.70	0.56
1:E:572:VAL:HG12	2:F:753:VAL:HG22	1.87	0.56
1:C:614:ALA:HB1	1:C:632:THR:HA	1.86	0.56
2:B:925:LEU:HD11	2:B:1320:LEU:HD22	1.87	0.56
3:L:364:ASP:O	3:L:409:VAL:HG23	2.06	0.56
2:F:836:GLN:HG2	2:F:897:HIS:HE1	1.70	0.56
3:K:253:SER:HB2	3:K:326:SER:O	2.05	0.56
3:I:353:ASN:HB2	3:I:394:ARG:NH1	2.20	0.56
2:H:925:LEU:HD11	2:H:1320:LEU:HD22	1.88	0.56
2:F:923:ARG:NH2	2:F:940:ILE:HG12	2.19	0.56
2:B:1180:LEU:HD23	2:B:1221:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1055:TRP:CZ2	2:B:1108:ILE:HA	2.40	0.56
1:G:477:ARG:HH11	1:G:477:ARG:CG	2.16	0.56
1:C:441:THR:HG21	1:E:441:THR:HG21	1.88	0.56
3:I:253:SER:HB2	3:I:326:SER:O	2.05	0.56
1:E:116:ILE:HD11	1:E:203:LYS:HB3	1.88	0.56
2:B:1535:ASP:O	2:B:1536:PHE:HB3	2.05	0.56
2:H:836:GLN:HG2	2:H:897:HIS:HE1	1.70	0.56
3:J:438:ASP:OD2	4:Q:28:VAL:HG13	2.05	0.56
1:A:10:ASN:HB2	1:A:621:GLY:C	2.25	0.56
2:D:1180:LEU:HD23	2:D:1221:LEU:HD11	1.88	0.56
3:J:253:SER:HB2	3:J:326:SER:O	2.06	0.56
3:L:381:ARG:CG	3:L:381:ARG:NH2	2.68	0.56
2:F:1337:ASN:O	2:F:1338:LYS:CB	2.53	0.56
2:D:1279:PRO:HG2	2:D:1306:GLU:HB3	1.88	0.56
2:D:923:ARG:HH22	2:D:940:ILE:HG12	1.70	0.56
3:I:364:ASP:O	3:I:409:VAL:HG23	2.06	0.56
4:N:6:THR:H	4:N:9:GLU:CB	2.16	0.56
2:H:964:PRO:HG3	2:H:1270:LEU:HD11	1.88	0.56
3:L:513:LYS:HZ2	3:L:524:GLU:HG2	1.71	0.56
2:D:1291:TRP:O	2:D:1292:GLU:C	2.45	0.56
2:H:809:ILE:HD11	2:H:892:ALA:HB3	1.87	0.56
3:L:353:ASN:HB2	3:L:394:ARG:NH1	2.20	0.56
2:F:1143:LEU:HB3	2:F:1144:PRO:HD3	1.86	0.56
3:J:364:ASP:O	3:J:409:VAL:HG23	2.06	0.56
4:P:6:THR:H	4:P:9:GLU:CB	2.16	0.56
1:A:477:ARG:HH11	1:A:477:ARG:CG	2.16	0.56
2:F:1012:TRP:HB3	2:F:1017:LEU:HD23	1.88	0.56
2:F:1566:ILE:O	2:F:1569:ARG:HG3	2.06	0.55
2:B:966:ALA:O	2:B:967:GLN:CB	2.54	0.55
3:I:461:LYS:HG2	4:M:28:VAL:CG1	2.36	0.55
3:K:267:CYS:HB2	3:K:433:MET:HE1	1.87	0.55
2:D:1291:TRP:CD1	2:D:1292:GLU:N	2.75	0.55
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.88	0.55
2:F:804:MET:HG2	2:F:805:GLN:H	1.72	0.55
2:F:925:LEU:HD11	2:F:1320:LEU:HD22	1.88	0.55
2:D:1516:GLU:HB3	2:D:1517:PRO:HD2	1.88	0.55
2:B:1338:LYS:HA	2:B:1371:ARG:HB2	1.88	0.55
2:F:1516:GLU:HB3	2:F:1517:PRO:HD2	1.88	0.55
1:G:143:VAL:C	1:G:144:ASN:HD22	2.10	0.55
2:B:1563:ILE:HB	2:B:1599:ILE:HD13	1.88	0.55
1:A:569:ALA:HB2	2:B:788:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1640:PRO:O	2:F:1641:ASN:HB2	2.07	0.55
2:H:839:LYS:HE2	4:N:60:PHE:CD1	2.41	0.55
1:C:477:ARG:CG	1:C:477:ARG:HH11	2.16	0.55
2:F:738:ASN:ND2	4:P:45:LYS:HE2	2.19	0.55
1:A:143:VAL:C	1:A:144:ASN:HD22	2.09	0.55
1:C:465:ILE:HD11	1:C:515:LEU:HD22	1.89	0.55
2:H:1525:THR:HG22	2:H:1543:ILE:HA	1.88	0.55
2:B:804:MET:HG2	2:B:805:GLN:H	1.71	0.55
2:H:1563:ILE:HB	2:H:1599:ILE:HD13	1.89	0.55
1:G:116:ILE:HD11	1:G:203:LYS:HB3	1.88	0.55
2:B:1566:ILE:O	2:B:1569:ARG:HG3	2.07	0.55
2:F:740:VAL:O	4:P:42:ARG:HD3	2.06	0.55
3:K:353:ASN:HB2	3:K:394:ARG:NH1	2.21	0.55
2:H:1338:LYS:CA	2:H:1371:ARG:HB2	2.36	0.55
2:F:1498:ILE:HD12	2:F:1498:ILE:N	2.21	0.55
2:D:836:GLN:HG2	2:D:897:HIS:HE1	1.70	0.55
1:C:350:LEU:HD21	1:C:400:ILE:HG21	1.88	0.55
1:E:143:VAL:C	1:E:144:ASN:HD22	2.10	0.55
1:E:13:ARG:HH22	1:E:476:GLY:HA3	1.71	0.55
2:D:1012:TRP:HB3	2:D:1017:LEU:HD23	1.88	0.55
2:B:1291:TRP:CD1	2:B:1292:GLU:N	2.75	0.55
2:F:1525:THR:HG22	2:F:1543:ILE:HA	1.88	0.55
2:F:776:SER:HB2	2:F:780:TRP:CZ2	2.42	0.55
1:C:252:GLY:HA2	1:C:262:LEU:HG	1.89	0.55
2:H:1498:ILE:CD1	2:H:1605:TRP:HA	2.35	0.55
2:B:877:VAL:H	2:B:1451:GLN:NE2	2.03	0.55
2:B:1012:TRP:HB3	2:B:1017:LEU:HD23	1.88	0.55
1:G:252:GLY:HA2	1:G:262:LEU:HG	1.89	0.55
2:F:896:HIS:HB3	4:M:61:LYS:HD3	1.88	0.55
1:G:473:MET:CE	1:G:603:ILE:HD11	2.37	0.55
1:G:386:LYS:HD3	1:G:440:ARG:HG2	1.87	0.55
2:B:1417:SER:HB2	4:Q:14:LYS:HZ3	1.71	0.55
2:H:1516:GLU:HB3	2:H:1517:PRO:HD2	1.88	0.55
1:G:465:ILE:HD11	1:G:515:LEU:HD22	1.89	0.55
2:F:1268:GLN:O	2:F:1269:GLU:CG	2.55	0.55
2:F:1291:TRP:O	2:F:1292:GLU:C	2.44	0.55
2:D:1338:LYS:HA	2:D:1371:ARG:HB2	1.89	0.55
2:F:1084:TRP:CD1	2:F:1088:GLU:HG3	2.42	0.55
1:A:116:ILE:HD11	1:A:203:LYS:HB3	1.88	0.55
2:F:1338:LYS:CA	2:F:1371:ARG:HB2	2.37	0.55
1:C:116:ILE:HD11	1:C:203:LYS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1641:ASN:HD21	3:J:366:LEU:HB3	1.72	0.55
3:J:353:ASN:HB2	3:J:394:ARG:NH1	2.21	0.55
1:G:508:ARG:NH1	1:G:604:GLY:HA3	2.22	0.54
2:F:1279:PRO:HG2	2:F:1306:GLU:HB3	1.88	0.54
2:D:776:SER:HB2	2:D:780:TRP:CZ2	2.42	0.54
2:F:1180:LEU:HD23	2:F:1221:LEU:HD11	1.88	0.54
1:E:10:ASN:HA	1:E:623:THR:HG23	1.89	0.54
3:L:461:LYS:HG2	4:N:28:VAL:CG1	2.37	0.54
2:H:1279:PRO:HG2	2:H:1306:GLU:HB3	1.88	0.54
2:D:1525:THR:HG22	2:D:1543:ILE:HA	1.89	0.54
2:H:744:GLU:C	2:H:746:PRO:HD3	2.28	0.54
2:H:1291:TRP:O	2:H:1292:GLU:C	2.45	0.54
2:B:776:SER:HB2	2:B:780:TRP:CZ2	2.42	0.54
1:C:143:VAL:C	1:C:144:ASN:HD22	2.10	0.54
2:H:1445:PHE:CE2	4:N:7:SER:HA	2.43	0.54
1:E:478:LEU:HD21	1:E:622:LEU:HD21	1.88	0.54
2:B:1291:TRP:O	2:B:1292:GLU:C	2.45	0.54
3:J:368:ASN:ND2	3:J:368:ASN:H	2.06	0.54
2:H:1289:ILE:HD13	2:H:1298:ARG:HE	1.73	0.54
1:E:252:GLY:HA2	1:E:262:LEU:HG	1.89	0.54
1:A:465:ILE:HD11	1:A:515:LEU:HD22	1.89	0.54
3:L:535:ASN:O	3:L:547:PHE:HB3	2.07	0.54
3:I:535:ASN:O	3:I:547:PHE:HB3	2.07	0.54
3:K:535:ASN:O	3:K:547:PHE:HB3	2.07	0.54
2:H:804:MET:HG2	2:H:805:GLN:H	1.72	0.54
2:D:804:MET:HG2	2:D:805:GLN:H	1.71	0.54
2:D:1566:ILE:O	2:D:1569:ARG:HG3	2.07	0.54
2:H:1268:GLN:CG	2:H:1269:GLU:N	2.70	0.54
1:E:555:PRO:HB3	2:F:775:ASP:HA	1.90	0.54
2:D:966:ALA:O	2:D:967:GLN:CB	2.54	0.54
1:E:396:LYS:HG3	1:E:397:PRO:HD2	1.90	0.54
2:B:1084:TRP:CD1	2:B:1088:GLU:HG3	2.42	0.54
3:L:478:ARG:NE	3:L:481:LYS:HD2	2.23	0.54
3:K:631:CYS:SG	3:K:714:ARG:HD2	2.48	0.54
2:D:837:GLU:HG2	4:P:64:SER:OG	2.07	0.54
2:D:1563:ILE:HB	2:D:1599:ILE:HD13	1.88	0.54
1:G:534:LYS:HD2	1:G:535:ASP:H	1.72	0.54
2:F:1289:ILE:HD13	2:F:1298:ARG:HE	1.73	0.54
2:B:1525:THR:HG22	2:B:1543:ILE:HA	1.89	0.54
1:A:269:ILE:HD13	1:A:278:VAL:HB	1.90	0.54
3:J:631:CYS:SG	3:J:714:ARG:HD2	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:478:ARG:NE	3:K:481:LYS:HD2	2.23	0.54
1:E:481:ALA:N	5:E:1646:NDG:H8C3	2.23	0.54
1:G:396:LYS:HG3	1:G:397:PRO:HD2	1.90	0.54
2:F:1563:ILE:HB	2:F:1599:ILE:HD13	1.89	0.54
3:K:381:ARG:CG	3:K:381:ARG:NH2	2.68	0.53
2:B:819:ARG:NH1	2:B:819:ARG:HG2	2.19	0.53
3:L:436:LEU:HB3	3:L:440:PHE:HE2	1.73	0.53
2:B:1582:MET:HA	2:B:1605:TRP:O	2.08	0.53
2:D:1084:TRP:CD1	2:D:1088:GLU:HG3	2.41	0.53
2:B:923:ARG:NH2	2:B:940:ILE:HG12	2.23	0.53
2:F:804:MET:HG2	2:F:805:GLN:N	2.23	0.53
1:A:13:ARG:HH22	1:A:476:GLY:HA3	1.73	0.53
1:C:505:PRO:HG3	1:C:595:TRP:CE3	2.42	0.53
1:E:568:GLY:HA2	2:F:757:LYS:HE2	1.89	0.53
1:C:436:LEU:HD11	1:C:511:ALA:HB3	1.90	0.53
2:B:1279:PRO:HG2	2:B:1306:GLU:HB3	1.88	0.53
2:D:997:THR:N	2:D:998:PRO:HD2	2.24	0.53
1:G:451:VAL:HB	1:G:495:LEU:HB3	1.91	0.53
2:D:804:MET:HG2	2:D:805:GLN:N	2.23	0.53
1:A:472:ILE:HD13	1:A:509:LEU:HD23	1.90	0.53
3:J:535:ASN:O	3:J:547:PHE:HB3	2.07	0.53
3:K:435:ASN:ND2	3:K:460:ARG:HH21	2.06	0.53
2:F:744:GLU:C	2:F:746:PRO:HD3	2.29	0.53
3:L:631:CYS:SG	3:L:714:ARG:HD2	2.48	0.53
2:F:940:ILE:HD12	2:F:1308:PHE:CE1	2.44	0.53
1:A:436:LEU:HD11	1:A:511:ALA:HB3	1.90	0.53
1:A:252:GLY:HA2	1:A:262:LEU:HG	1.89	0.53
1:E:465:ILE:HD11	1:E:515:LEU:HD22	1.89	0.53
3:J:478:ARG:NE	3:J:481:LYS:HD2	2.23	0.53
2:D:1289:ILE:HD13	2:D:1298:ARG:HE	1.74	0.53
1:G:269:ILE:HD13	1:G:278:VAL:HB	1.90	0.53
1:E:219:LYS:NZ	1:E:356:ASN:HD22	2.07	0.53
2:D:1582:MET:HA	2:D:1605:TRP:O	2.08	0.53
2:D:967:GLN:O	2:D:968:MET:HB2	2.08	0.53
2:H:940:ILE:HD12	2:H:1308:PHE:CE1	2.43	0.53
2:D:923:ARG:NH2	2:D:940:ILE:HG12	2.23	0.53
2:B:997:THR:N	2:B:998:PRO:HD2	2.24	0.53
1:A:451:VAL:HB	1:A:495:LEU:HB3	1.91	0.53
1:C:269:ILE:HD13	1:C:278:VAL:HB	1.90	0.53
1:E:477:ARG:HG2	1:E:477:ARG:NH1	2.21	0.53
3:I:478:ARG:NE	3:I:481:LYS:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1521:TYR:HB2	2:H:1523:TYR:CE2	2.44	0.53
2:B:804:MET:HG2	2:B:805:GLN:N	2.23	0.53
3:K:456:VAL:HG13	3:K:467:LYS:HA	1.91	0.53
4:M:6:THR:H	4:M:9:GLU:CB	2.16	0.53
1:A:506:SER:CB	1:A:530:TRP:HE1	2.21	0.53
2:F:937:LYS:HD2	2:F:937:LYS:O	2.09	0.53
3:L:438:ASP:OD2	4:N:28:VAL:HG13	2.09	0.53
2:H:776:SER:HB2	2:H:780:TRP:CZ2	2.42	0.53
3:J:456:VAL:HG13	3:J:467:LYS:HA	1.91	0.53
3:I:456:VAL:HG13	3:I:467:LYS:HA	1.91	0.53
2:F:1387:THR:CG2	2:F:1451:GLN:H	2.21	0.53
2:D:877:VAL:H	2:D:1451:GLN:NE2	2.07	0.53
3:K:436:LEU:HB3	3:K:440:PHE:HE2	1.73	0.53
3:J:436:LEU:HB3	3:J:440:PHE:HE2	1.73	0.53
2:F:973:VAL:HG12	2:F:975:ALA:H	1.73	0.53
2:D:1470:PHE:CB	2:D:1478:GLY:HA3	2.39	0.53
2:F:997:THR:N	2:F:998:PRO:HD2	2.24	0.53
2:F:822:GLN:OE1	2:F:1479:LYS:HA	2.09	0.53
2:D:865:THR:OG1	4:P:11:GLN:HG2	2.08	0.53
1:E:505:PRO:HG3	1:E:595:TRP:CE3	2.44	0.53
3:I:631:CYS:SG	3:I:714:ARG:HD2	2.48	0.53
2:H:740:VAL:O	4:Q:42:ARG:HD3	2.09	0.52
1:C:439:LEU:HD12	1:C:439:LEU:H	1.74	0.52
1:G:569:ALA:HB2	2:H:788:SER:HB2	1.90	0.52
1:E:590:THR:HG22	1:E:592:SER:H	1.75	0.52
2:B:1289:ILE:HD13	2:B:1298:ARG:HE	1.73	0.52
3:K:654:ARG:HA	3:K:722:GLN:HG3	1.91	0.52
2:B:962:GLY:C	2:B:964:PRO:HD3	2.29	0.52
3:K:438:ASP:OD2	4:P:28:VAL:HG13	2.09	0.52
2:F:978:LEU:HG	2:F:1240:TYR:HB3	1.91	0.52
1:G:472:ILE:HD13	1:G:509:LEU:HD23	1.90	0.52
1:G:342:PHE:CE1	1:G:391:THR:HG21	2.45	0.52
3:L:368:ASN:ND2	3:L:368:ASN:H	2.08	0.52
2:D:1196:ASN:HD22	2:D:1196:ASN:N	2.07	0.52
1:C:19:THR:HB	1:C:478:LEU:HB2	1.91	0.52
3:K:461:LYS:HD2	4:P:29:ASN:OD1	2.10	0.52
1:E:439:LEU:H	1:E:439:LEU:HD12	1.74	0.52
2:D:1387:THR:CG2	2:D:1451:GLN:H	2.22	0.52
2:B:1387:THR:CG2	2:B:1451:GLN:H	2.22	0.52
1:G:527:ASP:CA	1:G:616:VAL:HG11	2.40	0.52
2:B:1446:ASN:CB	4:Q:4:LEU:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1470:PHE:CB	2:B:1478:GLY:HA3	2.39	0.52
2:H:804:MET:HG2	2:H:805:GLN:N	2.23	0.52
1:C:569:ALA:HB2	2:D:788:SER:HB2	1.89	0.52
1:C:396:LYS:HG3	1:C:397:PRO:HD2	1.90	0.52
3:K:598:LEU:HA	3:K:603:ILE:HD13	1.91	0.52
3:J:654:ARG:HA	3:J:722:GLN:HG3	1.91	0.52
2:B:978:LEU:HG	2:B:1240:TYR:HB3	1.91	0.52
2:B:973:VAL:HG12	2:B:975:ALA:H	1.73	0.52
1:E:451:VAL:HB	1:E:495:LEU:HB3	1.91	0.52
2:D:1360:ASN:O	2:D:1361:THR:C	2.48	0.52
2:F:932:ARG:HH11	3:L:339:SER:HB2	1.73	0.52
3:I:461:LYS:HD2	4:M:29:ASN:OD1	2.09	0.52
2:D:973:VAL:HG12	2:D:975:ALA:H	1.73	0.52
2:B:1344:THR:HG21	2:B:1346:LYS:HE2	1.92	0.52
1:G:339:PRO:HB3	1:G:608:GLY:O	2.09	0.52
2:D:1521:TYR:HB2	2:D:1523:TYR:CE2	2.44	0.52
3:K:531:HIS:CD2	3:K:533:ASN:H	2.27	0.52
2:H:1578:LYS:HD3	2:H:1608:HIS:HE1	1.74	0.52
1:G:436:LEU:HD11	1:G:511:ALA:HB3	1.90	0.52
1:C:451:VAL:HB	1:C:495:LEU:HB3	1.91	0.52
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.75	0.52
1:A:344:PRO:HD2	1:A:433:TYR:CE1	2.44	0.52
3:J:598:LEU:HA	3:J:603:ILE:HD13	1.91	0.52
1:E:434:LEU:HB2	1:E:513:TYR:HE2	1.75	0.52
10:H:2643:NAG:H82	10:H:2643:NAG:O3	2.10	0.52
3:I:513:LYS:HZ2	3:I:524:GLU:HG2	1.75	0.52
2:F:1521:TYR:HB2	2:F:1523:TYR:CE2	2.44	0.52
3:L:256:ILE:HD12	3:L:405:VAL:HG23	1.92	0.52
3:I:313:GLN:O	3:I:317:ILE:HG13	2.10	0.52
1:C:434:LEU:HB2	1:C:513:TYR:HE2	1.75	0.52
3:I:531:HIS:CD2	3:I:533:ASN:H	2.27	0.52
1:E:472:ILE:HD13	1:E:509:LEU:HD23	1.90	0.52
2:H:1470:PHE:HB2	2:H:1478:GLY:HA3	1.92	0.52
2:F:1196:ASN:N	2:F:1196:ASN:HD22	2.07	0.52
3:I:654:ARG:HA	3:I:722:GLN:HG3	1.91	0.52
3:I:292:TYR:HD1	3:I:325:LYS:HD3	1.74	0.52
1:C:472:ILE:HD13	1:C:509:LEU:HD23	1.90	0.52
3:L:292:TYR:HD1	3:L:325:LYS:HD3	1.74	0.52
1:A:214:VAL:HG23	1:A:321:ARG:HB2	1.92	0.52
3:I:368:ASN:H	3:I:368:ASN:ND2	2.08	0.52
3:J:531:HIS:CD2	3:J:533:ASN:H	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:381:ARG:CG	3:J:381:ARG:NH2	2.68	0.52
1:G:506:SER:CB	1:G:530:TRP:HE1	2.21	0.52
2:H:1387:THR:CG2	2:H:1451:GLN:H	2.21	0.52
2:H:1359:LYS:HD2	4:N:4:LEU:CD1	2.40	0.52
2:D:978:LEU:HG	2:D:1240:TYR:HB3	1.91	0.52
2:H:1641:ASN:O	3:J:368:ASN:ND2	2.43	0.52
2:B:1521:TYR:HB2	2:B:1523:TYR:CE2	2.44	0.52
1:G:214:VAL:HG23	1:G:321:ARG:HB2	1.92	0.52
2:F:1470:PHE:HB2	2:F:1478:GLY:HA3	1.92	0.52
3:J:239:ASP:HB3	3:J:448:GLN:HB2	1.92	0.52
3:J:256:ILE:HD12	3:J:405:VAL:HG23	1.92	0.52
3:L:598:LEU:HA	3:L:603:ILE:HD13	1.91	0.52
1:A:404:THR:HG23	1:A:414:GLN:HB3	1.92	0.52
1:G:424:TYR:O	1:G:433:TYR:CE1	2.59	0.52
3:L:654:ARG:HA	3:L:722:GLN:HG3	1.91	0.52
3:I:436:LEU:HB3	3:I:440:PHE:HE2	1.73	0.52
4:P:30:GLU:HA	4:P:44:ILE:HD13	1.92	0.52
1:E:269:ILE:HD13	1:E:278:VAL:HB	1.90	0.52
1:A:396:LYS:HG3	1:A:397:PRO:HD2	1.90	0.52
1:E:436:LEU:HD11	1:E:511:ALA:HB3	1.90	0.52
3:L:239:ASP:HB3	3:L:448:GLN:HB2	1.92	0.51
2:F:1228:PRO:HB2	2:F:1229:PRO:HD3	1.92	0.51
2:B:1196:ASN:N	2:B:1196:ASN:HD22	2.07	0.51
2:H:860:HIS:CE1	2:H:862:GLN:HE22	2.29	0.51
3:K:368:ASN:H	3:K:368:ASN:ND2	2.07	0.51
3:L:531:HIS:CD2	3:L:533:ASN:H	2.27	0.51
2:B:1360:ASN:O	2:B:1361:THR:C	2.48	0.51
3:K:313:GLN:O	3:K:317:ILE:HG13	2.10	0.51
4:N:30:GLU:HA	4:N:44:ILE:HD13	1.92	0.51
1:A:439:LEU:HD12	1:A:439:LEU:H	1.74	0.51
1:C:126:ARG:HG2	1:C:168:PRO:HA	1.93	0.51
1:E:214:VAL:HG23	1:E:321:ARG:HB2	1.92	0.51
1:E:410:SER:O	1:E:414:GLN:HG2	2.11	0.51
3:I:598:LEU:HA	3:I:603:ILE:HD13	1.91	0.51
2:D:1228:PRO:HB2	2:D:1229:PRO:HD3	1.92	0.51
3:J:292:TYR:HD1	3:J:325:LYS:HD3	1.74	0.51
2:D:972:ALA:HB1	2:D:1005:TYR:OH	2.10	0.51
2:F:754:GLU:HG3	2:F:769:MET:SD	2.51	0.51
1:A:590:THR:HG22	1:A:592:SER:H	1.75	0.51
2:D:1344:THR:HG21	2:D:1346:LYS:HE2	1.92	0.51
3:L:313:GLN:O	3:L:317:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:70:LEU:HG	4:M:74:TYR:CE2	2.46	0.51
1:C:568:GLY:HA2	2:D:757:LYS:HE2	1.93	0.51
2:F:1578:LYS:HD3	2:F:1608:HIS:HE1	1.74	0.51
2:D:1381:LEU:HD23	2:D:1457:VAL:HG12	1.92	0.51
2:F:972:ALA:HB1	2:F:1005:TYR:OH	2.09	0.51
3:K:256:ILE:HD12	3:K:405:VAL:HG23	1.92	0.51
1:C:478:LEU:HD21	1:C:622:LEU:HD21	1.91	0.51
3:J:461:LYS:HD2	4:Q:29:ASN:OD1	2.10	0.51
2:D:754:GLU:HG3	2:D:769:MET:SD	2.51	0.51
3:K:292:TYR:HD1	3:K:325:LYS:HD3	1.74	0.51
2:B:972:ALA:HB1	2:B:1005:TYR:OH	2.10	0.51
1:G:36:THR:HG23	1:G:48:SER:HA	1.93	0.51
1:E:506:SER:CB	1:E:530:TRP:HE1	2.21	0.51
1:E:19:THR:HB	1:E:478:LEU:HB2	1.93	0.51
2:B:1126:LEU:HD23	2:B:1173:ALA:HB1	1.93	0.51
3:L:235:LYS:O	3:L:236:ILE:HB	2.11	0.51
3:L:456:VAL:HG13	3:L:467:LYS:HA	1.91	0.51
2:B:754:GLU:HG3	2:B:769:MET:SD	2.51	0.51
1:G:590:THR:HG22	1:G:592:SER:H	1.74	0.51
1:A:640:CYS:HB3	1:A:641:PRO:HD2	1.93	0.51
2:D:1233:TRP:O	2:D:1237:GLN:HG2	2.11	0.51
2:B:1381:LEU:HD23	2:B:1457:VAL:HG12	1.92	0.51
2:H:937:LYS:HD2	2:H:937:LYS:O	2.10	0.51
1:G:439:LEU:HD12	1:G:439:LEU:H	1.74	0.51
1:A:36:THR:HG23	1:A:48:SER:HA	1.93	0.51
1:A:410:SER:O	1:A:414:GLN:HG2	2.11	0.51
1:G:404:THR:HG23	1:G:414:GLN:HB3	1.92	0.51
2:D:1126:LEU:HD23	2:D:1173:ALA:HB1	1.93	0.51
2:B:860:HIS:CE1	2:B:862:GLN:HE22	2.29	0.51
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.91	0.51
2:D:1480:LEU:HB3	2:D:1493:GLU:OE2	2.10	0.51
1:C:214:VAL:HG23	1:C:321:ARG:HB2	1.93	0.51
1:G:640:CYS:HB3	1:G:641:PRO:HD2	1.93	0.51
2:D:819:ARG:HG2	2:D:819:ARG:NH1	2.19	0.51
4:Q:70:LEU:HG	4:Q:74:TYR:CE2	2.46	0.51
4:Q:30:GLU:HA	4:Q:44:ILE:HD13	1.92	0.51
1:G:126:ARG:HG2	1:G:168:PRO:HA	1.93	0.51
1:C:590:THR:HG22	1:C:592:SER:H	1.75	0.51
2:B:839:LYS:HE2	4:Q:60:PHE:CD1	2.46	0.51
3:I:381:ARG:CG	3:I:381:ARG:NH2	2.68	0.51
3:L:339:SER:HA	3:L:342:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:738:ASN:ND2	4:Q:45:LYS:HE2	2.22	0.51
2:F:966:ALA:O	2:F:967:GLN:CB	2.57	0.51
3:I:334:LEU:HB3	3:I:376:VAL:HG11	1.93	0.51
2:F:1126:LEU:HD23	2:F:1173:ALA:HB1	1.93	0.51
2:D:772:PHE:CD1	4:M:37:ASN:ND2	2.78	0.51
1:C:640:CYS:HB3	1:C:641:PRO:HD2	1.93	0.51
2:H:754:GLU:HG3	2:H:769:MET:SD	2.51	0.51
1:G:434:LEU:HB2	1:G:513:TYR:HE2	1.75	0.51
3:L:724:LEU:HB3	3:L:725:PRO:HD3	1.92	0.51
2:B:1578:LYS:HD3	2:B:1608:HIS:HE1	1.75	0.51
2:F:1233:TRP:O	2:F:1237:GLN:HG2	2.11	0.51
2:F:860:HIS:CE1	2:F:862:GLN:HE22	2.29	0.51
1:E:36:THR:HG23	1:E:48:SER:HA	1.93	0.50
3:J:563:TYR:CZ	3:J:569:PRO:HG3	2.47	0.50
4:P:70:LEU:HG	4:P:74:TYR:CE2	2.46	0.50
3:K:724:LEU:HB3	3:K:725:PRO:HD3	1.92	0.50
3:I:256:ILE:HD12	3:I:405:VAL:HG23	1.92	0.50
1:C:36:THR:HG23	1:C:48:SER:HA	1.93	0.50
1:E:404:THR:HG23	1:E:414:GLN:HB3	1.92	0.50
3:L:334:LEU:HB3	3:L:376:VAL:HG11	1.93	0.50
1:E:640:CYS:HB3	1:E:641:PRO:HD2	1.93	0.50
2:D:1593:LYS:HG2	2:D:1596:LEU:HD11	1.94	0.50
2:H:1381:LEU:HD23	2:H:1457:VAL:HG12	1.93	0.50
2:F:882:LYS:HG3	2:F:886:GLN:NE2	2.27	0.50
3:I:724:LEU:HB3	3:I:725:PRO:HD3	1.92	0.50
1:C:410:SER:O	1:C:414:GLN:HG2	2.11	0.50
3:L:439:VAL:HG22	4:N:31:LEU:HD21	1.91	0.50
2:F:1344:THR:HG21	2:F:1346:LYS:HE2	1.93	0.50
2:B:1233:TRP:O	2:B:1237:GLN:HG2	2.11	0.50
3:J:313:GLN:O	3:J:317:ILE:HG13	2.10	0.50
2:B:772:PHE:HD1	4:N:37:ASN:ND2	2.10	0.50
3:K:239:ASP:HB3	3:K:448:GLN:HB2	1.92	0.50
1:G:554:VAL:HG13	1:G:555:PRO:HD2	1.94	0.50
3:L:641:TYR:HE2	3:L:650:VAL:HB	1.77	0.50
3:L:278:TYR:HA	3:L:455:MET:HE1	1.92	0.50
3:J:334:LEU:HB3	3:J:376:VAL:HG11	1.93	0.50
3:L:465:TYR:CD1	3:L:517:GLY:HA2	2.46	0.50
3:I:239:ASP:HB3	3:I:448:GLN:HB2	1.92	0.50
2:B:1569:ARG:CG	2:B:1569:ARG:HH11	2.25	0.50
2:F:819:ARG:HH11	2:F:819:ARG:CG	2.22	0.50
1:C:404:THR:HG23	1:C:414:GLN:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:410:SER:O	1:G:414:GLN:HG2	2.11	0.50
3:I:641:TYR:HE2	3:I:650:VAL:HB	1.77	0.50
2:B:964:PRO:HG3	2:B:1270:LEU:HD11	1.92	0.50
3:I:563:TYR:CZ	3:I:569:PRO:HG3	2.46	0.50
2:B:940:ILE:HD12	2:B:1308:PHE:CE1	2.47	0.50
2:D:1578:LYS:HD3	2:D:1608:HIS:HE1	1.75	0.50
2:H:882:LYS:HG3	2:H:886:GLN:NE2	2.27	0.50
2:D:860:HIS:CE1	2:D:862:GLN:HE22	2.29	0.50
3:J:724:LEU:HB3	3:J:725:PRO:HD3	1.92	0.50
1:G:369:VAL:HG12	1:G:370:GLN:H	1.77	0.50
3:J:235:LYS:O	3:J:236:ILE:HB	2.11	0.50
3:K:641:TYR:HE2	3:K:650:VAL:HB	1.77	0.50
3:L:513:LYS:NZ	3:L:524:GLU:HG2	2.27	0.50
3:J:465:TYR:CD1	3:J:517:GLY:HA2	2.46	0.50
2:B:1593:LYS:HG2	2:B:1596:LEU:HD11	1.94	0.50
2:B:882:LYS:HG3	2:B:886:GLN:NE2	2.27	0.50
4:M:30:GLU:HA	4:M:44:ILE:HD13	1.92	0.50
3:J:339:SER:HA	3:J:342:SER:HB3	1.93	0.50
2:F:964:PRO:HG3	2:F:1270:LEU:HD11	1.93	0.50
1:E:126:ARG:HG2	1:E:168:PRO:HA	1.93	0.50
1:E:268:ARG:HD3	2:F:1378:MET:SD	2.51	0.50
1:A:126:ARG:HG2	1:A:168:PRO:HA	1.93	0.50
3:K:339:SER:HA	3:K:342:SER:HB3	1.93	0.50
2:H:1617:ASP:O	2:H:1621:GLN:HG3	2.12	0.50
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.94	0.50
2:H:962:GLY:C	2:H:964:PRO:HD3	2.31	0.50
3:J:478:ARG:CG	3:J:479:PRO:HD2	2.42	0.50
2:H:839:LYS:HE2	4:N:60:PHE:CE1	2.47	0.50
2:F:1617:ASP:O	2:F:1621:GLN:HG3	2.12	0.50
2:H:907:LEU:HD23	2:H:907:LEU:H	1.77	0.50
3:I:339:SER:HA	3:I:342:SER:HB3	1.93	0.50
2:F:855:THR:HB	2:F:1602:LYS:HZ3	1.76	0.50
2:D:907:LEU:H	2:D:907:LEU:HD23	1.77	0.50
2:F:1268:GLN:O	2:F:1269:GLU:CB	2.59	0.50
1:C:10:ASN:HA	1:C:623:THR:HG23	1.93	0.50
3:K:334:LEU:HB3	3:K:376:VAL:HG11	1.93	0.50
1:E:222:TYR:HB3	1:E:225:ASN:HB2	1.94	0.50
1:C:222:TYR:HB3	1:C:225:ASN:HB2	1.94	0.50
3:K:563:TYR:CZ	3:K:569:PRO:HG3	2.47	0.50
3:L:431:LYS:HG3	4:N:27:ASN:ND2	2.27	0.50
2:H:1488:LEU:HG	2:H:1590:TRP:CH2	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:641:TYR:HE2	3:J:650:VAL:HB	1.77	0.49
3:J:267:CYS:HB2	3:J:433:MET:HE1	1.94	0.49
1:A:568:GLY:HA2	2:B:757:LYS:HE2	1.94	0.49
2:B:1617:ASP:O	2:B:1621:GLN:HG3	2.12	0.49
1:A:103:LEU:HB3	1:A:193:GLN:HE21	1.77	0.49
2:D:733:ILE:HG12	2:D:734:ILE:N	2.26	0.49
3:K:465:TYR:CD1	3:K:517:GLY:HA2	2.46	0.49
1:A:426:THR:HG21	1:A:432:ASN:H	1.77	0.49
3:I:465:TYR:CD1	3:I:517:GLY:HA2	2.46	0.49
2:F:1593:LYS:HG2	2:F:1596:LEU:HD11	1.94	0.49
2:D:841:ARG:HH11	2:D:841:ARG:CG	2.23	0.49
1:C:351:MET:SD	1:C:440:ARG:HD2	2.53	0.49
3:J:435:ASN:HD21	3:J:460:ARG:HH21	1.57	0.49
3:I:438:ASP:OD2	4:M:28:VAL:HG13	2.12	0.49
2:D:940:ILE:HD12	2:D:1308:PHE:CE1	2.47	0.49
1:G:572:VAL:CG2	2:H:785:VAL:HB	2.42	0.49
2:D:882:LYS:HG3	2:D:886:GLN:NE2	2.27	0.49
2:D:1617:ASP:O	2:D:1621:GLN:HG3	2.12	0.49
1:E:554:VAL:HG13	1:E:555:PRO:HD2	1.94	0.49
3:L:478:ARG:CG	3:L:479:PRO:HD2	2.42	0.49
4:N:70:LEU:HG	4:N:74:TYR:CE2	2.46	0.49
2:F:1495:ASN:O	2:F:1602:LYS:HA	2.13	0.49
3:I:328:THR:HB	3:I:367:HIS:HA	1.94	0.49
3:K:235:LYS:O	3:K:236:ILE:HB	2.11	0.49
2:B:1505:VAL:HG23	2:B:1505:VAL:O	2.12	0.49
2:D:1505:VAL:HG23	2:D:1505:VAL:O	2.12	0.49
2:F:1569:ARG:HH11	2:F:1569:ARG:CG	2.26	0.49
2:F:841:ARG:CG	2:F:841:ARG:HH11	2.23	0.49
2:H:733:ILE:HG12	2:H:734:ILE:N	2.26	0.49
3:J:513:LYS:NZ	3:J:524:GLU:HG2	2.27	0.49
1:G:439:LEU:HD12	1:G:439:LEU:N	2.28	0.49
2:H:1593:LYS:HG2	2:H:1596:LEU:HD11	1.94	0.49
3:L:328:THR:HB	3:L:367:HIS:HA	1.94	0.49
2:B:1239:TYR:OH	2:B:1246:SER:HB2	2.13	0.49
2:H:1344:THR:HG21	2:H:1346:LYS:HE2	1.93	0.49
2:H:1635:VAL:HG23	2:H:1636:VAL:H	1.78	0.49
3:L:563:TYR:CZ	3:L:569:PRO:HG3	2.47	0.49
2:D:1485:ARG:HD3	2:D:1536:PHE:HZ	1.78	0.49
3:K:328:THR:HB	3:K:367:HIS:HA	1.95	0.49
1:E:108:LEU:HB2	1:E:196:PHE:CD1	2.48	0.49
2:F:1381:LEU:HD23	2:F:1457:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:573:PRO:HB3	3:I:721:PHE:CZ	2.48	0.49
2:D:1569:ARG:CG	2:D:1569:ARG:HH11	2.24	0.49
3:L:268:LEU:O	3:L:272:ILE:HG13	2.13	0.49
1:C:554:VAL:HG13	1:C:555:PRO:HD2	1.94	0.49
1:G:369:VAL:HG12	1:G:370:GLN:N	2.28	0.49
2:F:907:LEU:HD23	2:F:907:LEU:H	1.77	0.49
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.48	0.49
1:A:222:TYR:HB3	1:A:225:ASN:HB2	1.94	0.49
3:I:235:LYS:O	3:I:236:ILE:HB	2.11	0.49
2:B:813:LEU:HD23	2:B:907:LEU:HB3	1.95	0.49
1:A:567:HIS:ND1	2:B:760:PRO:HG3	2.27	0.49
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.48	0.49
2:B:738:ASN:HD22	4:N:45:LYS:HE2	1.78	0.49
1:G:477:ARG:CG	1:G:477:ARG:NH1	2.76	0.48
1:A:477:ARG:NH1	1:A:477:ARG:CG	2.76	0.48
2:D:833:ARG:CG	2:D:833:ARG:NH1	2.76	0.48
3:J:268:LEU:O	3:J:272:ILE:HG13	2.13	0.48
2:H:813:LEU:HD23	2:H:907:LEU:HB3	1.95	0.48
2:D:813:LEU:HD23	2:D:907:LEU:HB3	1.95	0.48
2:B:907:LEU:HD23	2:B:907:LEU:H	1.77	0.48
3:L:573:PRO:HB3	3:L:721:PHE:CZ	2.48	0.48
3:L:372:ASP:O	3:L:375:THR:HG22	2.13	0.48
3:J:573:PRO:HB3	3:J:721:PHE:CZ	2.48	0.48
2:D:1417:SER:HB2	4:P:14:LYS:NZ	2.27	0.48
2:D:1239:TYR:OH	2:D:1246:SER:HB2	2.13	0.48
1:G:454:LEU:HA	1:G:491:ASP:O	2.13	0.48
2:H:1492:ALA:O	2:H:1494:GLU:N	2.46	0.48
1:C:477:ARG:CG	1:C:477:ARG:NH1	2.76	0.48
2:H:1446:ASN:HB2	4:N:4:LEU:HB2	1.94	0.48
3:K:513:LYS:NZ	3:K:524:GLU:HG2	2.27	0.48
3:L:620:VAL:HG12	3:L:667:PRO:HD2	1.95	0.48
3:K:372:ASP:O	3:K:375:THR:HG22	2.13	0.48
3:I:620:VAL:HG12	3:I:667:PRO:HD2	1.95	0.48
2:H:1499:GLN:HG2	2:H:1500:LYS:N	2.27	0.48
3:K:268:LEU:O	3:K:272:ILE:HG13	2.13	0.48
3:K:478:ARG:CG	3:K:479:PRO:HD2	2.42	0.48
2:H:1338:LYS:H	2:H:1371:ARG:HD2	1.78	0.48
3:I:513:LYS:NZ	3:I:524:GLU:HG2	2.27	0.48
3:I:372:ASP:O	3:I:375:THR:HG22	2.13	0.48
3:J:372:ASP:O	3:J:375:THR:HG22	2.13	0.48
2:F:1635:VAL:HG23	2:F:1636:VAL:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:328:THR:HB	3:J:367:HIS:HA	1.95	0.48
3:I:268:LEU:O	3:I:272:ILE:HG13	2.13	0.48
3:J:493:GLU:HG3	3:J:563:TYR:OH	2.14	0.48
5:E:1646:NDG:H6C1	5:E:1647:NAG:H83	1.94	0.48
1:A:439:LEU:HD12	1:A:439:LEU:N	2.28	0.48
3:J:620:VAL:HG12	3:J:667:PRO:HD2	1.95	0.48
1:C:108:LEU:HB2	1:C:196:PHE:CD1	2.48	0.48
3:I:270:ASN:N	3:I:270:ASN:HD22	2.12	0.48
2:H:1569:ARG:CG	2:H:1569:ARG:HH11	2.26	0.48
3:I:478:ARG:CG	3:I:479:PRO:HD2	2.42	0.48
2:F:1239:TYR:OH	2:F:1246:SER:HB2	2.13	0.48
2:D:744:GLU:C	2:D:746:PRO:HD3	2.34	0.48
2:F:1445:PHE:CE2	4:M:7:SER:HA	2.48	0.48
1:G:108:LEU:HB2	1:G:196:PHE:CD1	2.48	0.48
3:K:267:CYS:HB2	3:K:433:MET:CE	2.44	0.48
2:B:1485:ARG:HD3	2:B:1536:PHE:HZ	1.78	0.48
3:K:362:MET:HG2	3:K:403:PHE:HB2	1.95	0.48
3:J:270:ASN:N	3:J:270:ASN:HD22	2.11	0.48
4:N:11:GLN:NE2	4:N:11:GLN:H	2.11	0.48
3:L:493:GLU:HG3	3:L:563:TYR:OH	2.14	0.48
4:P:11:GLN:H	4:P:11:GLN:NE2	2.11	0.48
4:Q:11:GLN:NE2	4:Q:11:GLN:H	2.11	0.48
2:D:738:ASN:HD22	4:M:45:LYS:HE2	1.77	0.48
3:K:378:ASP:HA	3:K:381:ARG:HB2	1.96	0.48
1:C:506:SER:CB	1:C:530:TRP:HE1	2.21	0.48
1:G:222:TYR:HB3	1:G:225:ASN:HB2	1.94	0.48
3:I:493:GLU:HG3	3:I:563:TYR:OH	2.14	0.48
3:I:465:TYR:CE1	3:I:517:GLY:HA2	2.49	0.48
1:E:369:VAL:HG12	1:E:370:GLN:H	1.78	0.48
3:K:573:PRO:HB3	3:K:721:PHE:CZ	2.48	0.48
3:I:439:VAL:HG22	4:M:31:LEU:HD21	1.95	0.48
3:L:544:ILE:HD13	3:L:650:VAL:HG12	1.96	0.48
1:G:624:PHE:HB3	1:G:632:THR:HG23	1.96	0.48
2:D:1291:TRP:O	2:D:1294:ALA:N	2.47	0.48
2:D:1361:THR:HA	2:D:1441:VAL:O	2.14	0.48
3:J:465:TYR:CE1	3:J:517:GLY:HA2	2.49	0.48
3:K:465:TYR:CE1	3:K:517:GLY:HA2	2.49	0.48
3:L:328:THR:O	3:L:367:HIS:HB2	2.14	0.48
4:M:11:GLN:NE2	4:M:11:GLN:H	2.11	0.48
2:F:819:ARG:HG2	2:F:819:ARG:NH1	2.19	0.48
1:C:439:LEU:HD12	1:C:439:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:606:THR:HB	1:E:619:ASP:HB3	1.96	0.48
1:G:528:SER:N	1:G:616:VAL:HG13	2.29	0.48
3:K:493:GLU:HG3	3:K:563:TYR:OH	2.14	0.48
1:A:624:PHE:HB3	1:A:632:THR:HG23	1.96	0.48
2:B:865:THR:OG1	4:Q:11:GLN:HG2	2.14	0.48
2:H:932:ARG:O	2:H:934:GLY:N	2.47	0.48
2:F:733:ILE:HG12	2:F:734:ILE:N	2.26	0.47
1:G:35:VAL:HG21	1:G:64:VAL:HG21	1.96	0.47
3:J:539:LYS:HD2	3:J:539:LYS:N	2.30	0.47
1:E:439:LEU:HD12	1:E:439:LEU:N	2.28	0.47
2:D:964:PRO:HB3	2:D:1270:LEU:HD11	1.95	0.47
3:J:267:CYS:HB2	3:J:433:MET:CE	2.44	0.47
3:K:328:THR:O	3:K:367:HIS:HB2	2.14	0.47
2:B:1361:THR:HA	2:B:1441:VAL:O	2.14	0.47
3:L:465:TYR:CE1	3:L:517:GLY:HA2	2.49	0.47
3:L:361:LEU:O	3:L:402:VAL:HA	2.14	0.47
1:A:470:TYR:HA	1:A:510:VAL:O	2.14	0.47
1:A:382:ASP:OD2	1:A:440:ARG:NH2	2.47	0.47
1:C:35:VAL:HG21	1:C:64:VAL:HG21	1.96	0.47
3:I:278:TYR:HA	3:I:455:MET:HE1	1.97	0.47
2:F:877:VAL:H	2:F:1451:GLN:NE2	2.12	0.47
1:G:510:VAL:HG21	1:G:622:LEU:HD12	1.96	0.47
1:G:470:TYR:HA	1:G:510:VAL:O	2.14	0.47
2:F:1338:LYS:H	2:F:1371:ARG:HD2	1.79	0.47
5:A:1646:NDG:H4	5:A:1647:NAG:H2	1.61	0.47
3:I:544:ILE:HD13	3:I:650:VAL:HG12	1.96	0.47
1:A:6:ILE:HD12	1:A:21:VAL:O	2.15	0.47
2:D:1521:TYR:HB2	2:D:1523:TYR:CZ	2.50	0.47
1:G:345:GLY:HA2	1:G:391:THR:O	2.14	0.47
3:K:620:VAL:HG12	3:K:667:PRO:HD2	1.95	0.47
3:J:378:ASP:HA	3:J:381:ARG:HB2	1.96	0.47
1:C:555:PRO:HB3	2:D:775:ASP:HA	1.96	0.47
3:L:334:LEU:HD12	3:L:373:PRO:HB3	1.97	0.47
2:B:1291:TRP:O	2:B:1294:ALA:N	2.47	0.47
2:F:813:LEU:HD23	2:F:907:LEU:HB3	1.95	0.47
2:D:965:VAL:O	2:D:1267:HIS:HD2	1.97	0.47
4:N:10:TYR:HE2	4:N:14:LYS:HE3	1.80	0.47
3:J:362:MET:HG2	3:J:403:PHE:HB2	1.95	0.47
3:I:378:ASP:HA	3:I:381:ARG:HB2	1.96	0.47
3:I:538:GLY:C	3:I:539:LYS:HD2	2.35	0.47
2:H:1270:LEU:O	2:H:1290:HIS:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:334:LEU:HD12	3:K:373:PRO:HB3	1.97	0.47
1:E:624:PHE:HB3	1:E:632:THR:HG23	1.96	0.47
1:C:624:PHE:HB3	1:C:632:THR:HG23	1.96	0.47
1:E:13:ARG:NH2	1:E:476:GLY:HA3	2.28	0.47
2:B:1521:TYR:HB2	2:B:1523:TYR:CZ	2.50	0.47
1:E:369:VAL:HG12	1:E:370:GLN:N	2.29	0.47
4:M:10:TYR:HE2	4:M:14:LYS:HE3	1.79	0.47
2:F:932:ARG:O	2:F:934:GLY:N	2.47	0.47
3:J:538:GLY:C	3:J:539:LYS:HD2	2.35	0.47
1:E:35:VAL:HG21	1:E:64:VAL:HG21	1.96	0.47
3:I:334:LEU:HD12	3:I:373:PRO:HB3	1.97	0.47
1:G:606:THR:HB	1:G:619:ASP:HB3	1.96	0.47
1:C:166:VAL:O	1:C:168:PRO:HD3	2.15	0.47
3:I:361:LEU:O	3:I:402:VAL:HA	2.14	0.47
3:I:349:PRO:O	3:I:352:TRP:HD1	1.98	0.47
3:I:362:MET:HG2	3:I:403:PHE:HB2	1.95	0.47
3:J:349:PRO:O	3:J:352:TRP:HD1	1.98	0.47
2:F:1269:GLU:HG3	2:F:1269:GLU:O	2.15	0.47
1:C:10:ASN:HB2	1:C:621:GLY:HA2	1.95	0.47
3:K:544:ILE:HD13	3:K:650:VAL:HG12	1.96	0.47
2:H:1359:LYS:HD2	4:N:4:LEU:CG	2.45	0.47
3:L:539:LYS:N	3:L:539:LYS:HD2	2.30	0.47
1:A:35:VAL:HG21	1:A:64:VAL:HG21	1.96	0.47
2:F:1270:LEU:O	2:F:1290:HIS:HA	2.15	0.47
3:J:513:LYS:HZ2	3:J:524:GLU:HG2	1.78	0.47
2:H:1521:TYR:HB2	2:H:1523:TYR:CZ	2.49	0.47
3:J:236:ILE:HG21	3:J:443:MET:O	2.15	0.47
3:L:362:MET:HG2	3:L:403:PHE:HB2	1.95	0.47
1:C:470:TYR:HA	1:C:510:VAL:O	2.14	0.47
2:B:967:GLN:O	2:B:968:MET:HB2	2.13	0.47
3:K:538:GLY:C	3:K:539:LYS:HD2	2.35	0.47
3:J:544:ILE:HD13	3:J:650:VAL:HG12	1.96	0.47
2:H:1446:ASN:CB	4:N:4:LEU:HB2	2.44	0.47
1:A:606:THR:HB	1:A:619:ASP:HB3	1.96	0.47
3:I:236:ILE:O	3:I:236:ILE:HG23	2.15	0.47
3:J:328:THR:O	3:J:367:HIS:HB2	2.15	0.47
3:K:363:THR:HG23	3:K:365:GLY:H	1.80	0.47
2:H:1498:ILE:HG13	2:H:1605:TRP:CZ3	2.50	0.47
1:E:6:ILE:HG22	1:E:625:THR:O	2.14	0.47
2:H:1291:TRP:O	2:H:1294:ALA:N	2.48	0.47
3:K:354:ARG:HB2	15:K:1749:NDG:C8	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1521:TYR:HB2	2:F:1523:TYR:CZ	2.49	0.47
1:E:219:LYS:HZ2	1:E:356:ASN:HD22	1.63	0.47
3:K:236:ILE:HG21	3:K:443:MET:O	2.15	0.47
1:C:510:VAL:HG12	1:C:528:SER:HB3	1.97	0.47
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.97	0.47
1:G:522:ARG:HG2	1:G:628:SER:CB	2.44	0.47
3:K:539:LYS:N	3:K:539:LYS:HD2	2.30	0.47
3:L:236:ILE:HG23	3:L:236:ILE:O	2.15	0.47
1:E:470:TYR:HA	1:E:510:VAL:O	2.14	0.47
1:C:325:PRO:HG2	1:C:357:PRO:HB2	1.97	0.47
3:K:270:ASN:N	3:K:270:ASN:HD22	2.12	0.47
2:B:733:ILE:HD13	2:B:841:ARG:HD3	1.98	0.46
2:F:1269:GLU:CG	2:F:1315:LYS:HB3	2.40	0.46
2:B:1640:PRO:HA	3:L:326:SER:OG	2.14	0.46
3:L:236:ILE:HG21	3:L:443:MET:O	2.15	0.46
1:C:378:LEU:HD13	1:E:446:GLY:O	2.16	0.46
1:E:34:THR:HG22	1:E:51:LYS:HE3	1.97	0.46
2:F:1524:LYS:HB3	2:F:1545:GLN:HG2	1.97	0.46
1:C:541:LEU:HD22	2:D:786:SER:HB3	1.96	0.46
2:D:1524:LYS:HB3	2:D:1545:GLN:HG2	1.97	0.46
2:F:733:ILE:HD13	2:F:841:ARG:HD3	1.97	0.46
1:C:6:ILE:HD12	1:C:21:VAL:O	2.14	0.46
2:F:1265:PRO:O	2:F:1266:ASP:CB	2.64	0.46
2:D:1172:TYR:CE1	2:D:1216:LEU:HB3	2.51	0.46
1:E:481:ALA:H	5:E:1646:NDG:H8C3	1.80	0.46
1:A:166:VAL:O	1:A:168:PRO:HD3	2.15	0.46
3:I:328:THR:O	3:I:367:HIS:HB2	2.14	0.46
1:A:213:ILE:HG22	1:A:215:GLU:HG3	1.97	0.46
2:B:1524:LYS:HB3	2:B:1545:GLN:HG2	1.97	0.46
2:D:990:GLU:O	2:D:994:ILE:HG13	2.16	0.46
1:C:369:VAL:HG12	1:C:370:GLN:N	2.31	0.46
3:L:270:ASN:HD22	3:L:270:ASN:N	2.11	0.46
1:G:477:ARG:NH1	1:G:477:ARG:HG2	2.21	0.46
1:E:6:ILE:HD12	1:E:21:VAL:O	2.14	0.46
3:L:538:GLY:C	3:L:539:LYS:HD2	2.35	0.46
2:F:1291:TRP:O	2:F:1294:ALA:N	2.48	0.46
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.51	0.46
2:H:1444:TYR:HB2	4:N:10:TYR:CE1	2.50	0.46
3:L:700:CYS:O	3:L:701:LYS:C	2.53	0.46
2:F:990:GLU:O	2:F:994:ILE:HG13	2.16	0.46
14:K:1745:MAN:O3	14:K:1748:MAN:H61	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:361:LEU:O	3:J:402:VAL:HA	2.14	0.46
1:E:207:LEU:HA	1:E:208:PRO:HD2	1.82	0.46
3:I:700:CYS:O	3:I:701:LYS:C	2.53	0.46
1:G:34:THR:HG22	1:G:51:LYS:HE3	1.97	0.46
3:L:679:ILE:HG21	3:L:686:PHE:HB3	1.97	0.46
3:L:378:ASP:HA	3:L:381:ARG:HB2	1.96	0.46
2:B:733:ILE:HG12	2:B:734:ILE:N	2.26	0.46
4:Q:10:TYR:HE2	4:Q:14:LYS:HE3	1.79	0.46
1:E:166:VAL:O	1:E:168:PRO:HD3	2.15	0.46
3:K:700:CYS:O	3:K:701:LYS:C	2.53	0.46
2:B:990:GLU:O	2:B:994:ILE:HG13	2.16	0.46
4:Q:73:ILE:O	4:Q:77:ILE:HG13	2.16	0.46
3:K:361:LEU:O	3:K:402:VAL:HA	2.14	0.46
1:E:80:ARG:HD2	2:F:1010:GLU:HG3	1.97	0.46
1:A:34:THR:HG22	1:A:51:LYS:HE3	1.97	0.46
2:H:833:ARG:CG	2:H:833:ARG:NH1	2.75	0.46
2:F:740:VAL:CB	4:P:42:ARG:HB2	2.43	0.46
3:I:539:LYS:HD2	3:I:539:LYS:N	2.30	0.46
3:J:236:ILE:O	3:J:236:ILE:HG23	2.15	0.46
3:I:236:ILE:HG21	3:I:443:MET:O	2.15	0.46
3:K:349:PRO:O	3:K:352:TRP:HD1	1.98	0.46
3:L:349:PRO:O	3:L:352:TRP:HD1	1.98	0.46
1:G:154:LYS:HD2	1:G:171:TRP:CD1	2.51	0.46
3:J:700:CYS:O	3:J:701:LYS:C	2.53	0.46
3:I:363:THR:HG23	3:I:365:GLY:H	1.80	0.46
1:G:6:ILE:HD12	1:G:21:VAL:O	2.15	0.46
2:F:1172:TYR:CE1	2:F:1216:LEU:HB3	2.51	0.46
3:I:531:HIS:HD2	3:I:533:ASN:H	1.64	0.46
3:K:236:ILE:O	3:K:236:ILE:HG23	2.15	0.46
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.51	0.46
1:C:213:ILE:HG22	1:C:215:GLU:HG3	1.97	0.46
10:H:2644:MAN:H62	10:H:2645:MAN:H2	1.43	0.46
4:M:73:ILE:O	4:M:77:ILE:HG13	2.16	0.46
1:C:639:GLN:NE2	1:C:639:GLN:H	2.14	0.46
1:C:606:THR:HB	1:C:619:ASP:HB3	1.96	0.46
2:H:837:GLU:HB3	2:H:868:PRO:HD3	1.97	0.46
3:J:531:HIS:HD2	3:J:533:ASN:H	1.64	0.46
3:K:292:TYR:CD1	3:K:325:LYS:HD3	2.51	0.46
2:F:1494:GLU:HB2	2:F:1602:LYS:HB3	1.97	0.46
1:G:247:ALA:HB2	1:G:308:VAL:HG22	1.97	0.46
3:L:363:THR:HG23	3:L:365:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:PHE:CE1	1:E:391:THR:HG21	2.50	0.46
3:L:345:ASP:HB3	3:L:346:ASP:H	1.49	0.46
3:L:531:HIS:HD2	3:L:533:ASN:H	1.64	0.46
4:N:73:ILE:O	4:N:77:ILE:HG13	2.15	0.46
1:C:47:LEU:HD13	1:C:66:PHE:HB2	1.97	0.46
2:D:1393:THR:O	2:D:1397:LYS:HD3	2.16	0.46
1:G:354:VAL:HG11	1:G:365:VAL:HG11	1.98	0.46
3:K:679:ILE:HG21	3:K:686:PHE:HB3	1.97	0.46
2:B:1393:THR:O	2:B:1397:LYS:HD3	2.16	0.46
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.97	0.46
3:K:261:PHE:HB3	3:K:319:TYR:HD1	1.81	0.46
1:C:154:LYS:HD2	1:C:171:TRP:CD1	2.51	0.46
3:J:363:THR:HG23	3:J:365:GLY:H	1.80	0.46
2:B:744:GLU:C	2:B:746:PRO:HD3	2.35	0.46
14:K:1743:NDG:H6C1	14:K:1744:NAG:C7	2.45	0.46
1:C:6:ILE:HG22	1:C:625:THR:O	2.16	0.46
3:J:334:LEU:HD12	3:J:373:PRO:HB3	1.97	0.46
2:F:1290:HIS:O	2:F:1291:TRP:O	2.34	0.46
1:E:10:ASN:HB2	1:E:621:GLY:C	2.36	0.46
2:F:811:LEU:HG	2:F:813:LEU:HD13	1.98	0.46
3:I:700:CYS:HA	3:I:704:LYS:O	2.16	0.46
8:F:2645:BMA:H62	8:F:2647:BMA:H2	1.36	0.46
4:P:73:ILE:O	4:P:77:ILE:HG13	2.16	0.46
3:L:261:PHE:HB3	3:L:319:TYR:HD1	1.81	0.46
1:A:639:GLN:NE2	1:A:639:GLN:H	2.14	0.46
1:E:147:ASN:HB2	1:E:148:PRO:CD	2.46	0.46
3:I:267:CYS:HB2	3:I:433:MET:CE	2.44	0.46
1:G:144:ASN:HD22	1:G:144:ASN:N	2.14	0.46
1:G:166:VAL:O	1:G:168:PRO:HD3	2.15	0.46
1:E:354:VAL:HG11	1:E:365:VAL:HG11	1.98	0.46
1:G:47:LEU:HD13	1:G:66:PHE:HB2	1.97	0.46
4:M:66:ALA:HA	4:M:69:GLN:HB2	1.98	0.46
2:B:819:ARG:HH11	2:B:819:ARG:CG	2.22	0.45
4:P:10:TYR:HE2	4:P:14:LYS:HE3	1.79	0.45
1:C:34:THR:HG22	1:C:51:LYS:HE3	1.97	0.45
1:G:213:ILE:HG22	1:G:215:GLU:HG3	1.97	0.45
3:K:646:ASP:OD2	3:K:648:SER:HB3	2.17	0.45
4:N:66:ALA:HA	4:N:69:GLN:HB2	1.98	0.45
3:J:679:ILE:HG21	3:J:686:PHE:HB3	1.97	0.45
3:L:653:PRO:CD	3:L:654:ARG:HH12	2.27	0.45
1:A:426:THR:HG22	1:A:427:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG12	1:A:370:GLN:N	2.31	0.45
3:I:646:ASP:OD2	3:I:648:SER:HB3	2.16	0.45
1:E:351:MET:SD	1:E:440:ARG:HD2	2.57	0.45
1:A:144:ASN:HD22	1:A:144:ASN:N	2.14	0.45
3:L:292:TYR:CD1	3:L:325:LYS:HD3	2.51	0.45
1:A:427:VAL:HB	1:A:523:GLU:HG3	1.99	0.45
3:J:700:CYS:HA	3:J:704:LYS:O	2.16	0.45
1:E:47:LEU:HD13	1:E:66:PHE:HB2	1.97	0.45
1:A:538:VAL:HB	2:B:791:LYS:O	2.16	0.45
3:I:261:PHE:HB3	3:I:319:TYR:HD1	1.81	0.45
2:H:1524:LYS:HB3	2:H:1545:GLN:HG2	1.97	0.45
1:G:639:GLN:H	1:G:639:GLN:NE2	2.14	0.45
1:G:473:MET:HE2	1:G:603:ILE:HD11	1.98	0.45
2:B:819:ARG:O	2:B:820:ASN:HB2	2.17	0.45
2:H:733:ILE:HD13	2:H:841:ARG:HD3	1.98	0.45
2:B:837:GLU:HB3	2:B:868:PRO:HD3	1.97	0.45
2:F:837:GLU:HB3	2:F:868:PRO:HD3	1.97	0.45
3:K:239:ASP:HA	3:K:240:PRO:HD3	1.86	0.45
1:E:154:LYS:HD2	1:E:171:TRP:CD1	2.51	0.45
3:L:702:ASN:O	3:L:703:GLN:HG3	2.17	0.45
3:K:702:ASN:O	3:K:703:GLN:HG3	2.17	0.45
3:J:705:ARG:O	3:J:706:GLN:CB	2.60	0.45
1:G:567:HIS:CG	2:H:760:PRO:HG3	2.52	0.45
1:G:100:LEU:HD21	1:G:638:LEU:CD2	2.44	0.45
2:B:1264:ALA:HA	2:B:1265:PRO:HD3	1.73	0.45
2:D:1288:ARG:HD3	2:D:1290:HIS:NE2	2.32	0.45
2:D:1223:ASP:O	2:D:1227:VAL:HG23	2.17	0.45
3:J:646:ASP:OD2	3:J:648:SER:HB3	2.17	0.45
2:D:1280:SER:O	2:D:1281:ARG:C	2.55	0.45
3:I:679:ILE:HG21	3:I:686:PHE:HB3	1.97	0.45
5:D:2642:NDG:H6C1	5:D:2643:NAG:C7	2.46	0.45
1:E:569:ALA:HB2	2:F:788:SER:HB2	1.99	0.45
2:D:1364:LEU:HD23	2:D:1439:PHE:CZ	2.52	0.45
2:H:1492:ALA:O	2:H:1493:GLU:C	2.55	0.45
1:G:424:TYR:OH	1:G:613:TYR:HB3	2.16	0.45
2:B:1288:ARG:HD3	2:B:1290:HIS:NE2	2.32	0.45
3:I:292:TYR:CD1	3:I:325:LYS:HD3	2.51	0.45
1:E:510:VAL:HG12	1:E:528:SER:HB3	1.97	0.45
2:H:1495:ASN:O	2:H:1496:CYS:C	2.54	0.45
2:D:1192:ALA:HB2	2:D:1198:TRP:CZ2	2.52	0.45
2:B:1123:ALA:O	2:B:1127:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:PHE:CE1	1:C:391:THR:HG21	2.52	0.45
3:L:646:ASP:OD2	3:L:648:SER:HB3	2.16	0.45
3:J:261:PHE:HB3	3:J:319:TYR:HD1	1.81	0.45
1:C:427:VAL:HB	1:C:523:GLU:HG3	1.99	0.45
2:H:819:ARG:O	2:H:820:ASN:HB2	2.17	0.45
3:I:653:PRO:CD	3:I:654:ARG:HH12	2.27	0.45
3:K:653:PRO:CD	3:K:654:ARG:HH12	2.27	0.45
2:F:1470:PHE:CB	2:F:1478:GLY:HA3	2.47	0.45
2:B:1203:LYS:HD2	2:B:1206:TYR:CE2	2.52	0.45
4:P:66:ALA:HA	4:P:69:GLN:HB2	1.98	0.45
3:K:428:PHE:CE1	4:P:31:LEU:HD11	2.52	0.45
2:B:1192:ALA:HB2	2:B:1198:TRP:CZ2	2.52	0.45
2:H:1497:PHE:C	2:H:1498:ILE:HD13	2.37	0.45
2:D:837:GLU:HB3	2:D:868:PRO:HD3	1.97	0.45
3:J:292:TYR:CD1	3:J:325:LYS:HD3	2.51	0.45
2:D:811:LEU:HG	2:D:813:LEU:HD13	1.98	0.45
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.98	0.45
2:B:851:CYS:HB2	2:B:1491:CYS:HB2	1.90	0.45
2:F:1182:GLY:HA3	2:F:1183:PRO:HD2	1.82	0.45
2:D:1123:ALA:O	2:D:1127:ILE:HG13	2.17	0.45
1:A:354:VAL:HG11	1:A:365:VAL:HG11	1.98	0.45
2:B:1280:SER:O	2:B:1281:ARG:C	2.55	0.45
1:G:516:ILE:N	1:G:516:ILE:HD12	2.32	0.45
2:B:729:LEU:HD22	2:B:729:LEU:O	2.17	0.45
2:F:1288:ARG:HD3	2:F:1290:HIS:NE2	2.32	0.45
2:F:962:GLY:C	2:F:964:PRO:HD3	2.37	0.45
2:H:811:LEU:HG	2:H:813:LEU:HD13	1.98	0.45
2:F:1364:LEU:HD23	2:F:1439:PHE:CZ	2.52	0.45
2:F:1280:SER:O	2:F:1281:ARG:C	2.55	0.45
7:G:1648:BMA:H3	9:G:1651:MAN:C1	2.46	0.45
1:E:213:ILE:HG22	1:E:215:GLU:HG3	1.97	0.45
2:F:1203:LYS:HD2	2:F:1206:TYR:CE2	2.52	0.45
1:E:639:GLN:H	1:E:639:GLN:NE2	2.14	0.45
2:D:937:LYS:HD2	2:D:937:LYS:O	2.17	0.45
2:H:1498:ILE:HD13	2:H:1498:ILE:N	2.32	0.45
2:D:733:ILE:HD13	2:D:841:ARG:HD3	1.98	0.45
2:H:734:ILE:N	2:H:734:ILE:HD12	2.32	0.45
3:L:272:ILE:HG12	3:L:284:TYR:CE1	2.52	0.45
2:D:1126:LEU:HD21	2:D:1177:MET:HE3	1.99	0.45
3:L:432:ASP:HA	4:N:27:ASN:HD21	1.82	0.45
2:D:1444:TYR:HB2	4:P:10:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG12	1:A:370:GLN:H	1.82	0.45
3:K:554:LEU:H	3:K:726:TRP:HH2	1.65	0.45
2:F:1506:THR:OG1	2:F:1509:GLU:HG2	2.17	0.45
3:J:702:ASN:O	3:J:703:GLN:HG3	2.17	0.45
1:E:477:ARG:NH1	1:E:477:ARG:CG	2.76	0.44
3:L:705:ARG:O	3:L:706:GLN:CB	2.60	0.44
2:H:1290:HIS:O	2:H:1291:TRP:O	2.34	0.44
3:K:238:LEU:HD22	3:K:280:VAL:HG21	1.99	0.44
2:B:1126:LEU:HD21	2:B:1177:MET:HE3	1.99	0.44
3:K:531:HIS:HD2	3:K:533:ASN:H	1.64	0.44
2:B:1223:ASP:O	2:B:1227:VAL:HG23	2.17	0.44
3:L:700:CYS:HA	3:L:704:LYS:O	2.16	0.44
2:F:1192:ALA:HB2	2:F:1198:TRP:CZ2	2.52	0.44
1:C:344:PRO:HD2	1:C:433:TYR:CE1	2.51	0.44
1:C:354:VAL:HG11	1:C:365:VAL:HG11	1.98	0.44
2:H:1497:PHE:O	2:H:1498:ILE:C	2.56	0.44
3:J:272:ILE:HG12	3:J:284:TYR:CE1	2.52	0.44
1:G:526:ALA:HB2	1:G:617:PHE:CE2	2.52	0.44
2:F:1126:LEU:O	2:F:1130:GLN:HG3	2.17	0.44
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.46	0.44
2:F:1223:ASP:O	2:F:1227:VAL:HG23	2.17	0.44
1:C:369:VAL:HG12	1:C:370:GLN:H	1.82	0.44
3:L:554:LEU:H	3:L:726:TRP:HH2	1.65	0.44
3:K:491:VAL:HB	3:K:572:LEU:HD11	1.99	0.44
3:J:554:LEU:H	3:J:726:TRP:HH2	1.65	0.44
1:A:516:ILE:HD12	1:A:516:ILE:N	2.32	0.44
2:D:819:ARG:O	2:D:820:ASN:HB2	2.17	0.44
2:B:734:ILE:N	2:B:734:ILE:HD12	2.33	0.44
3:K:489:ALA:HB2	3:K:677:PRO:CG	2.45	0.44
2:B:1126:LEU:O	2:B:1130:GLN:HG3	2.17	0.44
3:I:433:MET:HE3	3:I:433:MET:HB3	1.83	0.44
2:H:1470:PHE:CB	2:H:1478:GLY:HA3	2.47	0.44
7:G:1647:NAG:H3	7:G:1649:BMA:O3	2.17	0.44
2:F:1360:ASN:O	2:F:1361:THR:O	2.36	0.44
2:D:1203:LYS:HD2	2:D:1206:TYR:CE2	2.52	0.44
1:A:100:LEU:HD21	1:A:638:LEU:HD23	2.00	0.44
2:B:1283:SER:O	2:B:1284:LYS:HG2	2.18	0.44
2:F:734:ILE:HD12	2:F:734:ILE:N	2.33	0.44
2:H:1288:ARG:HD3	2:H:1290:HIS:NE2	2.32	0.44
1:E:144:ASN:N	1:E:144:ASN:HD22	2.14	0.44
2:H:943:ALA:O	2:H:1305:ASN:ND2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ILE:HG22	1:C:305:SER:HB3	2.00	0.44
2:B:847:ASN:HA	2:B:848:PRO:HD2	1.83	0.44
1:A:459:ARG:HH21	1:G:459:ARG:HE	1.66	0.44
1:E:427:VAL:HB	1:E:523:GLU:HG3	1.99	0.44
2:H:1360:ASN:O	2:H:1361:THR:O	2.36	0.44
2:H:1364:LEU:HD23	2:H:1439:PHE:CZ	2.52	0.44
2:F:943:ALA:O	2:F:1305:ASN:ND2	2.49	0.44
1:E:247:ALA:HB2	1:E:308:VAL:HG22	1.98	0.44
3:I:272:ILE:HG12	3:I:284:TYR:CE1	2.52	0.44
1:A:555:PRO:HB3	2:B:775:ASP:HA	1.98	0.44
3:K:238:LEU:HD11	3:K:278:TYR:CB	2.46	0.44
2:B:1639:CYS:HB2	3:L:368:ASN:OD1	2.18	0.44
1:A:342:PHE:CE1	1:A:391:THR:HG21	2.53	0.44
2:H:847:ASN:HA	2:H:848:PRO:HD2	1.83	0.44
2:B:1364:LEU:HD23	2:B:1439:PHE:CZ	2.52	0.44
3:L:491:VAL:HB	3:L:572:LEU:HD11	1.99	0.44
2:H:1280:SER:O	2:H:1281:ARG:C	2.55	0.44
3:I:554:LEU:H	3:I:726:TRP:HH2	1.65	0.44
3:K:446:GLU:OE2	3:K:457:TRP:NE1	2.50	0.44
2:D:1265:PRO:O	2:D:1266:ASP:CB	2.65	0.44
2:D:1292:GLU:HG2	2:D:1293:SER:H	1.83	0.44
2:D:1639:CYS:HB2	3:I:368:ASN:OD1	2.18	0.44
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.98	0.44
3:L:375:THR:O	3:L:379:GLU:HG3	2.18	0.44
3:I:375:THR:O	3:I:379:GLU:HG3	2.18	0.44
4:Q:66:ALA:HA	4:Q:69:GLN:HB2	1.98	0.44
2:F:847:ASN:HA	2:F:848:PRO:HD2	1.83	0.44
1:C:22:LEU:HD13	1:C:33:VAL:HG11	2.00	0.44
2:B:840:VAL:HG22	2:B:894:VAL:HG12	2.00	0.44
1:E:567:HIS:CG	2:F:760:PRO:HG3	2.53	0.44
1:G:147:ASN:HB2	1:G:148:PRO:CD	2.46	0.44
3:J:375:THR:O	3:J:379:GLU:HG3	2.18	0.44
1:A:459:ARG:HE	1:G:459:ARG:NH2	2.16	0.44
1:E:516:ILE:N	1:E:516:ILE:HD12	2.32	0.44
2:D:1446:ASN:HB2	4:P:4:LEU:HB2	1.99	0.44
1:E:558:GLN:HB3	2:F:770:ASN:HD21	1.82	0.44
2:F:1370:TYR:CD1	2:F:1376:ALA:HB2	2.52	0.44
2:B:937:LYS:HD2	2:B:937:LYS:O	2.17	0.44
3:K:245:ASN:OD1	3:K:283:ARG:HB2	2.18	0.44
2:F:1126:LEU:HD21	2:F:1177:MET:HE3	1.99	0.44
2:F:1264:ALA:HA	2:F:1265:PRO:HD3	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:433:MET:HE1	3:J:436:LEU:HD21	1.99	0.44
2:B:1462:ASN:C	2:B:1462:ASN:HD22	2.21	0.44
3:J:366:LEU:HB2	17:J:2002:HOH:O	2.18	0.44
1:A:329:SER:HA	1:A:330:PRO:HD3	1.78	0.44
2:D:1283:SER:O	2:D:1284:LYS:HG2	2.18	0.44
2:F:1375:ASP:OD1	2:F:1431:HIS:HD2	2.01	0.44
2:H:1375:ASP:OD1	2:H:1431:HIS:HD2	2.01	0.44
2:H:1283:SER:O	2:H:1284:LYS:HG2	2.18	0.44
3:I:543:GLY:O	3:I:545:PRO:HD3	2.18	0.44
2:D:734:ILE:N	2:D:734:ILE:HD12	2.33	0.44
3:J:654:ARG:HG3	3:J:722:GLN:CB	2.48	0.44
1:C:10:ASN:HB2	1:C:621:GLY:CA	2.48	0.44
3:K:272:ILE:HG12	3:K:284:TYR:CE1	2.52	0.44
3:J:238:LEU:HD22	3:J:280:VAL:HG21	1.99	0.44
2:H:1292:GLU:HG2	2:H:1293:SER:H	1.83	0.44
2:D:1338:LYS:H	2:D:1371:ARG:HD2	1.83	0.44
1:G:510:VAL:HG12	1:G:528:SER:HB3	1.99	0.44
2:D:1462:ASN:HD21	2:D:1464:GLU:HB2	1.83	0.44
3:K:375:THR:O	3:K:379:GLU:HG3	2.18	0.44
1:A:407:GLN:C	1:A:409:LEU:H	2.21	0.44
1:G:407:GLN:C	1:G:409:LEU:H	2.21	0.44
3:J:491:VAL:HB	3:J:572:LEU:HD11	1.99	0.44
3:I:702:ASN:O	3:I:703:GLN:HG3	2.17	0.44
2:F:1123:ALA:O	2:F:1127:ILE:HG13	2.17	0.44
2:D:1375:ASP:OD1	2:D:1431:HIS:HD2	2.01	0.44
2:F:819:ARG:O	2:F:820:ASN:HB2	2.17	0.43
3:K:654:ARG:HG3	3:K:722:GLN:CB	2.48	0.43
2:D:1126:LEU:O	2:D:1130:GLN:HG3	2.17	0.43
1:C:144:ASN:HD22	1:C:144:ASN:N	2.14	0.43
3:K:700:CYS:HA	3:K:704:LYS:O	2.16	0.43
3:I:491:VAL:HB	3:I:572:LEU:HD11	1.99	0.43
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.18	0.43
2:F:1497:PHE:CZ	2:F:1572:LEU:HD23	2.52	0.43
1:E:407:GLN:C	1:E:409:LEU:H	2.21	0.43
3:I:263:GLY:HA3	12:I:1743:NDG:H8C1	2.00	0.43
1:A:207:LEU:HA	1:A:208:PRO:HD2	1.81	0.43
2:F:1359:LYS:HB2	4:M:4:LEU:HD21	2.00	0.43
1:A:19:THR:HB	1:A:478:LEU:HB2	1.99	0.43
2:H:840:VAL:HG22	2:H:894:VAL:HG12	2.00	0.43
2:F:1462:ASN:HD21	2:F:1464:GLU:HB2	1.84	0.43
12:I:1743:NDG:H6C1	12:I:1744:NAG:C7	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ALA:HB2	1:A:308:VAL:HG22	1.99	0.43
2:F:1283:SER:O	2:F:1284:LYS:HG2	2.18	0.43
2:B:1038:ARG:NH1	2:B:1077:VAL:HG22	2.33	0.43
2:H:1370:TYR:CD1	2:H:1376:ALA:HB2	2.52	0.43
1:E:343:LYS:HB2	1:E:346:MET:HB2	2.00	0.43
3:J:653:PRO:CD	3:J:654:ARG:HH12	2.27	0.43
3:L:654:ARG:HG3	3:L:722:GLN:CB	2.48	0.43
3:K:513:LYS:HZ2	3:K:524:GLU:HG2	1.82	0.43
2:F:1038:ARG:NH1	2:F:1077:VAL:HG22	2.33	0.43
1:G:343:LYS:N	1:G:343:LYS:HD2	2.33	0.43
2:H:887:GLU:OE2	2:H:904:ARG:HD2	2.18	0.43
2:D:1056:LEU:O	2:D:1060:VAL:HG23	2.19	0.43
2:D:887:GLU:OE2	2:D:904:ARG:HD2	2.19	0.43
3:J:543:GLY:O	3:J:545:PRO:HD3	2.18	0.43
1:G:473:MET:HE1	1:G:603:ILE:HD11	1.99	0.43
3:I:245:ASN:OD1	3:I:283:ARG:HB2	2.18	0.43
2:F:833:ARG:NH1	2:F:833:ARG:CG	2.75	0.43
2:F:1639:CYS:HA	2:F:1640:PRO:HD3	1.69	0.43
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.54	0.43
1:E:208:PRO:CD	1:E:583:LEU:HD11	2.48	0.43
7:G:1647:NAG:H61	7:G:1648:BMA:H2	1.99	0.43
1:G:427:VAL:HB	1:G:523:GLU:HG3	1.99	0.43
1:G:341:TYR:CE1	1:G:611:LYS:HB3	2.53	0.43
1:E:22:LEU:HD13	1:E:33:VAL:HG11	2.00	0.43
1:A:22:LEU:HD13	1:A:33:VAL:HG11	2.00	0.43
3:L:238:LEU:HD22	3:L:280:VAL:HG21	1.99	0.43
2:B:1338:LYS:H	2:B:1371:ARG:HD2	1.83	0.43
2:F:1462:ASN:C	2:F:1462:ASN:HD22	2.21	0.43
1:E:343:LYS:HD2	1:E:343:LYS:N	2.33	0.43
1:C:407:GLN:C	1:C:409:LEU:H	2.21	0.43
2:B:1482:LYS:HA	2:B:1492:ALA:HB3	2.00	0.43
1:E:250:ILE:HG12	1:E:251:PHE:H	1.84	0.43
1:C:516:ILE:HD12	1:C:516:ILE:N	2.32	0.43
3:J:245:ASN:OD1	3:J:283:ARG:HB2	2.18	0.43
3:I:654:ARG:HG3	3:I:722:GLN:CB	2.48	0.43
2:D:1336:CYS:O	2:D:1337:ASN:O	2.36	0.43
2:B:1336:CYS:O	2:B:1337:ASN:O	2.37	0.43
2:D:840:VAL:HG22	2:D:894:VAL:HG12	2.00	0.43
2:B:1290:HIS:O	2:B:1291:TRP:O	2.37	0.43
2:H:1506:THR:OG1	2:H:1509:GLU:HG2	2.17	0.43
1:G:2:PRO:HA	1:G:25:HIS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1375:ASP:OD1	2:B:1431:HIS:HD2	2.01	0.43
3:I:238:LEU:HD22	3:I:280:VAL:HG21	1.99	0.43
2:F:840:VAL:HG22	2:F:894:VAL:HG12	2.00	0.43
1:G:572:VAL:HG23	2:H:785:VAL:HB	2.01	0.43
2:B:944:ASP:O	2:B:945:LEU:C	2.57	0.43
3:K:543:GLY:O	3:K:545:PRO:HD3	2.18	0.43
2:F:1078:LEU:HD23	2:F:1135:ILE:HG21	2.01	0.43
1:E:282:ARG:CZ	1:E:286:LEU:HD11	2.49	0.43
3:L:543:GLY:O	3:L:545:PRO:HD3	2.18	0.43
3:K:655:PHE:HD2	3:K:716:PHE:HB3	1.84	0.43
2:D:944:ASP:O	2:D:945:LEU:C	2.57	0.43
1:C:343:LYS:HD2	1:C:343:LYS:N	2.33	0.43
1:G:526:ALA:O	1:G:616:VAL:HG21	2.19	0.43
1:E:251:PHE:CG	1:E:280:LEU:HD22	2.54	0.43
1:E:2:PRO:HA	1:E:25:HIS:O	2.19	0.43
1:A:343:LYS:HD2	1:A:343:LYS:N	2.33	0.43
1:C:2:PRO:HA	1:C:25:HIS:O	2.19	0.43
3:I:655:PHE:HD2	3:I:716:PHE:HB3	1.84	0.43
3:I:446:GLU:H	3:I:446:GLU:HG3	1.66	0.43
1:G:343:LYS:HB2	1:G:346:MET:HB2	2.00	0.43
1:G:250:ILE:HG12	1:G:251:PHE:H	1.84	0.43
1:C:282:ARG:CZ	1:C:286:LEU:HD11	2.49	0.43
1:C:503:PHE:HD1	1:C:507:PHE:CG	2.37	0.43
3:I:431:LYS:HG3	4:M:27:ASN:ND2	2.34	0.43
2:H:1528:VAL:HG21	2:H:1559:GLN:HE21	1.84	0.43
1:C:506:SER:HB2	1:C:530:TRP:NE1	2.27	0.43
3:L:238:LEU:HD11	3:L:278:TYR:CB	2.46	0.43
2:B:1386:MET:O	2:B:1387:THR:C	2.57	0.43
2:B:1462:ASN:HD21	2:B:1464:GLU:HB2	1.83	0.43
2:D:1523:TYR:HB3	2:D:1543:ILE:HG23	2.01	0.43
2:B:1523:TYR:HB3	2:B:1543:ILE:HG23	2.01	0.43
1:E:481:ALA:HB3	5:E:1646:NDG:H8C3	1.99	0.43
2:F:1227:VAL:HB	2:F:1228:PRO:HD3	2.01	0.43
2:H:1376:ALA:HB3	2:H:1429:VAL:CG2	2.49	0.43
2:B:824:GLU:OE2	2:B:875:PRO:HB3	2.19	0.43
2:B:896:HIS:HB3	4:Q:61:LYS:HD3	2.00	0.43
2:B:887:GLU:OE2	2:B:904:ARG:HD2	2.18	0.43
2:F:1056:LEU:O	2:F:1060:VAL:HG23	2.19	0.43
2:D:1038:ARG:NH1	2:D:1077:VAL:HG22	2.33	0.43
3:K:407:PRO:CD	14:K:1743:NDG:H8C1	2.46	0.42
2:H:1462:ASN:HD21	2:H:1464:GLU:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:PHE:CG	1:C:280:LEU:HD22	2.54	0.42
2:H:851:CYS:HB2	2:H:1491:CYS:HB2	1.81	0.42
1:A:577:ASP:CG	2:B:778:THR:HG21	2.40	0.42
3:K:503:PHE:HB2	3:K:530:PHE:CZ	2.54	0.42
1:A:251:PHE:CG	1:A:280:LEU:HD22	2.54	0.42
1:G:282:ARG:CZ	1:G:286:LEU:HD11	2.49	0.42
1:C:538:VAL:HB	2:D:791:LYS:O	2.18	0.42
3:J:607:PHE:CE1	3:J:669:THR:HG22	2.54	0.42
3:K:607:PHE:CE1	3:K:669:THR:HG22	2.54	0.42
2:B:1334:LEU:HD13	2:B:1334:LEU:HA	1.80	0.42
2:D:819:ARG:NH1	2:D:819:ARG:CG	2.80	0.42
3:L:245:ASN:OD1	3:L:283:ARG:HB2	2.18	0.42
3:I:238:LEU:HD11	3:I:278:TYR:CB	2.46	0.42
2:F:1292:GLU:HG2	2:F:1293:SER:H	1.83	0.42
3:J:446:GLU:HG3	3:J:446:GLU:H	1.66	0.42
2:B:1215:LEU:O	2:B:1219:LEU:HG	2.19	0.42
2:F:745:PHE:N	2:F:746:PRO:HD3	2.32	0.42
2:B:772:PHE:CD1	4:N:37:ASN:ND2	2.87	0.42
2:H:824:GLU:OE2	2:H:875:PRO:HB3	2.19	0.42
1:C:247:ALA:HB2	1:C:308:VAL:HG22	2.02	0.42
2:H:1500:LYS:NZ	2:H:1504:LYS:HB2	2.34	0.42
1:G:22:LEU:HD13	1:G:33:VAL:HG11	2.00	0.42
3:I:449:SER:HA	3:I:452:LEU:HD13	2.01	0.42
2:B:1265:PRO:O	2:B:1266:ASP:CB	2.64	0.42
2:B:1292:GLU:HG2	2:B:1293:SER:H	1.83	0.42
1:A:439:LEU:CD1	1:A:439:LEU:H	2.32	0.42
7:G:1647:NAG:N2	7:G:1649:BMA:O3	2.52	0.42
1:C:343:LYS:HB2	1:C:346:MET:HB2	2.00	0.42
2:D:824:GLU:OE2	2:D:875:PRO:HB3	2.19	0.42
2:B:932:ARG:O	2:B:933:GLU:C	2.57	0.42
3:J:655:PHE:HD2	3:J:716:PHE:HB3	1.84	0.42
3:L:655:PHE:HD2	3:L:716:PHE:HB3	1.84	0.42
2:D:1482:LYS:HA	2:D:1492:ALA:HB3	2.01	0.42
1:E:111:GLN:O	1:E:125:TYR:HA	2.20	0.42
3:J:437:GLU:CD	3:J:458:GLU:HB2	2.40	0.42
1:A:549:GLU:O	1:A:550:ASP:HB2	2.20	0.42
2:B:1446:ASN:HB2	4:Q:4:LEU:CD1	2.49	0.42
3:I:607:PHE:CE1	3:I:669:THR:HG22	2.55	0.42
1:A:503:PHE:HD1	1:A:507:PHE:CG	2.37	0.42
2:D:932:ARG:O	2:D:933:GLU:C	2.57	0.42
3:L:607:PHE:CE1	3:L:669:THR:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:ILE:N	1:G:127:ILE:HD12	2.35	0.42
1:A:10:ASN:HB2	1:A:621:GLY:HA2	2.01	0.42
2:H:745:PHE:N	2:H:746:PRO:HD3	2.35	0.42
12:I:1744:NAG:H82	12:I:1744:NAG:H2	1.91	0.42
3:I:432:ASP:HA	4:M:27:ASN:HD21	1.84	0.42
1:C:111:GLN:O	1:C:125:TYR:HA	2.20	0.42
2:F:1528:VAL:HG21	2:F:1559:GLN:HE21	1.84	0.42
2:D:1082:VAL:HG13	2:D:1129:LEU:HD22	2.01	0.42
2:F:969:THR:O	2:F:970:GLU:C	2.57	0.42
2:D:1078:LEU:HD23	2:D:1135:ILE:HG21	2.01	0.42
1:A:282:ARG:CZ	1:A:286:LEU:HD11	2.49	0.42
3:I:709:VAL:HA	3:I:710:PRO:HD3	1.92	0.42
1:A:127:ILE:HD12	1:A:127:ILE:N	2.35	0.42
3:L:489:ALA:HB2	3:L:677:PRO:CG	2.45	0.42
3:K:353:ASN:OD1	15:K:1749:NDG:C7	2.67	0.42
2:D:1290:HIS:O	2:D:1291:TRP:O	2.37	0.42
2:D:1215:LEU:O	2:D:1219:LEU:HG	2.19	0.42
1:G:251:PHE:CG	1:G:280:LEU:HD22	2.54	0.42
3:I:289:TYR:HA	3:I:293:PRO:HA	2.01	0.42
2:B:1506:THR:OG1	2:B:1509:GLU:HG2	2.20	0.42
1:E:454:LEU:HA	1:E:491:ASP:O	2.19	0.42
2:D:1506:THR:OG1	2:D:1509:GLU:HG2	2.20	0.42
1:A:40:PHE:HA	1:A:41:PRO:HA	1.84	0.42
2:H:1485:ARG:HH21	2:H:1590:TRP:HE1	1.67	0.42
1:C:147:ASN:HB2	1:C:148:PRO:CD	2.46	0.42
2:H:1516:GLU:HB3	2:H:1517:PRO:CD	2.50	0.42
3:J:531:HIS:CD2	3:J:533:ASN:HB2	2.55	0.42
1:G:439:LEU:H	1:G:439:LEU:CD1	2.32	0.42
2:B:1227:VAL:HB	2:B:1228:PRO:HD3	2.01	0.42
1:C:218:GLU:C	1:C:220:PHE:H	2.23	0.42
1:E:127:ILE:HD12	1:E:127:ILE:N	2.35	0.42
2:H:1386:MET:O	2:H:1387:THR:C	2.58	0.42
1:E:6:ILE:HD11	1:E:20:MET:CG	2.50	0.42
1:G:512:TYR:CE1	1:G:624:PHE:HE1	2.37	0.42
2:F:1215:LEU:O	2:F:1219:LEU:HG	2.19	0.42
2:F:1216:LEU:HD21	2:F:1256:ALA:HA	2.02	0.42
1:E:219:LYS:NZ	1:E:356:ASN:ND2	2.68	0.42
3:I:531:HIS:CD2	3:I:533:ASN:HB2	2.55	0.42
3:L:531:HIS:CD2	3:L:533:ASN:HB2	2.55	0.42
1:A:218:GLU:C	1:A:220:PHE:H	2.23	0.42
3:L:503:PHE:HB2	3:L:530:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:943:ALA:O	2:D:1305:ASN:ND2	2.53	0.42
3:L:289:TYR:HA	3:L:293:PRO:HA	2.02	0.42
2:B:1078:LEU:HD23	2:B:1135:ILE:HG21	2.01	0.42
2:F:944:ASP:O	2:F:945:LEU:C	2.57	0.42
2:F:887:GLU:OE2	2:F:904:ARG:HD2	2.19	0.42
1:C:127:ILE:N	1:C:127:ILE:HD12	2.35	0.42
2:H:944:ASP:O	2:H:945:LEU:C	2.57	0.42
3:K:244:MET:HG2	3:K:245:ASN:N	2.35	0.42
3:I:705:ARG:O	3:I:706:GLN:CB	2.60	0.42
3:I:676:GLY:HA2	3:I:677:PRO:HD3	1.83	0.42
2:D:1386:MET:O	2:D:1387:THR:C	2.58	0.42
4:Q:84:LYS:O	4:Q:84:LYS:HG3	2.20	0.42
3:J:443:MET:HB3	3:J:443:MET:HE2	1.86	0.42
1:C:330:PRO:HG2	1:C:409:LEU:HD21	2.01	0.42
1:A:250:ILE:HG22	1:A:305:SER:HB3	2.01	0.42
1:G:574:VAL:HG13	2:H:783:LEU:HB3	2.01	0.42
2:B:1376:ALA:HB3	2:B:1429:VAL:CG2	2.49	0.42
1:G:111:GLN:O	1:G:125:TYR:HA	2.20	0.42
2:H:1334:LEU:HD13	2:H:1334:LEU:HA	1.80	0.42
2:F:1269:GLU:O	2:F:1271:ASN:N	2.52	0.42
1:G:19:THR:HG22	1:G:20:MET:N	2.35	0.42
2:D:1518:GLY:CA	2:D:1585:LEU:HD22	2.48	0.42
2:D:1462:ASN:HD22	2:D:1462:ASN:C	2.21	0.42
3:L:443:MET:HE2	3:L:443:MET:HB3	1.87	0.42
1:C:250:ILE:HG12	1:C:251:PHE:H	1.84	0.42
1:G:503:PHE:HD1	1:G:507:PHE:CG	2.37	0.42
2:F:1522:VAL:HG22	2:F:1583:TRP:HB3	2.02	0.42
2:D:1009:THR:HB	2:D:1011:GLN:HE21	1.85	0.42
2:F:1009:THR:HB	2:F:1011:GLN:HE21	1.85	0.42
3:L:298:LYS:HB2	3:L:301:GLU:HG3	2.02	0.42
3:J:503:PHE:HB2	3:J:530:PHE:CZ	2.54	0.42
3:I:503:PHE:HB2	3:I:530:PHE:CZ	2.54	0.42
2:H:841:ARG:CG	2:H:841:ARG:HH11	2.23	0.41
2:H:877:VAL:H	2:H:1451:GLN:HE21	1.68	0.41
1:C:6:ILE:HD11	1:C:20:MET:CG	2.50	0.41
1:G:6:ILE:HD11	1:G:20:MET:CG	2.50	0.41
1:C:439:LEU:CD1	1:C:439:LEU:H	2.32	0.41
1:G:526:ALA:CB	1:G:617:PHE:CE2	3.03	0.41
2:H:1338:LYS:N	2:H:1371:ARG:HB2	2.34	0.41
2:F:1336:CYS:O	2:F:1337:ASN:C	2.59	0.41
2:H:854:ALA:HB2	2:H:860:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1227:VAL:HB	2:D:1228:PRO:HD3	2.01	0.41
2:B:1082:VAL:HG13	2:B:1129:LEU:HD22	2.02	0.41
4:M:23:LEU:HD21	4:M:51:ALA:HB3	2.02	0.41
2:F:1390:ALA:HA	2:F:1391:PRO:HD3	1.91	0.41
4:N:56:LYS:HG3	4:N:57:SER:N	2.34	0.41
3:J:489:ALA:HB2	3:J:677:PRO:CG	2.45	0.41
1:G:350:LEU:CD2	1:G:400:ILE:HG21	2.50	0.41
3:L:239:ASP:HA	3:L:240:PRO:HD3	1.86	0.41
1:A:330:PRO:HG2	1:A:409:LEU:HD21	2.00	0.41
2:B:932:ARG:O	2:B:934:GLY:N	2.53	0.41
2:D:932:ARG:O	2:D:934:GLY:N	2.53	0.41
1:A:80:ARG:HD2	2:B:1010:GLU:HG3	2.01	0.41
4:Q:23:LEU:HD21	4:Q:51:ALA:HB3	2.02	0.41
2:B:943:ALA:O	2:B:1305:ASN:ND2	2.53	0.41
2:B:1165:TYR:HD1	2:B:1210:ALA:HB2	1.85	0.41
4:M:56:LYS:HG3	4:M:57:SER:N	2.34	0.41
2:D:1528:VAL:HG21	2:D:1559:GLN:HE21	1.84	0.41
3:K:540:LYS:HB2	3:K:540:LYS:NZ	2.36	0.41
3:J:244:MET:HG2	3:J:245:ASN:N	2.35	0.41
1:E:386:LYS:HD3	1:E:440:ARG:HG2	2.02	0.41
1:C:19:THR:HG22	1:C:20:MET:N	2.35	0.41
2:B:1541:MET:HE3	2:B:1541:MET:HB2	1.96	0.41
2:H:1611:GLU:HG3	2:H:1612:GLU:N	2.34	0.41
4:N:84:LYS:O	4:N:84:LYS:HG3	2.20	0.41
3:J:433:MET:HE3	3:J:433:MET:HB3	1.82	0.41
1:E:126:ARG:CZ	1:E:572:VAL:HB	2.50	0.41
3:K:531:HIS:CD2	3:K:533:ASN:HB2	2.55	0.41
3:K:443:MET:HE2	3:K:443:MET:HB3	1.87	0.41
3:I:666:ASP:HA	3:I:667:PRO:HD3	1.95	0.41
8:F:2644:BMA:H5	8:F:2645:BMA:H2	2.01	0.41
1:E:365:VAL:HA	1:E:366:PRO:HD2	1.80	0.41
1:G:341:TYR:CD2	1:G:610:GLY:HA2	2.56	0.41
3:L:503:PHE:CZ	3:L:555:ILE:HD11	2.55	0.41
2:D:1370:TYR:CG	2:D:1376:ALA:HB2	2.55	0.41
2:D:1376:ALA:HB3	2:D:1429:VAL:CG2	2.49	0.41
2:B:1009:THR:HB	2:B:1011:GLN:HE21	1.85	0.41
2:F:1165:TYR:HD1	2:F:1210:ALA:HB2	1.85	0.41
3:J:298:LYS:HB2	3:J:301:GLU:HG3	2.02	0.41
4:Q:56:LYS:HG3	4:Q:57:SER:N	2.34	0.41
2:F:915:ARG:O	2:F:916:MET:HG3	2.21	0.41
3:L:494:TYR:O	3:L:556:LYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG13	1:A:267:LYS:HB2	2.02	0.41
2:F:1472:HIS:HA	2:F:1473:PRO:HD3	1.94	0.41
2:B:1528:VAL:HG21	2:B:1559:GLN:HE21	1.84	0.41
1:A:111:GLN:O	1:A:125:TYR:HA	2.20	0.41
3:L:540:LYS:NZ	3:L:540:LYS:HB2	2.36	0.41
2:F:932:ARG:HH11	3:L:339:SER:CB	2.34	0.41
2:H:740:VAL:CB	4:Q:42:ARG:HB2	2.45	0.41
3:K:259:SER:HB3	14:K:1743:NDG:O7	2.20	0.41
3:L:278:TYR:CE2	3:L:455:MET:SD	3.13	0.41
2:F:1518:GLY:CA	2:F:1585:LEU:HD22	2.48	0.41
4:P:84:LYS:HG3	4:P:84:LYS:O	2.20	0.41
2:F:1055:TRP:CD1	2:F:1111:LEU:HD22	2.56	0.41
2:B:1055:TRP:CD1	2:B:1111:LEU:HD22	2.56	0.41
4:N:41:LYS:O	4:N:45:LYS:HG3	2.21	0.41
14:K:1745:MAN:H62	14:K:1746:MAN:H2	1.74	0.41
1:A:343:LYS:HB2	1:A:346:MET:HB2	2.00	0.41
3:I:503:PHE:CZ	3:I:555:ILE:HD11	2.55	0.41
3:J:494:TYR:O	3:J:556:LYS:HA	2.21	0.41
1:C:100:LEU:HD12	1:C:101:VAL:H	1.86	0.41
1:G:218:GLU:C	1:G:220:PHE:H	2.23	0.41
2:H:1514:ALA:O	2:H:1519:VAL:HG11	2.20	0.41
1:A:454:LEU:HA	1:A:491:ASP:O	2.21	0.41
3:I:244:MET:HG2	3:I:245:ASN:N	2.35	0.41
2:F:932:ARG:O	2:F:933:GLU:C	2.58	0.41
3:J:676:GLY:HA2	3:J:677:PRO:HD3	1.83	0.41
3:J:461:LYS:HG2	4:Q:28:VAL:HG12	2.03	0.41
2:H:1359:LYS:CB	4:N:4:LEU:HD21	2.50	0.41
3:K:446:GLU:H	3:K:446:GLU:HG3	1.66	0.41
2:B:1451:GLN:HA	2:B:1452:PRO:HD3	1.94	0.41
2:F:759:PRO:HA	2:F:760:PRO:HD3	1.84	0.41
2:H:1462:ASN:HD22	2:H:1462:ASN:C	2.21	0.41
2:D:1055:TRP:CD1	2:D:1111:LEU:HD22	2.56	0.41
2:D:1516:GLU:HB3	2:D:1517:PRO:CD	2.50	0.41
1:A:13:ARG:NH2	1:A:476:GLY:HA3	2.35	0.41
3:J:289:TYR:HA	3:J:293:PRO:HA	2.02	0.41
3:K:503:PHE:CZ	3:K:555:ILE:HD11	2.55	0.41
1:A:250:ILE:HG12	1:A:251:PHE:H	1.84	0.41
1:A:2:PRO:HA	1:A:25:HIS:O	2.19	0.41
2:F:1082:VAL:HG13	2:F:1129:LEU:HD22	2.02	0.41
1:C:549:GLU:O	1:C:550:ASP:HB2	2.20	0.41
2:H:1500:LYS:HE3	2:H:1504:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:549:GLU:O	1:G:550:ASP:HB2	2.20	0.41
4:M:84:LYS:O	4:M:84:LYS:HG3	2.20	0.41
3:J:368:ASN:ND2	3:J:368:ASN:N	2.69	0.41
2:B:813:LEU:HD23	2:B:907:LEU:HD22	2.02	0.41
4:P:56:LYS:HG3	4:P:57:SER:N	2.34	0.41
2:D:1357:ASP:C	2:D:1359:LYS:H	2.24	0.41
2:F:824:GLU:OE2	2:F:875:PRO:HB3	2.19	0.41
3:J:540:LYS:NZ	3:J:540:LYS:HB2	2.35	0.41
2:F:1334:LEU:HA	2:F:1334:LEU:HD13	1.80	0.41
2:F:1386:MET:O	2:F:1387:THR:C	2.58	0.41
2:H:1518:GLY:CA	2:H:1585:LEU:HD22	2.48	0.41
2:D:1611:GLU:HG3	2:D:1612:GLU:N	2.34	0.41
1:A:10:ASN:HA	1:A:623:THR:HG23	2.03	0.41
2:B:854:ALA:HB2	2:B:860:HIS:HB3	2.02	0.41
1:A:459:ARG:NH2	1:G:459:ARG:HE	2.19	0.41
2:F:1514:ALA:O	2:F:1519:VAL:HG11	2.20	0.41
2:B:1522:VAL:HG22	2:B:1583:TRP:HB3	2.02	0.41
3:I:494:TYR:O	3:I:556:LYS:HA	2.21	0.41
2:D:851:CYS:HB2	2:D:1491:CYS:HB2	1.78	0.41
3:K:298:LYS:HB2	3:K:301:GLU:HG3	2.02	0.41
1:G:7:ILE:HG21	1:G:471:LEU:HD22	2.02	0.41
1:E:503:PHE:HD1	1:E:507:PHE:CG	2.37	0.41
2:D:1522:VAL:HG22	2:D:1583:TRP:HB3	2.02	0.41
1:E:549:GLU:O	1:E:550:ASP:HB2	2.20	0.41
2:B:841:ARG:HH11	2:B:841:ARG:CG	2.23	0.41
1:A:6:ILE:HD11	1:A:20:MET:CG	2.50	0.41
2:B:1444:TYR:HB2	4:Q:10:TYR:CE1	2.55	0.41
2:F:1338:LYS:N	2:F:1371:ARG:HB2	2.36	0.41
2:B:1216:LEU:HD21	2:B:1256:ALA:HA	2.02	0.41
3:L:428:PHE:CE1	3:L:439:VAL:HG13	2.56	0.41
2:H:813:LEU:HA	2:H:814:PRO:HD3	1.97	0.41
2:B:1522:VAL:HG12	2:B:1547:ILE:HD12	2.03	0.41
1:C:207:LEU:HA	1:C:208:PRO:HD2	1.82	0.41
1:G:249:VAL:HG13	1:G:267:LYS:HB2	2.02	0.41
1:G:23:GLU:OE1	1:G:469:THR:HG21	2.21	0.41
2:H:1639:CYS:HA	2:H:1640:PRO:HD3	1.76	0.41
1:A:363:TYR:CD2	1:A:381:GLY:HA2	2.56	0.41
1:A:506:SER:HB2	1:A:530:TRP:NE1	2.27	0.41
3:K:676:GLY:HA2	3:K:677:PRO:HD3	1.83	0.41
1:C:10:ASN:HB2	1:C:622:LEU:N	2.36	0.41
1:E:19:THR:HG22	1:E:20:MET:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:238:LEU:HD11	3:J:278:TYR:CB	2.46	0.41
2:H:1541:MET:HB2	2:H:1541:MET:HE3	1.96	0.41
3:J:423:ASN:ND2	3:J:423:ASN:N	2.68	0.41
2:D:1611:GLU:HB3	2:D:1614:GLU:HG3	2.03	0.41
1:E:218:GLU:C	1:E:220:PHE:H	2.23	0.41
2:B:1611:GLU:HB3	2:B:1614:GLU:HG3	2.03	0.41
12:J:1744:NAG:H2	12:J:1744:NAG:H82	1.91	0.41
2:H:1523:TYR:HB3	2:H:1543:ILE:HG23	2.02	0.41
2:F:745:PHE:HA	2:F:776:SER:OG	2.21	0.41
1:E:640:CYS:HB3	1:E:641:PRO:CD	2.51	0.41
3:I:239:ASP:HA	3:I:240:PRO:HD3	1.86	0.41
4:M:69:GLN:HB3	4:M:69:GLN:HE21	1.68	0.41
2:B:1192:ALA:HB2	2:B:1198:TRP:CE2	2.56	0.41
2:F:1376:ALA:HB3	2:F:1429:VAL:CG2	2.49	0.41
1:E:250:ILE:HG22	1:E:305:SER:HB3	2.03	0.41
1:E:250:ILE:HG12	1:E:251:PHE:N	2.36	0.41
1:A:250:ILE:HG12	1:A:251:PHE:N	2.36	0.41
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.55	0.41
3:J:503:PHE:CZ	3:J:555:ILE:HD11	2.55	0.41
1:C:454:LEU:HA	1:C:491:ASP:O	2.21	0.41
3:K:289:TYR:HA	3:K:293:PRO:HA	2.02	0.41
2:H:1522:VAL:HG22	2:H:1583:TRP:HB3	2.02	0.41
3:J:428:PHE:CE1	4:Q:31:LEU:HD11	2.55	0.41
4:P:23:LEU:HD21	4:P:51:ALA:HB3	2.02	0.41
2:D:1165:TYR:HD1	2:D:1210:ALA:HB2	1.85	0.41
1:A:552:GLN:HA	1:A:553:PRO:HD3	1.81	0.41
3:J:638:ALA:HA	3:J:639:PRO:HD3	1.98	0.41
1:E:324:ILE:HA	1:E:325:PRO:HD3	1.89	0.41
1:A:24:ALA:HB3	1:A:60:HIS:HB3	2.03	0.41
1:G:207:LEU:HA	1:G:208:PRO:HD2	1.82	0.41
1:C:477:ARG:HG2	1:C:477:ARG:NH1	2.21	0.41
3:K:244:MET:HG2	3:K:245:ASN:H	1.86	0.41
1:E:439:LEU:H	1:E:439:LEU:CD1	2.32	0.41
1:A:19:THR:HG22	1:A:20:MET:N	2.35	0.41
2:D:1216:LEU:HD21	2:D:1256:ALA:HA	2.02	0.41
1:G:391:THR:HG22	1:G:392:HIS:N	2.36	0.41
2:B:1229:PRO:HA	2:B:1232:ARG:NH1	2.36	0.41
2:H:1635:VAL:HG23	2:H:1636:VAL:N	2.36	0.41
2:F:813:LEU:HD23	2:F:907:LEU:HD22	2.02	0.41
2:D:745:PHE:N	2:D:746:PRO:HD3	2.35	0.41
2:B:729:LEU:C	2:B:729:LEU:HD13	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD12	1:A:101:VAL:H	1.86	0.41
2:F:1522:VAL:HG12	2:F:1547:ILE:HD12	2.03	0.41
3:I:503:PHE:HB2	3:I:530:PHE:HZ	1.86	0.41
3:J:428:PHE:CE1	3:J:439:VAL:HG13	2.56	0.41
1:E:438:VAL:HG13	1:E:449:LEU:HD11	2.03	0.41
2:H:965:VAL:HG23	2:H:1268:GLN:OE1	2.22	0.40
2:F:819:ARG:CG	2:F:819:ARG:NH1	2.80	0.40
4:P:41:LYS:O	4:P:45:LYS:HG3	2.21	0.40
1:G:400:ILE:N	1:G:400:ILE:HD12	2.36	0.40
1:A:400:ILE:HD12	1:A:400:ILE:N	2.36	0.40
2:F:1516:GLU:HB3	2:F:1517:PRO:CD	2.50	0.40
2:F:1229:PRO:HA	2:F:1232:ARG:NH1	2.36	0.40
2:F:854:ALA:HB2	2:F:860:HIS:HB3	2.02	0.40
4:M:41:LYS:O	4:M:45:LYS:HG3	2.21	0.40
2:D:1192:ALA:HB2	2:D:1198:TRP:CE2	2.56	0.40
3:K:439:VAL:HA	4:P:31:LEU:HD21	2.02	0.40
3:K:428:PHE:CE1	3:K:439:VAL:HG13	2.56	0.40
1:C:365:VAL:HA	1:C:366:PRO:HD2	1.81	0.40
2:H:1522:VAL:HG12	2:H:1547:ILE:HD12	2.03	0.40
2:H:915:ARG:O	2:H:916:MET:HG3	2.21	0.40
2:B:917:ASN:OD1	5:B:2642:NDG:O	2.38	0.40
1:E:541:LEU:HD22	2:F:786:SER:HB3	2.02	0.40
1:E:249:VAL:HG13	1:E:267:LYS:HB2	2.03	0.40
2:H:1503:ASP:O	2:H:1504:LYS:HG3	2.21	0.40
2:H:877:VAL:HG22	2:H:1451:GLN:NE2	2.28	0.40
2:F:1611:GLU:HB3	2:F:1614:GLU:HG3	2.03	0.40
1:A:344:PRO:HG3	1:A:423:PRO:HB3	2.02	0.40
2:H:813:LEU:HD23	2:H:907:LEU:HD22	2.02	0.40
1:E:391:THR:HG22	1:E:392:HIS:N	2.36	0.40
2:F:1192:ALA:HB2	2:F:1198:TRP:CE2	2.56	0.40
2:F:1370:TYR:CE2	2:F:1372:GLY:HA3	2.56	0.40
2:H:1370:TYR:CG	2:H:1376:ALA:HB2	2.56	0.40
1:E:24:ALA:HB3	1:E:60:HIS:HB3	2.03	0.40
1:G:558:GLN:HB3	2:H:770:ASN:HD21	1.86	0.40
1:E:552:GLN:HA	1:E:553:PRO:HD3	1.81	0.40
2:F:1000:VAL:HG22	2:F:1027:ILE:HG23	2.04	0.40
1:G:505:PRO:O	1:G:533:VAL:HB	2.21	0.40
1:G:480:LYS:HG2	1:G:481:ALA:N	2.37	0.40
1:G:506:SER:HB2	1:G:530:TRP:NE1	2.27	0.40
3:I:654:ARG:HG3	3:I:722:GLN:HB3	2.03	0.40
2:H:1527:LEU:HD22	2:H:1574:LEU:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:809:ILE:HD11	2:H:892:ALA:CB	2.52	0.40
2:F:1523:TYR:HB3	2:F:1543:ILE:HG23	2.02	0.40
1:E:480:LYS:HG2	1:E:481:ALA:N	2.36	0.40
1:G:126:ARG:HG3	2:H:751:TRP:CZ2	2.56	0.40
2:D:813:LEU:HD23	2:D:907:LEU:HD22	2.02	0.40
1:C:109:PHE:CZ	1:C:594:ILE:HG23	2.56	0.40
5:E:1648:BMA:H62	5:E:1649:BMA:H2	1.58	0.40
3:I:345:ASP:HB3	3:I:346:ASP:H	1.49	0.40
3:L:244:MET:HG2	3:L:245:ASN:N	2.35	0.40
3:I:461:LYS:CG	4:M:28:VAL:HG12	2.51	0.40
2:B:1446:ASN:HB2	4:Q:4:LEU:HD12	2.03	0.40
2:D:776:SER:HB2	2:D:780:TRP:HZ2	1.86	0.40
1:A:342:PHE:CZ	1:A:423:PRO:HG3	2.56	0.40
3:K:328:THR:N	3:K:368:ASN:HD21	2.20	0.40
2:D:1229:PRO:HA	2:D:1232:ARG:NH1	2.36	0.40
3:I:428:PHE:CE1	3:I:439:VAL:HG13	2.56	0.40
3:I:402:VAL:HG11	3:I:414:ILE:HG23	2.04	0.40
1:E:583:LEU:N	1:E:583:LEU:HD12	2.36	0.40
1:C:391:THR:HG22	1:C:392:HIS:N	2.36	0.40
1:C:392:HIS:C	1:C:394:SER:H	2.25	0.40
2:H:1370:TYR:CE2	2:H:1372:GLY:HA3	2.56	0.40
1:A:363:TYR:HD2	1:A:381:GLY:HA2	1.86	0.40
3:K:494:TYR:O	3:K:556:LYS:HA	2.21	0.40
3:I:298:LYS:HB2	3:I:301:GLU:HG3	2.02	0.40
2:H:1609:TRP:HD1	2:H:1610:PRO:O	2.04	0.40
1:E:100:LEU:HD12	1:E:101:VAL:H	1.86	0.40
1:C:583:LEU:HD12	1:C:583:LEU:N	2.36	0.40
3:I:540:LYS:HB2	3:I:540:LYS:NZ	2.35	0.40
2:D:1527:LEU:HD22	2:D:1574:LEU:HB3	2.04	0.40
2:F:1143:LEU:O	2:F:1147:ILE:HG13	2.22	0.40
1:C:400:ILE:HD12	1:C:400:ILE:N	2.36	0.40
3:J:292:TYR:HA	3:J:293:PRO:HD3	1.95	0.40
2:F:1632:GLU:HA	2:F:1635:VAL:HG22	2.04	0.40
1:G:220:PHE:CZ	1:G:330:PRO:HB3	2.56	0.40
1:C:480:LYS:HG2	1:C:481:ALA:N	2.37	0.40
1:C:24:ALA:HB3	1:C:60:HIS:HB3	2.03	0.40
1:C:199:GLU:HB2	1:C:587:ASN:OD1	2.22	0.40
1:E:642:GLN:O	1:E:644:ALA:N	2.54	0.40
2:B:1609:TRP:HD1	2:B:1610:PRO:O	2.04	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	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	30	73
1	C	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	30	73
1	E	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	30	73
1	G	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	30	73
2	B	893/915 (98%)	785 (88%)	80 (9%)	28 (3%)	5	44
2	D	893/915 (98%)	784 (88%)	82 (9%)	27 (3%)	5	44
2	F	894/915 (98%)	786 (88%)	78 (9%)	30 (3%)	5	42
2	H	890/915 (97%)	782 (88%)	75 (8%)	33 (4%)	4	39
3	I	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	12	56
3	J	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	12	56
3	K	505/507 (100%)	445 (88%)	52 (10%)	8 (2%)	12	56
3	L	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	12	56
4	M	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	16	61
4	N	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	16	61
4	P	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	16	61
4	Q	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	16	61
All	All	8446/8636 (98%)	7530 (89%)	746 (9%)	170 (2%)	9	52

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	933	GLU
2	B	967	GLN
2	B	1269	GLU
2	B	1281	ARG
2	B	1291	TRP
2	B	1292	GLU

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Mol	Chain	Res	Type
2	B	1294	ALA
2	B	1337	ASN
2	B	1338	LYS
2	B	1359	LYS
2	B	1377	THR
2	B	1503	ASP
2	D	933	GLU
2	D	967	GLN
2	D	1281	ARG
2	D	1291	TRP
2	D	1292	GLU
2	D	1294	ALA
2	D	1337	ASN
2	D	1338	LYS
2	D	1359	LYS
2	D	1377	THR
2	D	1503	ASP
2	F	933	GLU
2	F	967	GLN
2	F	1269	GLU
2	F	1281	ARG
2	F	1291	TRP
2	F	1292	GLU
2	F	1337	ASN
2	F	1338	LYS
2	F	1361	THR
2	F	1377	THR
2	F	1417	SER
2	F	1446	ASN
2	H	933	GLU
2	H	968	MET
2	H	1281	ARG
2	H	1291	TRP
2	H	1292	GLU
2	H	1337	ASN
2	H	1338	LYS
2	H	1361	THR
2	H	1377	THR
2	H	1417	SER
2	H	1446	ASN
2	H	1493	GLU
3	I	236	ILE

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Mol	Chain	Res	Type
3	I	407	PRO
3	I	701	LYS
3	I	706	GLN
3	J	236	ILE
3	J	407	PRO
3	J	701	LYS
3	J	706	GLN
3	K	236	ILE
3	K	407	PRO
3	K	701	LYS
3	K	706	GLN
3	L	236	ILE
3	L	407	PRO
3	L	701	LYS
3	L	706	GLN
2	B	911	PRO
2	B	1360	ASN
2	B	1361	THR
2	B	1476	GLU
2	B	1571	ALA
2	D	911	PRO
2	D	1360	ASN
2	D	1361	THR
2	D	1476	GLU
2	D	1480	LEU
2	D	1571	ALA
2	F	911	PRO
2	F	1267	HIS
2	F	1294	ALA
2	F	1476	GLU
2	F	1498	ILE
2	F	1571	ALA
2	H	1266	ASP
2	H	1269	GLU
2	H	1294	ALA
2	H	1476	GLU
2	H	1496	CYS
2	H	1498	ILE
2	H	1571	ALA
1	A	442	GLU
1	A	643	PRO
2	B	1387	THR

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Mol	Chain	Res	Type
2	B	1502	ASP
2	B	1573	LYS
1	C	442	GLU
1	C	643	PRO
2	D	1387	THR
2	D	1502	ASP
2	D	1573	LYS
1	E	442	GLU
1	E	643	PRO
2	F	1387	THR
2	F	1573	LYS
1	G	442	GLU
2	H	911	PRO
2	H	1387	THR
2	H	1573	LYS
3	I	707	LYS
3	J	516	VAL
3	J	707	LYS
3	K	516	VAL
3	K	707	LYS
3	L	707	LYS
1	A	505	PRO
2	B	1196	ASN
2	B	1265	PRO
2	B	1480	LEU
1	C	505	PRO
2	D	1196	ASN
2	D	1265	PRO
2	D	1269	GLU
1	E	505	PRO
2	F	1196	ASN
2	F	1265	PRO
2	F	1268	GLN
2	F	1331	LYS
2	F	1637	PHE
1	G	505	PRO
2	H	967	GLN
2	H	1267	HIS
2	H	1486	ASP
2	H	1495	ASN
2	H	1502	ASP
3	I	516	VAL

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Mol	Chain	Res	Type
3	L	516	VAL
4	M	7	SER
4	N	7	SER
4	P	7	SER
4	Q	7	SER
2	B	834	GLN
2	B	1201	PRO
2	B	1267	HIS
2	B	1536	PHE
2	D	834	GLN
2	D	1201	PRO
2	D	1536	PHE
2	F	834	GLN
2	F	1201	PRO
2	F	1270	LEU
2	F	1536	PHE
1	G	643	PRO
2	H	834	GLN
2	H	1196	ASN
2	H	1201	PRO
2	H	1264	ALA
2	H	1536	PHE
3	I	268	LEU
3	J	268	LEU
3	K	268	LEU
3	L	268	LEU
3	I	482	GLY
3	J	482	GLY
3	K	482	GLY
3	L	482	GLY
2	B	1517	PRO
2	D	1517	PRO
2	F	1517	PRO
2	H	1517	PRO
1	A	208	PRO
1	C	208	PRO
1	E	208	PRO
1	G	208	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	558/567 (98%)	549 (98%)	9 (2%)	70	88
1	C	558/567 (98%)	549 (98%)	9 (2%)	70	88
1	E	558/567 (98%)	549 (98%)	9 (2%)	70	88
1	G	558/567 (98%)	549 (98%)	9 (2%)	70	88
2	B	793/810 (98%)	769 (97%)	24 (3%)	48	78
2	D	790/810 (98%)	766 (97%)	24 (3%)	48	78
2	F	793/810 (98%)	769 (97%)	24 (3%)	48	78
2	H	793/810 (98%)	766 (97%)	27 (3%)	44	77
3	I	442/446 (99%)	429 (97%)	13 (3%)	50	79
3	J	442/446 (99%)	429 (97%)	13 (3%)	50	79
3	K	442/446 (99%)	429 (97%)	13 (3%)	50	79
3	L	442/446 (99%)	429 (97%)	13 (3%)	50	79
4	M	76/84 (90%)	73 (96%)	3 (4%)	39	74
4	N	76/84 (90%)	73 (96%)	3 (4%)	39	74
4	P	76/84 (90%)	73 (96%)	3 (4%)	39	74
4	Q	76/84 (90%)	73 (96%)	3 (4%)	39	74
All	All	7473/7628 (98%)	7274 (97%)	199 (3%)	52	80

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	81	ASN
1	A	144	ASN
1	A	155	GLN
1	A	289	VAL
1	A	398	LEU
1	A	404	THR
1	A	440	ARG

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Mol	Chain	Res	Type
1	A	551	ARG
2	B	757	LYS
2	B	770	ASN
2	B	833	ARG
2	B	834	GLN
2	B	841	ARG
2	B	937	LYS
2	B	945	LEU
2	B	953	GLU
2	B	1018	GLU
2	B	1196	ASN
2	B	1292	GLU
2	B	1334	LEU
2	B	1335	THR
2	B	1342	LYS
2	B	1361	THR
2	B	1416	PHE
2	B	1433	GLU
2	B	1445	PHE
2	B	1462	ASN
2	B	1520	ASP
2	B	1535	ASP
2	B	1536	PHE
2	B	1569	ARG
2	B	1637	PHE
1	C	10	ASN
1	C	81	ASN
1	C	144	ASN
1	C	155	GLN
1	C	289	VAL
1	C	398	LEU
1	C	404	THR
1	C	440	ARG
1	C	551	ARG
2	D	757	LYS
2	D	770	ASN
2	D	833	ARG
2	D	834	GLN
2	D	841	ARG
2	D	937	LYS
2	D	945	LEU
2	D	953	GLU

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Mol	Chain	Res	Type
2	D	1018	GLU
2	D	1196	ASN
2	D	1292	GLU
2	D	1334	LEU
2	D	1335	THR
2	D	1342	LYS
2	D	1361	THR
2	D	1416	PHE
2	D	1433	GLU
2	D	1445	PHE
2	D	1462	ASN
2	D	1520	ASP
2	D	1535	ASP
2	D	1536	PHE
2	D	1569	ARG
2	D	1637	PHE
1	E	10	ASN
1	E	81	ASN
1	E	144	ASN
1	E	155	GLN
1	E	289	VAL
1	E	398	LEU
1	E	404	THR
1	E	440	ARG
1	E	551	ARG
2	F	757	LYS
2	F	770	ASN
2	F	833	ARG
2	F	834	GLN
2	F	841	ARG
2	F	937	LYS
2	F	945	LEU
2	F	953	GLU
2	F	1018	GLU
2	F	1196	ASN
2	F	1268	GLN
2	F	1292	GLU
2	F	1334	LEU
2	F	1335	THR
2	F	1342	LYS
2	F	1397	LYS
2	F	1433	GLU

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Mol	Chain	Res	Type
2	F	1462	ASN
2	F	1520	ASP
2	F	1535	ASP
2	F	1536	PHE
2	F	1569	ARG
2	F	1572	LEU
2	F	1640	PRO
1	G	10	ASN
1	G	81	ASN
1	G	144	ASN
1	G	155	GLN
1	G	289	VAL
1	G	398	LEU
1	G	404	THR
1	G	440	ARG
1	G	551	ARG
2	H	757	LYS
2	H	770	ASN
2	H	833	ARG
2	H	834	GLN
2	H	841	ARG
2	H	937	LYS
2	H	945	LEU
2	H	953	GLU
2	H	968	MET
2	H	969	THR
2	H	1018	GLU
2	H	1196	ASN
2	H	1267	HIS
2	H	1292	GLU
2	H	1334	LEU
2	H	1335	THR
2	H	1342	LYS
2	H	1397	LYS
2	H	1433	GLU
2	H	1462	ASN
2	H	1498	ILE
2	H	1499	GLN
2	H	1520	ASP
2	H	1535	ASP
2	H	1536	PHE
2	H	1569	ARG

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Mol	Chain	Res	Type
2	H	1572	LEU
3	I	237	VAL
3	I	255	SER
3	I	322	HIS
3	I	329	ASN
3	I	368	ASN
3	I	381	ARG
3	I	423	ASN
3	I	446	GLU
3	I	539	LYS
3	I	540	LYS
3	I	654	ARG
3	I	702	ASN
3	I	703	GLN
3	J	237	VAL
3	J	255	SER
3	J	322	HIS
3	J	329	ASN
3	J	368	ASN
3	J	381	ARG
3	J	423	ASN
3	J	446	GLU
3	J	539	LYS
3	J	540	LYS
3	J	654	ARG
3	J	702	ASN
3	J	703	GLN
3	K	237	VAL
3	K	255	SER
3	K	322	HIS
3	K	329	ASN
3	K	368	ASN
3	K	381	ARG
3	K	423	ASN
3	K	446	GLU
3	K	539	LYS
3	K	540	LYS
3	K	654	ARG
3	K	702	ASN
3	K	703	GLN
3	L	237	VAL
3	L	255	SER

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Mol	Chain	Res	Type
3	L	322	HIS
3	L	329	ASN
3	L	368	ASN
3	L	381	ARG
3	L	423	ASN
3	L	446	GLU
3	L	539	LYS
3	L	540	LYS
3	L	654	ARG
3	L	702	ASN
3	L	703	GLN
4	M	11	GLN
4	M	69	GLN
4	M	71	GLN
4	N	11	GLN
4	N	69	GLN
4	N	71	GLN
4	P	11	GLN
4	P	69	GLN
4	P	71	GLN
4	Q	11	GLN
4	Q	69	GLN
4	Q	71	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (256) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	87	GLN
1	A	104	GLN
1	A	144	ASN
1	A	155	GLN
1	A	161	GLN
1	A	162	ASN
1	A	163	GLN
1	A	370	GLN
1	A	380	GLN
1	A	390	ASN
1	A	414	GLN
1	A	490	GLN
1	A	558	GLN
1	A	567	HIS

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Mol	Chain	Res	Type
1	A	634	GLN
1	A	639	GLN
2	B	738	ASN
2	B	752	ASN
2	B	762	ASN
2	B	770	ASN
2	B	820	ASN
2	B	834	GLN
2	B	860	HIS
2	B	886	GLN
2	B	896	HIS
2	B	897	HIS
2	B	1011	GLN
2	B	1069	ASN
2	B	1076	GLN
2	B	1114	ASN
2	B	1130	GLN
2	B	1141	ASN
2	B	1160	ASN
2	B	1196	ASN
2	B	1204	GLN
2	B	1267	HIS
2	B	1277	GLN
2	B	1333	GLN
2	B	1337	ASN
2	B	1401	ASN
2	B	1431	HIS
2	B	1451	GLN
2	B	1462	ASN
2	B	1559	GLN
2	B	1579	HIS
2	B	1608	HIS
2	B	1620	ASN
1	C	10	ASN
1	C	60	HIS
1	C	87	GLN
1	C	104	GLN
1	C	132	HIS
1	C	144	ASN
1	C	155	GLN
1	C	161	GLN
1	C	162	ASN

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Mol	Chain	Res	Type
1	C	163	GLN
1	C	356	ASN
1	C	370	GLN
1	C	380	GLN
1	C	390	ASN
1	C	414	GLN
1	C	450	ASN
1	C	490	GLN
1	C	558	GLN
1	C	567	HIS
1	C	634	GLN
1	C	639	GLN
2	D	738	ASN
2	D	752	ASN
2	D	762	ASN
2	D	770	ASN
2	D	820	ASN
2	D	834	GLN
2	D	860	HIS
2	D	897	HIS
2	D	1011	GLN
2	D	1069	ASN
2	D	1076	GLN
2	D	1114	ASN
2	D	1130	GLN
2	D	1141	ASN
2	D	1160	ASN
2	D	1196	ASN
2	D	1204	GLN
2	D	1267	HIS
2	D	1277	GLN
2	D	1333	GLN
2	D	1337	ASN
2	D	1401	ASN
2	D	1431	HIS
2	D	1451	GLN
2	D	1462	ASN
2	D	1559	GLN
2	D	1579	HIS
2	D	1608	HIS
2	D	1620	ASN
1	E	60	HIS

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Mol	Chain	Res	Type
1	E	87	GLN
1	E	104	GLN
1	E	132	HIS
1	E	144	ASN
1	E	155	GLN
1	E	161	GLN
1	E	162	ASN
1	E	163	GLN
1	E	356	ASN
1	E	370	GLN
1	E	380	GLN
1	E	390	ASN
1	E	414	GLN
1	E	450	ASN
1	E	490	GLN
1	E	558	GLN
1	E	567	HIS
1	E	639	GLN
2	F	738	ASN
2	F	752	ASN
2	F	762	ASN
2	F	770	ASN
2	F	820	ASN
2	F	834	GLN
2	F	860	HIS
2	F	897	HIS
2	F	1011	GLN
2	F	1069	ASN
2	F	1076	GLN
2	F	1114	ASN
2	F	1130	GLN
2	F	1141	ASN
2	F	1160	ASN
2	F	1196	ASN
2	F	1204	GLN
2	F	1267	HIS
2	F	1277	GLN
2	F	1333	GLN
2	F	1337	ASN
2	F	1401	ASN
2	F	1431	HIS
2	F	1451	GLN

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Mol	Chain	Res	Type
2	F	1462	ASN
2	F	1559	GLN
2	F	1579	HIS
2	F	1608	HIS
2	F	1620	ASN
2	F	1641	ASN
1	G	60	HIS
1	G	87	GLN
1	G	104	GLN
1	G	132	HIS
1	G	144	ASN
1	G	155	GLN
1	G	161	GLN
1	G	162	ASN
1	G	163	GLN
1	G	356	ASN
1	G	370	GLN
1	G	380	GLN
1	G	390	ASN
1	G	414	GLN
1	G	490	GLN
1	G	558	GLN
1	G	587	ASN
1	G	634	GLN
1	G	639	GLN
2	H	738	ASN
2	H	752	ASN
2	H	762	ASN
2	H	770	ASN
2	H	820	ASN
2	H	834	GLN
2	H	860	HIS
2	H	896	HIS
2	H	897	HIS
2	H	1277	GLN
2	H	1333	GLN
2	H	1337	ASN
2	H	1401	ASN
2	H	1431	HIS
2	H	1451	GLN
2	H	1462	ASN
2	H	1559	GLN

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Mol	Chain	Res	Type
2	H	1579	HIS
2	H	1608	HIS
2	H	1620	ASN
3	I	270	ASN
3	I	329	ASN
3	I	368	ASN
3	I	392	ASN
3	I	411	GLN
3	I	413	ASN
3	I	423	ASN
3	I	466	HIS
3	I	531	HIS
3	I	533	ASN
3	I	591	GLN
3	I	703	GLN
3	J	270	ASN
3	J	329	ASN
3	J	368	ASN
3	J	392	ASN
3	J	411	GLN
3	J	413	ASN
3	J	423	ASN
3	J	435	ASN
3	J	466	HIS
3	J	531	HIS
3	J	533	ASN
3	J	591	GLN
3	J	703	GLN
3	K	270	ASN
3	K	329	ASN
3	K	368	ASN
3	K	392	ASN
3	K	411	GLN
3	K	413	ASN
3	K	423	ASN
3	K	435	ASN
3	K	466	HIS
3	K	531	HIS
3	K	533	ASN
3	K	591	GLN
3	K	703	GLN
3	L	270	ASN

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Mol	Chain	Res	Type
3	L	329	ASN
3	L	368	ASN
3	L	392	ASN
3	L	411	GLN
3	L	413	ASN
3	L	423	ASN
3	L	466	HIS
3	L	531	HIS
3	L	533	ASN
3	L	591	GLN
3	L	703	GLN
4	M	11	GLN
4	M	27	ASN
4	M	49	GLN
4	M	69	GLN
4	M	71	GLN
4	N	11	GLN
4	N	27	ASN
4	N	49	GLN
4	N	69	GLN
4	N	71	GLN
4	P	11	GLN
4	P	27	ASN
4	P	49	GLN
4	P	69	GLN
4	P	71	GLN
4	Q	11	GLN
4	Q	27	ASN
4	Q	49	GLN
4	Q	69	GLN
4	Q	71	GLN

5.3.3 RNA (i)

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)

52 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	NDG	A	1646	1,5	14,14,15	0.44	0	15,19,21	0.80	1 (6%)
5	NAG	A	1647	5	14,14,15	0.61	0	15,19,21	1.85	4 (26%)
5	BMA	A	1648	5	11,11,12	0.54	0	14,15,17	1.33	2 (14%)
5	BMA	A	1649	5	11,11,12	0.64	0	14,15,17	1.39	2 (14%)
5	NDG	B	2642	2,5	14,14,15	0.53	0	15,19,21	1.20	2 (13%)
5	NAG	B	2643	5	14,14,15	0.51	0	15,19,21	2.18	1 (6%)
5	BMA	B	2644	5	11,11,12	0.91	0	14,15,17	1.97	3 (21%)
5	BMA	B	2645	5	11,11,12	0.70	0	14,15,17	0.81	0
7	NDG	C	1646	1,7	14,14,15	0.59	0	15,19,21	1.26	2 (13%)
7	NAG	C	1647	7	14,14,15	0.64	0	15,19,21	1.04	1 (6%)
7	BMA	C	1648	7	11,11,12	0.64	0	14,15,17	1.16	1 (7%)
7	BMA	C	1649	7	11,11,12	0.73	0	14,15,17	1.63	3 (21%)
7	BMA	C	1650	7	11,11,12	0.64	0	14,15,17	1.82	4 (28%)
5	NDG	D	2642	2,5	14,14,15	0.47	0	15,19,21	0.86	0
5	NAG	D	2643	5	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
5	BMA	D	2644	5	11,11,12	0.61	0	14,15,17	1.36	2 (14%)
5	BMA	D	2645	5	11,11,12	0.64	0	14,15,17	1.31	2 (14%)
5	NDG	E	1646	1,5	14,14,15	0.53	0	15,19,21	0.85	1 (6%)
5	NAG	E	1647	5	14,14,15	0.58	0	15,19,21	1.04	1 (6%)
5	BMA	E	1648	5	11,11,12	0.67	0	14,15,17	1.10	1 (7%)
5	BMA	E	1649	5	11,11,12	0.89	1 (9%)	14,15,17	1.81	3 (21%)
8	NDG	F	2642	8,2	14,14,15	0.37	0	15,19,21	1.10	2 (13%)
8	NAG	F	2643	8	14,14,15	0.43	0	15,19,21	1.74	3 (20%)
8	BMA	F	2644	8	11,11,12	0.57	0	14,15,17	1.58	4 (28%)
8	BMA	F	2645	8	11,11,12	0.96	1 (9%)	14,15,17	1.79	4 (28%)
8	BMA	F	2646	8	11,11,12	0.64	0	14,15,17	1.91	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BMA	F	2647	8	11,11,12	0.67	0	14,15,17	1.08	1 (7%)
7	NDG	G	1646	1,7	14,14,15	0.42	0	15,19,21	1.20	1 (6%)
7	NAG	G	1647	7	14,14,15	0.50	0	15,19,21	2.25	5 (33%)
7	BMA	G	1648	7	11,11,12	0.50	0	14,15,17	2.85	6 (42%)
7	BMA	G	1649	7	11,11,12	0.54	0	14,15,17	4.67	6 (42%)
7	BMA	G	1650	7	11,11,12	0.62	0	14,15,17	1.42	2 (14%)
10	NDG	H	2642	10,2	14,14,15	0.56	0	15,19,21	0.68	0
10	NAG	H	2643	10	14,14,15	0.46	0	15,19,21	0.78	0
10	MAN	H	2644	10	11,11,12	0.75	0	14,15,17	1.36	1 (7%)
10	MAN	H	2645	10	11,11,12	0.73	0	14,15,17	1.11	2 (14%)
12	NDG	I	1743	3,12	14,14,15	0.54	0	15,19,21	1.08	2 (13%)
12	NAG	I	1744	12	14,14,15	0.60	0	15,19,21	1.01	1 (6%)
12	MAN	I	1745	12	11,11,12	0.62	0	14,15,17	1.07	1 (7%)
13	NDG	I	1746	3,13	14,14,15	0.52	0	15,19,21	1.18	2 (13%)
13	NAG	I	1747	13	14,14,15	0.52	0	15,19,21	0.97	1 (6%)
12	NDG	J	1743	3,12	14,14,15	0.49	0	15,19,21	1.10	1 (6%)
12	NAG	J	1744	12	14,14,15	0.58	0	15,19,21	1.04	1 (6%)
12	MAN	J	1745	12	11,11,12	0.62	0	14,15,17	1.00	1 (7%)
14	NDG	K	1743	3,14	14,14,15	0.60	0	15,19,21	1.11	1 (6%)
14	NAG	K	1744	14	14,14,15	0.67	0	15,19,21	1.41	3 (20%)
14	MAN	K	1745	14	11,11,12	0.54	0	14,15,17	1.88	5 (35%)
14	MAN	K	1746	14	11,11,12	0.72	0	14,15,17	1.66	3 (21%)
14	MAN	K	1748	14	11,11,12	0.58	0	14,15,17	1.09	2 (14%)
16	NDG	L	1743	3,16	14,14,15	0.47	0	15,19,21	0.95	0
16	NAG	L	1744	16	14,14,15	0.58	0	15,19,21	1.08	1 (6%)
16	BMA	L	1745	16	11,11,12	0.62	0	14,15,17	0.91	1 (7%)

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	NDG	A	1646	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1647	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1648	5	-	0/2/19/22	0/1/1/1
5	BMA	A	1649	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NDG	B	2642	2,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	2643	5	-	0/6/23/26	0/1/1/1
5	BMA	B	2644	5	-	0/2/19/22	0/1/1/1
5	BMA	B	2645	5	-	0/2/19/22	0/1/1/1
7	NDG	C	1646	1,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	C	1647	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1648	7	-	0/2/19/22	0/1/1/1
7	BMA	C	1649	7	-	0/2/19/22	0/1/1/1
7	BMA	C	1650	7	-	0/2/19/22	0/1/1/1
5	NDG	D	2642	2,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	D	2643	5	-	0/6/23/26	0/1/1/1
5	BMA	D	2644	5	-	0/2/19/22	0/1/1/1
5	BMA	D	2645	5	-	0/2/19/22	0/1/1/1
5	NDG	E	1646	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	E	1647	5	-	0/6/23/26	0/1/1/1
5	BMA	E	1648	5	-	0/2/19/22	0/1/1/1
5	BMA	E	1649	5	-	0/2/19/22	0/1/1/1
8	NDG	F	2642	8,2	-	0/6/23/26	0/1/1/1
8	NAG	F	2643	8	-	0/6/23/26	0/1/1/1
8	BMA	F	2644	8	-	0/2/19/22	0/1/1/1
8	BMA	F	2645	8	-	0/2/19/22	0/1/1/1
8	BMA	F	2646	8	-	0/2/19/22	0/1/1/1
8	BMA	F	2647	8	-	0/2/19/22	0/1/1/1
7	NDG	G	1646	1,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	G	1647	7	-	0/6/23/26	0/1/1/1
7	BMA	G	1648	7	-	0/2/19/22	0/1/1/1
7	BMA	G	1649	7	-	0/2/19/22	0/1/1/1
7	BMA	G	1650	7	-	0/2/19/22	0/1/1/1
10	NDG	H	2642	10,2	1/1/5/7	0/6/23/26	0/1/1/1
10	NAG	H	2643	10	-	0/6/23/26	0/1/1/1
10	MAN	H	2644	10	1/1/4/5	0/2/19/22	0/1/1/1
10	MAN	H	2645	10	1/1/4/5	0/2/19/22	0/1/1/1
12	NDG	I	1743	3,12	1/1/5/7	0/6/23/26	0/1/1/1
12	NAG	I	1744	12	-	0/6/23/26	0/1/1/1
12	MAN	I	1745	12	1/1/4/5	0/2/19/22	0/1/1/1
13	NDG	I	1746	3,13	1/1/5/7	0/6/23/26	0/1/1/1
13	NAG	I	1747	13	-	0/6/23/26	0/1/1/1
12	NDG	J	1743	3,12	1/1/5/7	0/6/23/26	0/1/1/1
12	NAG	J	1744	12	-	0/6/23/26	0/1/1/1
12	MAN	J	1745	12	1/1/4/5	0/2/19/22	0/1/1/1
14	NDG	K	1743	3,14	1/1/5/7	0/6/23/26	0/1/1/1
14	NAG	K	1744	14	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MAN	K	1745	14	1/1/4/5	0/2/19/22	0/1/1/1
14	MAN	K	1746	14	1/1/4/5	0/2/19/22	0/1/1/1
14	MAN	K	1748	14	1/1/4/5	0/2/19/22	0/1/1/1
16	NDG	L	1743	3,16	1/1/5/7	0/6/23/26	0/1/1/1
16	NAG	L	1744	16	-	0/6/23/26	0/1/1/1
16	BMA	L	1745	16	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1649	BMA	O5-C1	-2.24	1.40	1.43
8	F	2645	BMA	O5-C1	-2.12	1.40	1.43

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	1649	BMA	C1-C2-C3	-10.99	96.54	109.54
7	G	1649	BMA	C1-O5-C5	-7.49	102.74	112.25
7	G	1649	BMA	C3-C4-C5	-7.24	97.58	110.20
7	G	1648	BMA	C1-C2-C3	-5.62	102.89	109.54
5	E	1649	BMA	C1-O5-C5	-4.80	106.16	112.25
8	F	2646	BMA	C1-C2-C3	-4.52	104.20	109.54
7	G	1648	BMA	C1-O5-C5	-4.35	106.73	112.25
7	C	1650	BMA	C1-C2-C3	-4.29	104.46	109.54
7	G	1648	BMA	C6-C5-C4	-4.15	102.77	113.02
5	B	2644	BMA	C1-O5-C5	-4.04	107.13	112.25
5	D	2644	BMA	C1-O5-C5	-4.02	107.14	112.25
14	K	1745	MAN	C1-O5-C5	-4.01	107.16	112.25
8	F	2644	BMA	O5-C1-C2	-3.51	105.17	110.86
7	G	1647	NAG	C4-C3-C2	-3.41	105.92	111.23
7	C	1649	BMA	O3-C3-C4	-3.36	102.78	110.34
5	A	1648	BMA	C1-O5-C5	-3.36	107.99	112.25
8	F	2646	BMA	O5-C1-C2	-3.28	105.53	110.86
7	G	1650	BMA	C1-C2-C3	-3.27	105.68	109.54
8	F	2643	NAG	C4-C3-C2	-3.25	106.18	111.23
12	I	1745	MAN	C1-O5-C5	-3.15	108.24	112.25
5	A	1649	BMA	O5-C1-C2	-3.03	105.94	110.86
5	A	1649	BMA	C1-C2-C3	-3.00	106.00	109.54
7	G	1650	BMA	O5-C1-C2	-2.97	106.03	110.86
5	E	1649	BMA	O5-C1-C2	-2.93	106.11	110.86
7	C	1650	BMA	C1-O5-C5	-2.92	108.54	112.25
7	C	1650	BMA	O5-C1-C2	-2.89	106.17	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1649	BMA	C1-C2-C3	-2.89	106.13	109.54
5	D	2645	BMA	O5-C1-C2	-2.88	106.19	110.86
14	K	1746	MAN	O5-C1-C2	-2.87	106.21	110.86
7	C	1648	BMA	C1-O5-C5	-2.78	108.72	112.25
5	D	2645	BMA	C1-C2-C3	-2.78	106.25	109.54
12	J	1745	MAN	C1-O5-C5	-2.77	108.73	112.25
14	K	1745	MAN	C1-C2-C3	-2.77	106.26	109.54
8	F	2645	BMA	C1-O5-C5	-2.76	108.75	112.25
8	F	2646	BMA	C1-O5-C5	-2.66	108.87	112.25
7	C	1649	BMA	C1-O5-C5	-2.65	108.88	112.25
5	E	1648	BMA	C1-O5-C5	-2.63	108.92	112.25
10	H	2645	MAN	C1-O5-C5	-2.54	109.03	112.25
8	F	2644	BMA	C2-C3-C4	-2.49	106.81	111.04
16	L	1745	BMA	C1-O5-C5	-2.34	109.27	112.25
5	A	1647	NAG	O4-C4-C3	-2.33	105.10	110.34
8	F	2644	BMA	C1-C2-C3	-2.28	106.84	109.54
14	K	1745	MAN	C2-C3-C4	-2.23	107.26	111.04
8	F	2642	NDG	C4-C3-C2	-2.22	107.77	111.23
8	F	2647	BMA	O5-C1-C2	-2.20	107.29	110.86
7	G	1647	NAG	C2-N2-C7	-2.16	120.27	123.04
10	H	2645	MAN	O5-C1-C2	-2.11	107.43	110.86
14	K	1746	MAN	C6-C5-C4	-2.11	107.81	113.02
14	K	1744	NAG	O4-C4-C3	-2.09	105.62	110.34
8	F	2644	BMA	C6-C5-C4	-2.02	108.03	113.02
7	G	1647	NAG	O4-C4-C3	2.03	114.92	110.34
7	C	1647	NAG	C4-C3-C2	2.04	114.41	111.23
5	E	1646	NDG	C3-C4-C5	2.07	113.81	110.20
5	A	1646	NDG	C1-O-C5	2.08	114.89	112.25
5	D	2644	BMA	O5-C5-C6	2.12	111.93	107.35
14	K	1748	MAN	C1-O5-C5	2.14	114.96	112.25
14	K	1748	MAN	C3-C4-C5	2.15	113.94	110.20
13	I	1746	NDG	C4-C3-C2	2.15	114.57	111.23
8	F	2642	NDG	O4-C4-C5	2.17	114.99	109.24
5	B	2642	NDG	C3-C4-C5	2.18	113.99	110.20
8	F	2645	BMA	C3-C4-C5	2.19	114.02	110.20
12	I	1743	NDG	C3-C4-C5	2.25	114.11	110.20
12	I	1743	NDG	C1-O-C5	2.25	115.11	112.25
12	I	1744	NAG	C4-C3-C2	2.27	114.76	111.23
12	J	1744	NAG	C4-C3-C2	2.29	114.79	111.23
5	B	2644	BMA	C2-C3-C4	2.31	114.97	111.04
7	G	1649	BMA	O3-C3-C2	2.33	114.21	110.00
16	L	1744	NAG	C4-C3-C2	2.35	114.89	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	2643	NAG	C1-O5-C5	2.40	115.29	112.25
7	C	1646	NDG	C1-O-C5	2.40	115.30	112.25
7	C	1650	BMA	C3-C4-C5	2.47	114.50	110.20
7	G	1646	NDG	C4-C3-C2	2.52	115.15	111.23
5	A	1648	BMA	O5-C5-C6	2.56	112.90	107.35
7	G	1648	BMA	O6-C6-C5	2.58	119.86	111.33
5	E	1647	NAG	C1-O5-C5	2.59	115.53	112.25
13	I	1747	NAG	C1-O5-C5	2.59	115.53	112.25
13	I	1746	NDG	C3-C4-C5	2.66	114.84	110.20
5	A	1647	NAG	C3-C4-C5	2.68	114.87	110.20
8	F	2646	BMA	C3-C4-C5	2.69	114.89	110.20
12	J	1743	NDG	C1-O-C5	2.75	115.73	112.25
14	K	1743	NDG	C3-C4-C5	2.79	115.05	110.20
8	F	2645	BMA	C2-C3-C4	2.87	115.91	111.04
14	K	1744	NAG	C3-C4-C5	2.87	115.19	110.20
8	F	2643	NAG	O4-C4-C3	2.90	116.87	110.34
14	K	1745	MAN	O3-C3-C2	2.91	115.25	110.00
14	K	1745	MAN	O5-C5-C6	2.99	113.83	107.35
7	G	1647	NAG	O4-C4-C5	3.02	117.25	109.24
7	C	1646	NDG	C3-C4-C5	3.07	115.54	110.20
5	B	2642	NDG	C1-O-C5	3.09	116.17	112.25
7	C	1649	BMA	C3-C4-C5	3.16	115.70	110.20
7	G	1648	BMA	C3-C4-C5	3.24	115.85	110.20
14	K	1744	NAG	C4-C3-C2	3.33	116.40	111.23
5	A	1647	NAG	C1-O5-C5	3.46	116.63	112.25
8	F	2643	NAG	C1-O5-C5	3.72	116.97	112.25
14	K	1746	MAN	C3-C4-C5	3.83	116.87	110.20
8	F	2645	BMA	C1-C2-C3	4.14	114.44	109.54
10	H	2644	MAN	C1-C2-C3	4.16	114.46	109.54
5	A	1647	NAG	C4-C3-C2	4.54	118.29	111.23
5	B	2644	BMA	C1-C2-C3	4.72	115.13	109.54
7	G	1648	BMA	O5-C5-C6	4.72	117.57	107.35
7	G	1649	BMA	O5-C5-C6	4.90	117.96	107.35
7	G	1649	BMA	O3-C3-C4	6.31	124.55	110.34
7	G	1647	NAG	C1-O5-C5	6.32	120.26	112.25
5	B	2643	NAG	C1-O5-C5	7.52	121.79	112.25

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	I	1743	NDG	C1
12	J	1745	MAN	C1

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Mol	Chain	Res	Type	Atom
16	L	1743	NDG	C1
5	B	2642	NDG	C1
5	D	2642	NDG	C1
14	K	1743	NDG	C1
14	K	1746	MAN	C1
10	H	2642	NDG	C1
12	I	1745	MAN	C1
12	J	1743	NDG	C1
7	C	1646	NDG	C1
5	E	1646	NDG	C1
10	H	2644	MAN	C1
10	H	2645	MAN	C1
13	I	1746	NDG	C1
14	K	1748	MAN	C1
14	K	1745	MAN	C1
7	G	1646	NDG	C1

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1646	NDG	1	0
5	A	1647	NAG	1	0
5	B	2642	NDG	1	0
7	C	1646	NDG	2	0
7	C	1647	NAG	1	0
5	D	2642	NDG	1	0
5	D	2643	NAG	1	0
5	E	1646	NDG	4	0
5	E	1647	NAG	1	0
5	E	1648	BMA	1	0
5	E	1649	BMA	1	0
8	F	2644	BMA	1	0
8	F	2645	BMA	2	0
8	F	2647	BMA	1	0
7	G	1646	NDG	2	0
7	G	1647	NAG	3	0
7	G	1648	BMA	2	0
7	G	1649	BMA	2	0
10	H	2643	NAG	1	0
10	H	2644	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	2645	MAN	1	0
12	I	1743	NDG	2	0
12	I	1744	NAG	2	0
12	J	1743	NDG	1	0
12	J	1744	NAG	2	0
14	K	1743	NDG	4	0
14	K	1744	NAG	1	0
14	K	1745	MAN	2	0
14	K	1746	MAN	1	0
14	K	1748	MAN	1	0

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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	BMA	B	2646	-	11,11,12	0.70	0	14,15,17	1.46	3 (21%)
9	MAN	G	1651	-	11,11,12	0.79	0	14,15,17	1.79	4 (28%)
6	BMA	K	1747	-	11,11,12	0.77	0	14,15,17	2.04	4 (28%)
15	NDG	K	1749	3	14,14,15	0.50	0	15,19,21	1.02	1 (6%)
15	NDG	L	1746	3	14,14,15	0.49	0	15,19,21	0.64	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
6	BMA	B	2646	-	-	0/2/19/22	0/1/1/1
9	MAN	G	1651	-	-	0/2/19/22	0/1/1/1
6	BMA	K	1747	-	-	0/2/19/22	0/1/1/1
15	NDG	K	1749	3	-	0/6/23/26	0/1/1/1
15	NDG	L	1746	3	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	1747	BMA	C1-O5-C5	-5.42	105.37	112.25
9	G	1651	MAN	C1-C2-C3	-4.09	104.70	109.54
6	K	1747	BMA	C1-C2-C3	-3.83	105.01	109.54
6	B	2646	BMA	C1-C2-C3	-3.40	105.52	109.54
9	G	1651	MAN	C1-O5-C5	-3.25	108.12	112.25
6	B	2646	BMA	C1-O5-C5	-2.34	109.28	112.25
15	K	1749	NDG	C2-N2-C7	2.07	125.69	123.04
6	K	1747	BMA	C3-C4-C5	2.20	114.03	110.20
6	B	2646	BMA	O5-C1-C2	2.45	114.83	110.86
6	K	1747	BMA	O5-C1-C2	2.49	114.90	110.86
9	G	1651	MAN	C3-C4-C5	2.73	114.96	110.20
9	G	1651	MAN	O5-C1-C2	2.81	115.41	110.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	L	1746	NDG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	1651	MAN	1	0
15	K	1749	NDG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	638/645 (98%)	0.19	17 (2%)	58	46	87, 142, 190, 237	0
1	C	638/645 (98%)	0.14	14 (2%)	65	54	80, 127, 176, 228	0
1	E	638/645 (98%)	0.13	10 (1%)	74	64	84, 142, 196, 245	0
1	G	638/645 (98%)	0.45	61 (9%)	10	7	93, 180, 241, 267	0
2	B	901/915 (98%)	0.18	27 (2%)	54	40	91, 167, 229, 260	0
2	D	901/915 (98%)	0.20	28 (3%)	52	40	81, 155, 216, 266	0
2	F	900/915 (98%)	0.39	51 (5%)	27	19	96, 179, 284, 329	0
2	H	605/915 (66%)	0.40	37 (6%)	25	16	98, 162, 231, 294	0
3	I	507/507 (100%)	0.00	4 (0%)	87	81	93, 142, 197, 240	0
3	J	507/507 (100%)	0.15	17 (3%)	49	37	127, 170, 220, 261	0
3	K	507/507 (100%)	0.23	23 (4%)	37	27	132, 183, 230, 284	0
3	L	507/507 (100%)	-0.02	5 (0%)	84	77	101, 144, 194, 239	0
4	M	84/92 (91%)	-0.05	1 (1%)	81	72	87, 110, 186, 221	0
4	N	84/92 (91%)	-0.02	2 (2%)	62	50	97, 116, 189, 227	0
4	P	84/92 (91%)	-0.00	2 (2%)	62	50	100, 124, 176, 211	0
4	Q	84/92 (91%)	-0.09	2 (2%)	62	50	100, 119, 186, 200	0
All	All	8223/8636 (95%)	0.21	301 (3%)	45	34	80, 155, 228, 329	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	645	ALA	9.1
1	G	421	ALA	6.8
2	F	1501	SER	5.8
1	G	399	SER	5.7
2	F	1038	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
2	H	1501	SER	5.3
1	G	645	ALA	5.3
1	A	645	ALA	5.2
2	D	1603	ASP	4.8
2	H	1328	ALA	4.7
2	F	1122	THR	4.7
2	F	1136	CYS	4.6
2	F	1049	LYS	4.6
3	K	574	CYS	4.5
1	G	398	LEU	4.5
1	G	626	SER	4.5
1	G	636	ALA	4.4
4	P	2	THR	4.4
2	H	967	GLN	4.3
3	L	708	GLN	4.3
1	G	368	ALA	4.2
1	G	400	ILE	4.2
2	F	1116	GLU	4.1
1	A	48	SER	4.1
2	B	1099	ASP	4.0
1	C	48	SER	4.0
1	G	373	ASP	3.9
2	H	1593	LYS	3.9
3	K	699	VAL	3.9
1	G	420	GLN	3.9
1	G	333	ILE	3.8
4	N	85	TYR	3.8
3	J	703	GLN	3.7
2	H	964	PRO	3.7
1	G	71	ASN	3.7
2	F	1329	LYS	3.6
4	M	85	TYR	3.6
2	H	947	ASP	3.6
2	F	1529	LYS	3.6
3	K	479	PRO	3.5
2	F	1328	ALA	3.5
2	H	1316	GLY	3.5
2	F	1593	LYS	3.5
2	F	1077	VAL	3.4
1	C	376	GLN	3.4
1	G	26	ASP	3.4
2	F	1048	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	488	PRO	3.4
2	F	967	GLN	3.4
2	H	935	VAL	3.4
1	G	28	GLN	3.4
2	F	1327	HIS	3.3
1	G	1	SER	3.3
2	H	1561	THR	3.3
3	J	480	SER	3.3
2	F	1079	CYS	3.3
2	H	1329	LYS	3.3
3	J	479	PRO	3.3
2	D	1358	ALA	3.3
3	J	235	LYS	3.3
3	K	668	ASN	3.2
2	F	1073	ILE	3.2
1	E	257	GLU	3.2
1	G	370	GLN	3.2
3	J	542	ALA	3.2
2	H	1268	GLN	3.2
2	F	1047	PHE	3.2
2	F	1594	PRO	3.2
4	Q	2	THR	3.2
2	B	1504	LYS	3.2
1	G	369	VAL	3.1
3	K	385	TYR	3.1
1	E	83	PHE	3.1
1	G	643	PRO	3.1
2	B	1622	LYS	3.1
3	K	544	ILE	3.1
3	K	527	VAL	3.1
2	D	1269	GLU	3.1
2	H	1598	TYR	3.1
2	H	1559	GLN	3.1
2	D	1267	HIS	3.1
2	H	1283	SER	3.1
3	J	510	HIS	3.1
1	G	644	ALA	3.1
1	G	609	SER	3.0
1	E	71	ASN	3.0
2	F	1074	ASP	3.0
2	D	1293	SER	3.0
2	H	1594	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
3	K	542	ALA	3.0
1	G	32	PRO	2.9
2	H	912	GLU	2.9
3	J	346	ASP	2.9
2	B	1097	GLN	2.9
2	B	1611	GLU	2.9
1	G	335	PHE	2.9
1	C	190	ASN	2.9
3	I	708	GLN	2.9
1	G	528	SER	2.9
1	G	419	MET	2.9
1	C	314	SER	2.8
1	E	521	GLN	2.8
2	H	1546	THR	2.8
1	A	437	SER	2.8
1	E	101	VAL	2.8
1	G	100	LEU	2.8
2	D	1618	GLU	2.8
2	D	1531	GLN	2.8
2	H	948	GLN	2.8
2	F	1143	LEU	2.8
1	G	518	ALA	2.7
1	G	519	SER	2.7
1	A	46	VAL	2.7
1	A	20	MET	2.7
3	K	480	SER	2.7
2	D	928	GLU	2.7
3	K	703	GLN	2.7
1	A	100	LEU	2.7
2	B	1180	LEU	2.7
2	F	1046	ALA	2.7
4	P	85	TYR	2.6
1	G	374	THR	2.6
2	F	1166	THR	2.6
3	J	699	VAL	2.6
2	B	1623	GLN	2.6
1	G	352	VAL	2.6
2	F	1194	ASP	2.6
3	J	544	ILE	2.6
2	B	964	PRO	2.6
3	J	641	TYR	2.6
2	F	1181	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	41	PRO	2.6
2	F	1119	MET	2.6
1	G	339	PRO	2.5
2	F	987	GLY	2.5
2	H	1502	ASP	2.5
3	J	385	TYR	2.5
2	B	1270	LEU	2.5
2	F	913	GLY	2.5
1	G	20	MET	2.5
2	B	1618	GLU	2.5
2	D	1155	GLU	2.5
2	H	1531	GLN	2.5
2	D	1486	ASP	2.5
1	G	258	GLN	2.5
1	G	527	ASP	2.5
2	D	1504	LYS	2.5
2	F	1035	LEU	2.5
2	F	1094	GLY	2.5
2	H	1374	GLN	2.5
2	H	1523	TYR	2.5
1	G	340	LYS	2.5
3	L	709	VAL	2.4
1	C	20	MET	2.4
2	D	1539	TYR	2.4
2	F	925	LEU	2.4
2	B	1621	GLN	2.4
2	F	953	GLU	2.4
3	K	739	LEU	2.4
1	A	101	VAL	2.4
1	G	491	ASP	2.4
1	A	644	ALA	2.4
1	E	636	ALA	2.4
3	K	512	ILE	2.4
1	C	450	ASN	2.4
2	F	1534	ASN	2.4
2	H	1325	MET	2.4
1	G	102	SER	2.4
2	D	1314	GLY	2.4
2	F	1294	ALA	2.4
2	D	1488	LEU	2.4
2	F	820	ASN	2.4
1	G	637	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	L	710	PRO	2.4
1	C	315	ASP	2.4
2	B	1488	LEU	2.3
2	B	1614	GLU	2.3
1	C	644	ALA	2.3
1	A	22	LEU	2.3
3	K	706	GLN	2.3
3	K	697	VAL	2.3
1	E	370	GLN	2.3
2	F	1374	GLN	2.3
2	F	1078	LEU	2.3
2	F	1039	GLN	2.3
3	K	640	GLY	2.3
3	K	346	ASP	2.3
1	G	433	TYR	2.3
2	H	921	ALA	2.3
2	D	1563	ILE	2.3
2	F	1502	ASP	2.3
1	G	460	ALA	2.3
2	H	1293	SER	2.3
2	B	963	THR	2.3
2	H	1560	ARG	2.3
2	F	1051	ALA	2.3
2	H	1292	GLU	2.3
1	E	437	SER	2.3
1	G	564	GLU	2.3
2	B	912	GLU	2.3
4	Q	85	TYR	2.3
2	F	1118	ASP	2.3
3	J	354	ARG	2.3
3	K	543	GLY	2.3
3	K	589	THR	2.3
1	C	636	ALA	2.3
1	G	365	VAL	2.3
1	G	411	GLU	2.3
3	K	510	HIS	2.3
2	H	1327	HIS	2.2
1	G	72	ARG	2.2
2	D	1158	TYR	2.2
2	D	1538	GLU	2.2
2	B	1267	HIS	2.2
2	H	1308	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLU	2.2
1	E	441	THR	2.2
4	N	83	SER	2.2
1	G	99	VAL	2.2
2	F	1135	ILE	2.2
2	B	1365	GLU	2.2
1	G	94	VAL	2.2
1	G	608	GLY	2.2
2	D	1537	ASP	2.2
2	F	1093	ASP	2.2
3	K	478	ARG	2.2
1	G	256	GLY	2.2
2	D	932	ARG	2.2
2	D	1332	ASP	2.2
1	E	1	SER	2.2
3	L	345	ASP	2.2
2	F	1076	GLN	2.2
2	H	916	MET	2.2
2	B	1539	TYR	2.2
2	B	965	VAL	2.2
2	F	912	GLU	2.2
1	A	190	ASN	2.2
2	D	1534	ASN	2.2
1	C	368	ALA	2.2
2	B	1606	VAL	2.2
2	D	1089	LYS	2.1
3	K	545	PRO	2.1
1	G	548	SER	2.1
2	H	1317	GLN	2.1
2	H	1547	ILE	2.1
2	B	763	GLY	2.1
1	A	69	PRO	2.1
1	G	523	GLU	2.1
1	C	420	GLN	2.1
1	G	452	ASN	2.1
2	F	1157	ASN	2.1
1	G	98	VAL	2.1
1	G	50	GLU	2.1
3	J	343	TRP	2.1
2	F	1559	GLN	2.1
3	L	706	GLN	2.1
1	G	81	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	1621	GLN	2.1
1	A	421	ALA	2.1
1	A	450	ASN	2.1
1	A	452	ASN	2.1
2	D	968	MET	2.1
3	J	389	ASP	2.1
1	G	40	PHE	2.1
2	H	1324	THR	2.1
2	B	1328	ALA	2.1
2	B	1269	GLU	2.1
2	B	1295	SER	2.1
2	D	1530	VAL	2.1
2	F	988	CYS	2.1
2	H	1310	VAL	2.1
2	H	1269	GLU	2.1
1	G	254	GLN	2.1
1	G	401	THR	2.1
3	J	350	GLU	2.1
2	D	1184	LEU	2.1
1	G	27	ALA	2.1
2	B	1594	PRO	2.1
2	F	1034	GLN	2.1
1	A	389	ILE	2.1
2	F	1514	ALA	2.1
1	G	630	GLN	2.1
3	I	703	GLN	2.1
2	H	1562	PHE	2.1
2	F	916	MET	2.0
2	F	1500	LYS	2.0
1	C	71	ASN	2.0
2	H	1540	ILE	2.0
2	B	1162	GLN	2.0
3	J	571	CYS	2.0
3	I	706	GLN	2.0
3	K	343	TRP	2.0
3	J	588	THR	2.0
1	G	332	GLN	2.0
3	I	702	ASN	2.0
1	C	419	MET	2.0
2	D	1183	PRO	2.0
2	B	1158	TYR	2.0
1	A	491	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	1510	ARG	2.0
3	K	705	ARG	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	NDG	L	1743	14/15	0.87	0.36	1.80	122,147,148,148	0
14	NDG	K	1743	14/15	0.87	0.28	0.75	174,204,206,207	0
12	NDG	I	1743	14/15	0.92	0.28	0.68	122,149,151,152	0
12	NDG	J	1743	14/15	0.90	0.27	0.33	158,188,189,189	0
7	NDG	C	1646	14/15	0.82	0.28	-0.76	163,191,192,193	0
5	NDG	E	1646	14/15	0.83	0.23	-0.92	174,204,206,206	0
8	NDG	F	2642	14/15	0.86	0.22	-1.27	169,193,194,194	0
5	NDG	A	1646	14/15	0.88	0.21	-2.67	156,185,187,188	0
7	NAG	G	1647	14/15	0.83	0.25	-	213,216,216,217	0
16	NAG	L	1744	14/15	0.85	0.43	-	185,187,189,189	0
12	NAG	J	1744	14/15	0.81	0.33	-	177,179,180,180	0
8	BMA	F	2644	11/12	0.84	0.15	-	232,233,234,234	0
5	NAG	A	1647	14/15	0.82	0.23	-	199,200,201,203	0
5	NAG	D	2643	14/15	0.88	0.21	-	200,201,202,203	0
5	BMA	A	1648	11/12	0.80	0.30	-	212,214,215,216	0
14	NAG	K	1744	14/15	0.83	0.27	-	196,199,201,202	0
5	NDG	B	2642	14/15	0.91	0.23	-	163,194,194,195	0
5	NDG	D	2642	14/15	0.89	0.20	-	147,176,178,179	0
8	BMA	F	2646	11/12	0.72	0.37	-	221,222,224,224	0
16	BMA	L	1745	11/12	0.76	0.24	-	197,201,202,202	0
14	MAN	K	1746	11/12	0.87	0.52	-	229,230,232,232	0
10	NDG	H	2642	14/15	0.90	0.21	-	183,213,214,215	0
7	BMA	C	1648	11/12	0.64	0.27	-	219,220,222,223	0
12	MAN	I	1745	11/12	0.79	0.24	-	205,207,208,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	BMA	G	1648	11/12	0.68	0.54	-	247,249,250,251	0
5	BMA	D	2645	11/12	0.86	0.28	-	229,232,233,234	0
5	BMA	E	1648	11/12	0.74	0.43	-	229,230,231,232	0
8	BMA	F	2645	11/12	0.83	0.23	-	248,249,249,250	0
7	BMA	G	1650	11/12	0.55	0.68	-	229,231,232,232	0
7	BMA	C	1650	11/12	0.70	0.33	-	231,233,235,235	0
12	MAN	J	1745	11/12	0.61	0.36	-	206,210,211,212	0
5	NAG	E	1647	14/15	0.83	0.21	-	223,225,227,227	0
7	NAG	C	1647	14/15	0.67	0.27	-	200,202,203,203	0
13	NAG	I	1747	14/15	0.63	0.66	-	222,223,224,224	0
12	NAG	I	1744	14/15	0.94	0.36	-	178,180,181,182	0
10	NAG	H	2643	14/15	0.82	0.26	-	221,222,224,225	0
10	MAN	H	2644	11/12	0.64	0.27	-	229,230,231,232	0
8	NAG	F	2643	14/15	0.91	0.21	-	200,202,204,204	0
5	NAG	B	2643	14/15	0.91	0.28	-	193,196,196,197	0
10	MAN	H	2645	11/12	0.68	0.61	-	234,236,237,238	0
5	BMA	B	2645	11/12	0.41	0.37	-	237,239,240,241	0
5	BMA	A	1649	11/12	0.83	0.44	-	226,227,228,228	0
13	NDG	I	1746	14/15	0.79	0.65	-	198,225,227,227	0
7	BMA	G	1649	11/12	0.59	0.37	-	226,228,229,230	0
5	BMA	E	1649	11/12	0.81	0.27	-	209,212,214,215	0
7	BMA	C	1649	11/12	0.65	0.29	-	235,237,239,240	0
14	MAN	K	1748	11/12	0.84	0.36	-	230,232,235,235	0
8	BMA	F	2647	11/12	0.70	0.50	-	214,215,217,217	0
14	MAN	K	1745	11/12	0.73	0.34	-	249,252,253,254	0
5	BMA	B	2644	11/12	0.39	0.35	-	218,220,222,223	0
5	BMA	D	2644	11/12	0.67	0.32	-	220,221,223,223	0
7	NDG	G	1646	14/15	0.90	0.16	-	198,201,208,215	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, 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
11	MG	L	1742	1/1	0.91	0.25	0.53	127,127,127,127	0
11	MG	I	1742	1/1	0.42	0.17	-0.61	120,120,120,120	0
11	MG	K	1742	1/1	0.84	0.11	-0.92	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	MG	J	1742	1/1	0.82	0.07	-2.08	148,148,148,148	0
6	BMA	B	2646	11/12	0.66	0.51	-	198,200,200,201	0
6	BMA	K	1747	11/12	0.76	0.52	-	194,195,196,196	0
15	NDG	L	1746	14/15	0.87	0.56	-	176,204,205,205	0
9	MAN	G	1651	11/12	0.45	0.54	-	222,225,227,228	0
15	NDG	K	1749	14/15	0.76	0.47	-	184,214,216,217	0

6.5 Other polymers

There are no such residues in this entry.