



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:13 pm BST

PDB ID : 3D29
Title : Proteasome Inhibition by Fellutamide B
Authors : Groll, M.; Hines, J.; Fahnestock, M.; Crews, M.C.
Deposited on : 2008-05-07
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

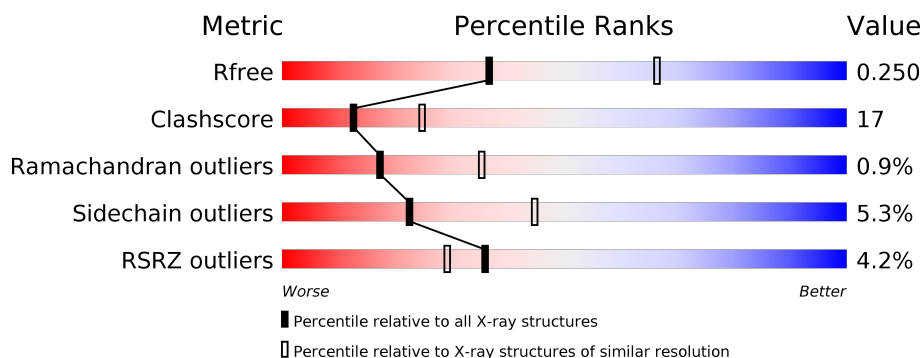
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>.</div> </div> </div>
1	O	250	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
2	B	244	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>37%</div> <div>.</div> </div> </div>
2	P	244	<div> <div>6%</div> <div> <div></div> <div>57%</div> <div>40%</div> <div>.</div> </div> </div>
3	C	241	<div> <div>11%</div> <div> <div></div> <div>61%</div> <div>37%</div> <div>.</div> </div> </div>
3	Q	241	<div> <div>15%</div> <div> <div></div> <div>61%</div> <div>37%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51114 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 Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	237	GLU	-	EXPRESSION TAG	UNP P40303
C	238	GLN	-	EXPRESSION TAG	UNP P40303
C	239	GLU	-	EXPRESSION TAG	UNP P40303
C	240	LYS	-	EXPRESSION TAG	UNP P40303
C	241	GLN	-	EXPRESSION TAG	UNP P40303
C	242	GLU	-	EXPRESSION TAG	UNP P40303
C	243	GLN	-	EXPRESSION TAG	UNP P40303
Q	237	GLU	-	EXPRESSION TAG	UNP P40303

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	238	GLN	-	EXPRESSION TAG	UNP P40303
Q	239	GLU	-	EXPRESSION TAG	UNP P40303
Q	240	LYS	-	EXPRESSION TAG	UNP P40303
Q	241	GLN	-	EXPRESSION TAG	UNP P40303
Q	242	GLU	-	EXPRESSION TAG	UNP P40303
Q	243	GLN	-	EXPRESSION TAG	UNP P40303

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	6	ALA	-	EXPRESSION TAG	UNP P21243
G	7	GLY	-	EXPRESSION TAG	UNP P21243
U	6	ALA	-	EXPRESSION TAG	UNP P21243
U	7	GLY	-	EXPRESSION TAG	UNP P21243

- Molecule 8 is a protein called Proteasome component PUP1 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

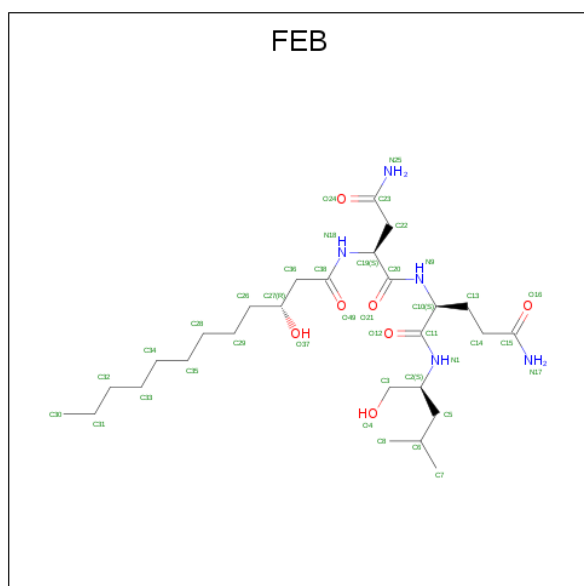
- Molecule 13 is a protein called Proteasome component PRE4 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is N 2 -[(3R)-3-hydroxydodecanoyl]-L-asparaginyl-N 1 -[(1S)-1-(hydroxymethyl)-3-methylbutyl]-L-glutamamide (three-letter code: FEB) (formula: C₂₇H₅₁N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			39	27	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			39	27	5	7		
15	N	1	Total	C	N	O	0	0
			39	27	5	7		
15	V	1	Total	C	N	O	0	0
			39	27	5	7		
15	Y	1	Total	C	N	O	0	0
			39	27	5	7		
15	2	1	Total	C	N	O	0	0
			39	27	5	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	55	Total	O	0	0
			55	55		
16	B	36	Total	O	0	0
			36	36		
16	C	46	Total	O	0	0
			46	46		
16	D	42	Total	O	0	0
			42	42		
16	E	23	Total	O	0	0
			23	23		
16	F	46	Total	O	0	0
			46	46		
16	G	62	Total	O	0	0
			62	62		
16	H	51	Total	O	0	0
			51	51		
16	I	66	Total	O	0	0
			66	66		
16	J	53	Total	O	0	0
			53	53		
16	K	42	Total	O	0	0
			42	42		
16	L	56	Total	O	0	0
			56	56		
16	M	68	Total	O	0	0
			68	68		
16	N	59	Total	O	0	0
			59	59		

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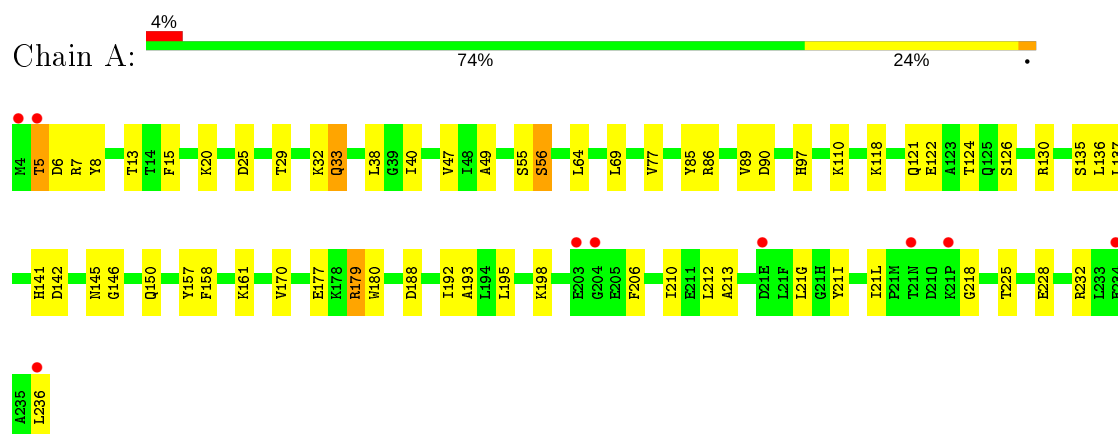
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	O	35	Total 35	O 35	0	0
16	P	29	Total 29	O 29	0	0
16	Q	26	Total 26	O 26	0	0
16	R	31	Total 31	O 31	0	0
16	S	20	Total 20	O 20	0	0
16	T	39	Total 39	O 39	0	0
16	U	61	Total 61	O 61	0	0
16	V	48	Total 48	O 48	0	0
16	W	59	Total 59	O 59	0	0
16	X	46	Total 46	O 46	0	0
16	Y	48	Total 48	O 48	0	0
16	Z	52	Total 52	O 52	0	0
16	1	74	Total 74	O 74	0	0
16	2	59	Total 59	O 59	0	0

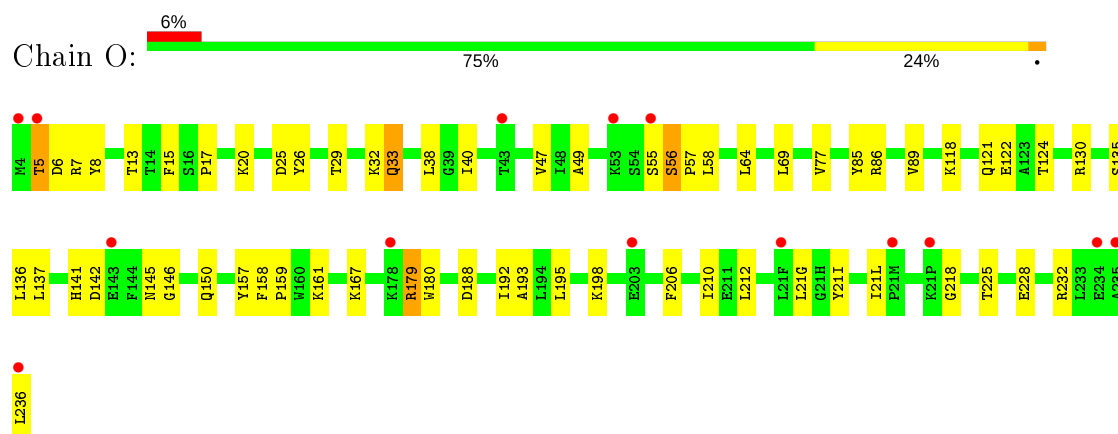
3 Residue-property plots [i](#)

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

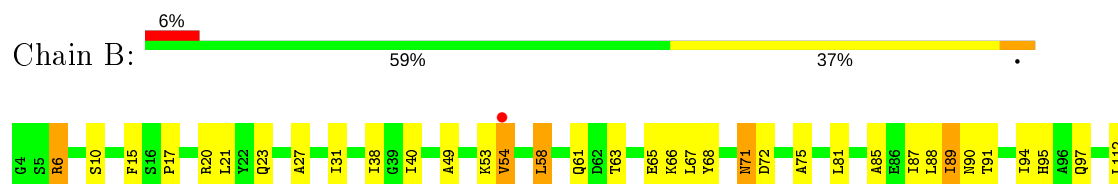
• Molecule 1: Proteasome component Y7

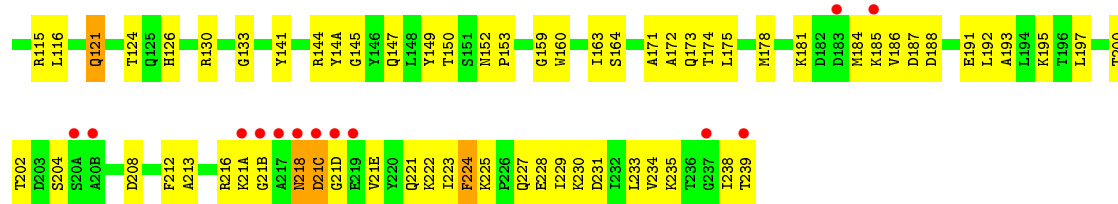


• Molecule 1: Proteasome component Y7

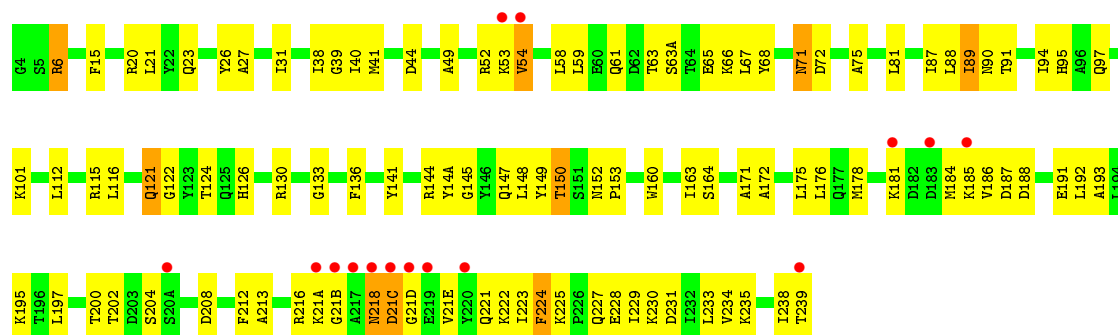


• Molecule 2: Proteasome component Y13

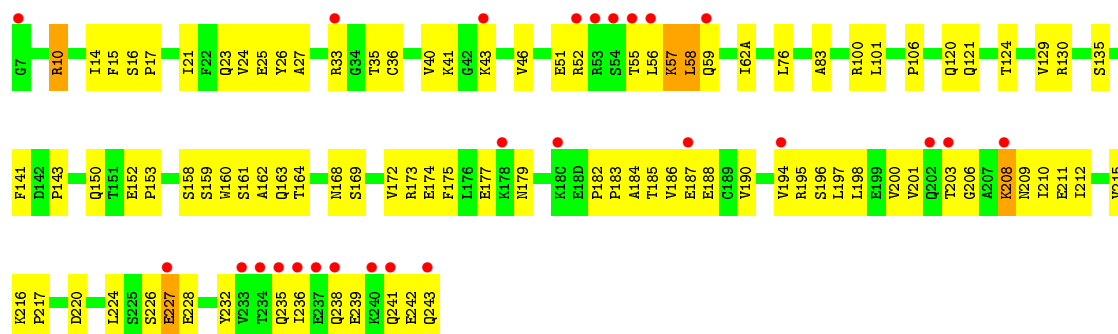




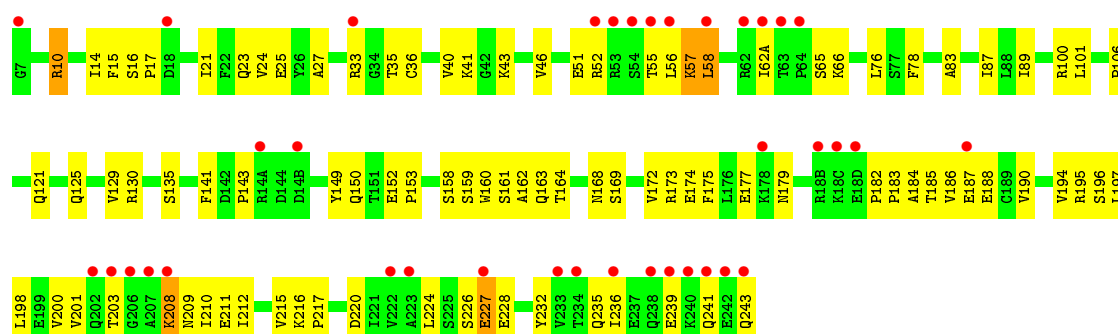
• Molecule 2: Proteasome component Y13



• Molecule 3: Proteasome component PRE6



• Molecule 3: Proteasome component PRE6



Chain D:

7% 75% 22%

D9 R10 G11 V12 Q23 V24 S27 L28 I40 G45 K52 P57 L58 L59 E60 S61 V68 G75 A85 I89 V97 Y102 E110 S111 L112 C117 L121 R122 F123 G12A E12B G12C A12D S12E G12F E12G I125 R126 L127 M128 S129 R130 P131 Y136 Q147 L148 F157 Y160 K163 E170 E175 L176 L177 S18D T185 L186 K187 E188 A189 E190 L191 L192 V193 L194 K195 L196 E202 E205 K206 L207 Q211 L212 I215 Q216 F221 L237 E241 A242 A243 E244

Chain R:

73% 25% 7%

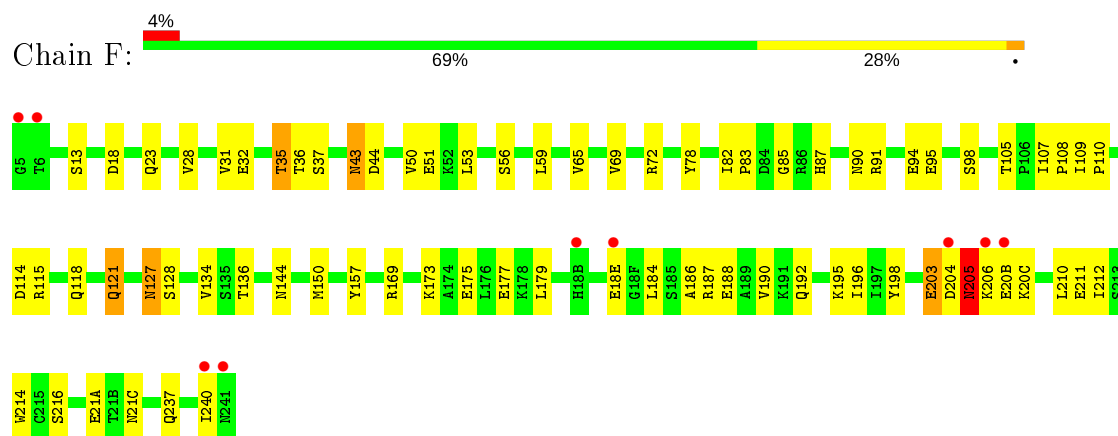
Chain E:

Category	Percentage
Red	4%
Green	66%
Yellow	29%
Orange	6%

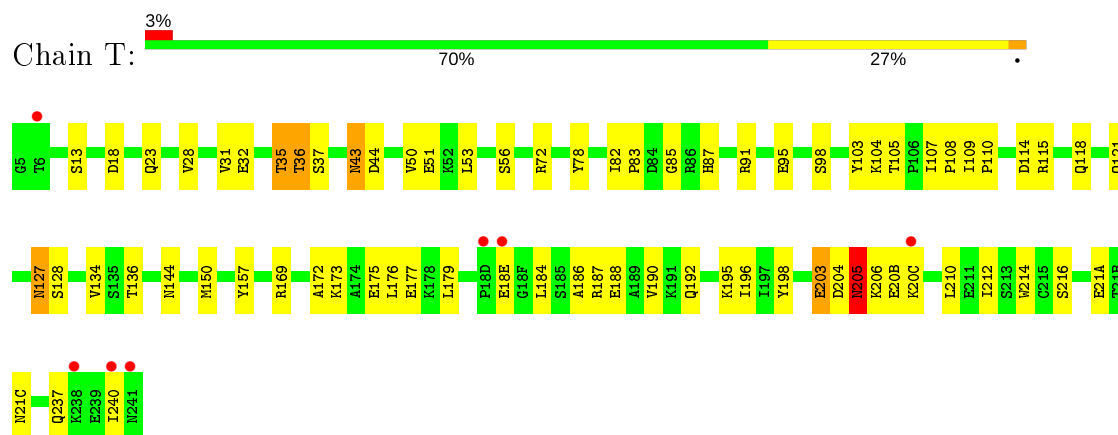
Chain S:

State	Category
F4	Red
R5	Red
N6	Red
N7	Red
T12	Red
T13	Red
T14	Red
F15	Red
F22	Red
Y26	Red
I31	Red
K32	Red
S35	Red
V36	Red
T37	Red
V38	Red
G39	Red
T44	Red
L48	Red
K52	Red
D56	Red
E57	Red
L58	Red
S59	Red
S60	Red
V63	Red
Q64	Red
R65	Red
K66	Red
I67	Red
H73	Red
H74	Red
G75	Red
L76	Red
A82	Red
R86	Red
N90	Red
Y91	Red
L92	Red
N97	Red
N104	Red
L107	Red
E111	Red
A112	Red
D113	Red
Q124	Red
R122	Red
M123	Red
T124	Red
Q125	Red
S126	Red
Y127	Red
R130	Red
P131	Red
Y132	Red
L136	Red
T139	Red
G140	Red
Y141	Red
L148	Red
F151	Red
Q152	Red
P153	Red
L160	Red
Y161	Red
G162	Red
T163	Red
Y175	Red
R176	Red
T179	Red
L180	Red
F180	Red
L18D	Red
K18E	Red
I18F	Red
D183	Red
G184	Red
N185	Red
L189	Red
Y194	Red
E195	Red
A196	Red
I197	Red
S198	Red
Q199	Red
S200	Red
L201	Red
R202	Red
D203	Red
E204	Red
S206	Red
L207	Red
T2B	Red
V2C	Red
D2D	Red
N2E	Red
I214	Red
V215	Red
G216	Red
K217	Red
P220	Red
F221	Red
T222	Red
I223	Red
G226	Red
E227	Red
A228	Red
V229	Red
A230	Red
K231	Red
Y232	Red
L233	Red

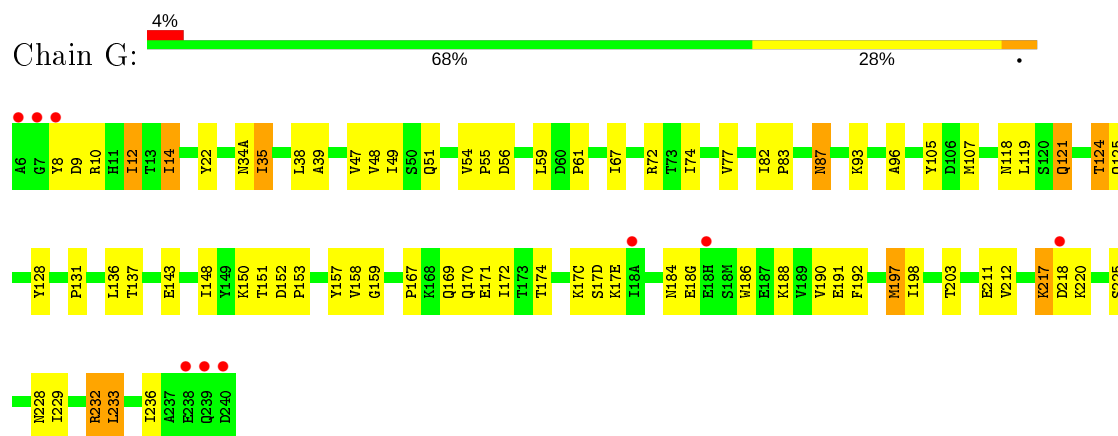
- Molecule 6: Proteasome component C1



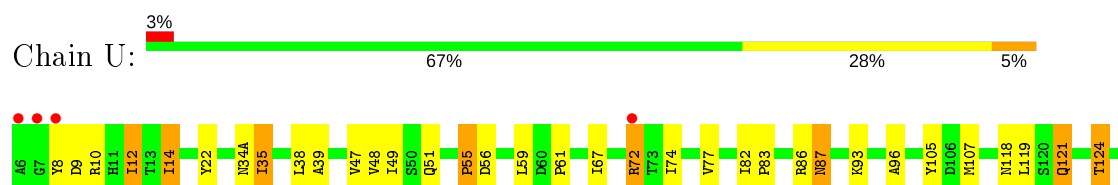
- Molecule 6: Proteasome component C1

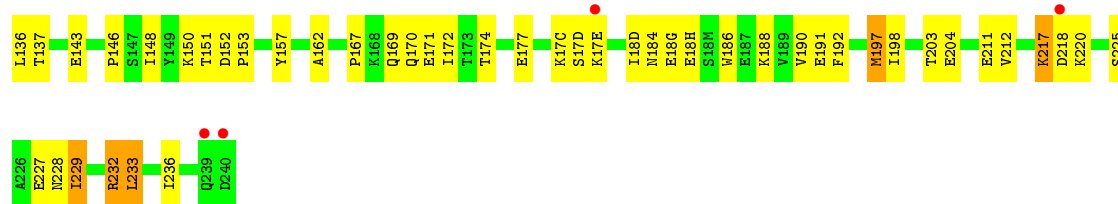


- Molecule 7: Proteasome component C7-alpha

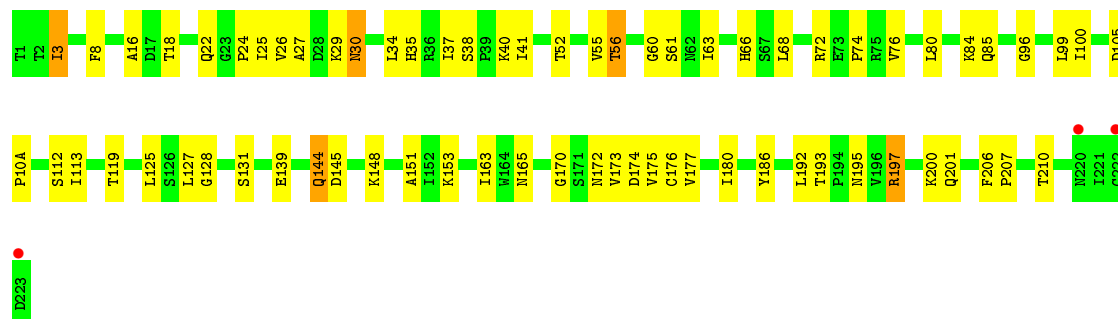


- Molecule 7: Proteasome component C7-alpha

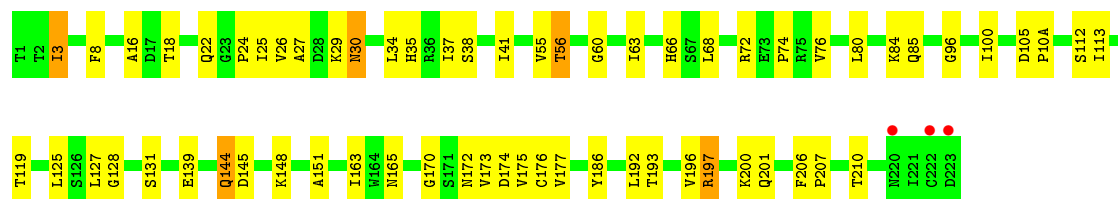




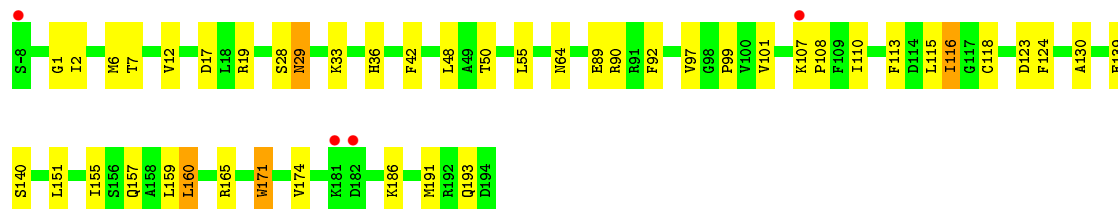
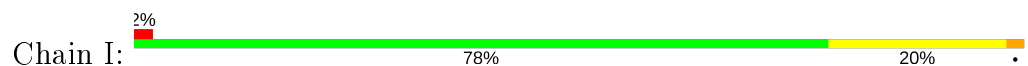
• Molecule 8: Proteasome component PUP1 precursor



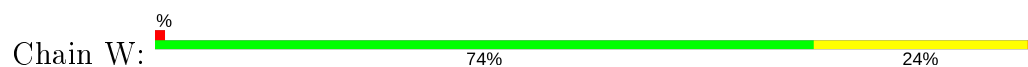
• Molecule 8: Proteasome component PUP1 precursor



• Molecule 9: Proteasome component PUP3



• Molecule 9: Proteasome component PUP3

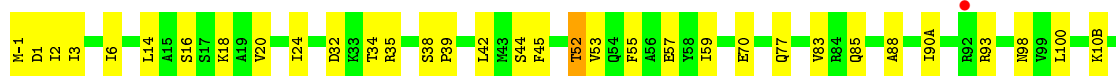




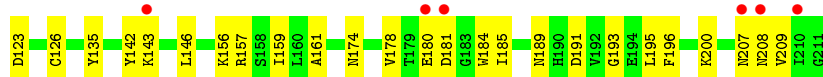
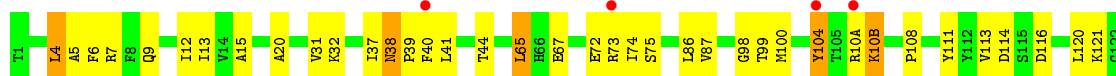
• Molecule 10: Proteasome component C11



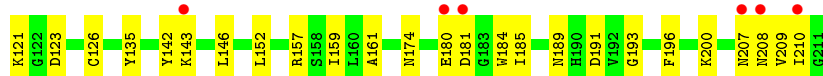
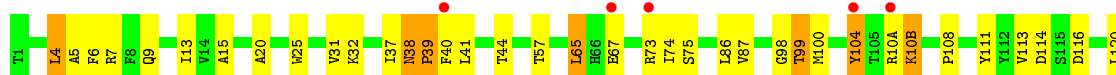
• Molecule 10: Proteasome component C11



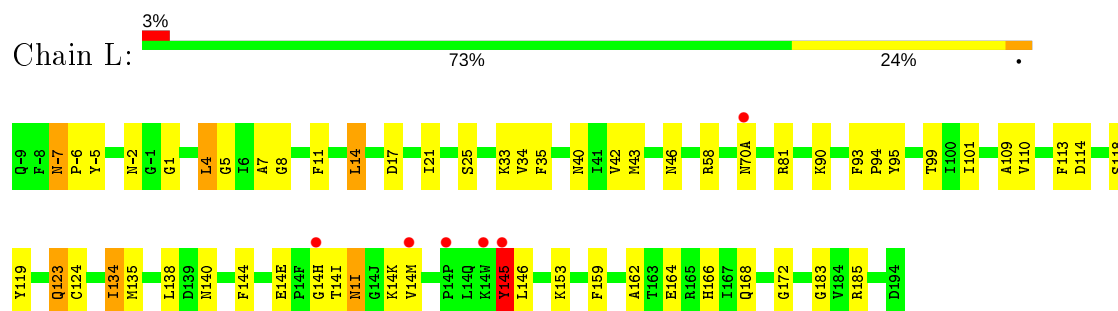
• Molecule 11: Proteasome component PRE2 precursor



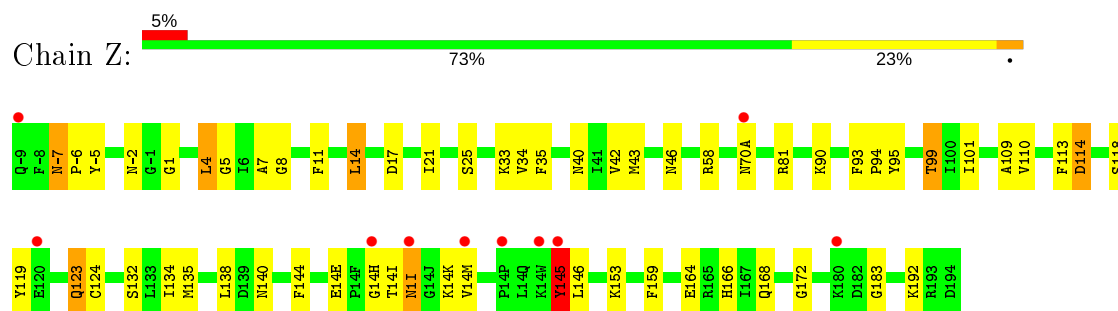
• Molecule 11: Proteasome component PRE2 precursor



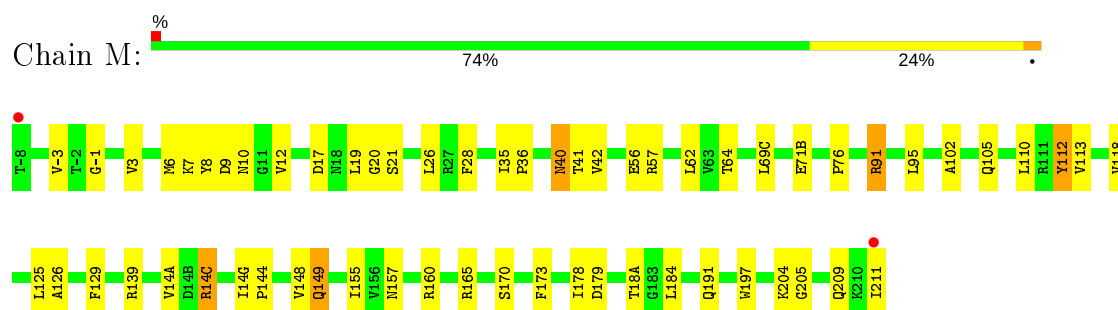
- Molecule 12: Proteasome component C5 precursor



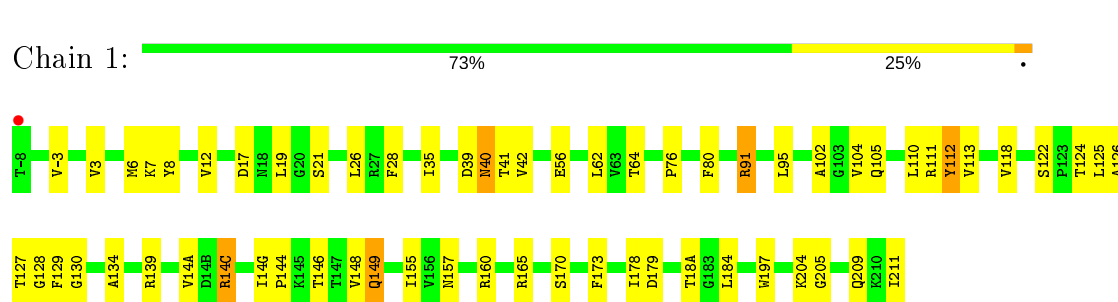
- Molecule 12: Proteasome component C5 precursor



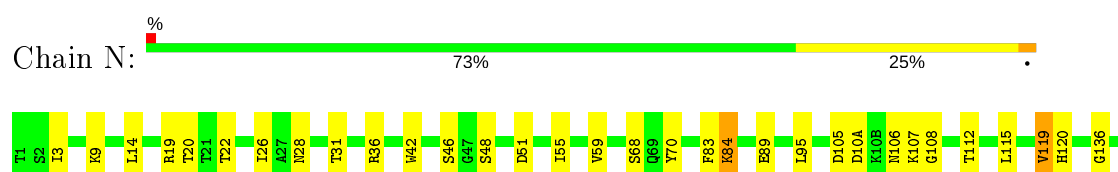
- Molecule 13: Proteasome component PRE4 precursor

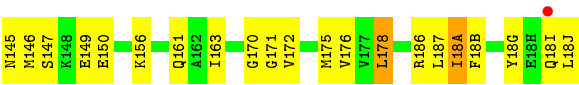


- Molecule 13: Proteasome component PRE4 precursor

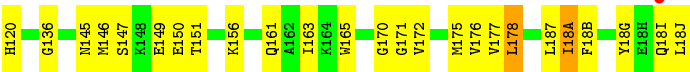


- Molecule 14: Proteasome component PRE3 precursor





● Molecule 14: Proteasome component PRE3 precursor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.27Å 301.58Å 143.45Å 90.00° 112.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 19.99 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.60) 98.0 (19.99-2.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.266 0.227 , 0.250	Depositor DCC
R_{free} test set	15699 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51114	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FEB

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	0.38	0/1952	0.63	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.35	0/1935	0.62	0/2618
2	P	0.36	0/1935	0.62	0/2618
3	C	0.35	0/1920	0.60	0/2598
3	Q	0.35	0/1920	0.61	0/2598
4	D	0.35	0/1887	0.62	0/2541
4	R	0.35	0/1887	0.62	0/2541
5	E	0.36	0/1823	0.62	0/2463
5	S	0.36	0/1823	0.62	0/2463
6	F	0.38	0/1937	0.62	0/2614
6	T	0.39	0/1937	0.62	0/2614
7	G	0.42	0/1959	0.65	0/2652
7	U	0.41	0/1959	0.64	0/2652
8	H	0.39	0/1716	0.66	0/2326
8	V	0.39	0/1716	0.66	0/2326
9	I	0.40	0/1611	0.67	0/2174
9	W	0.41	0/1611	0.68	0/2174
10	J	0.39	0/1613	0.65	0/2173
10	X	0.39	0/1613	0.65	0/2173
11	K	0.42	0/1681	0.69	1/2274 (0.0%)
11	Y	0.43	0/1681	0.69	1/2274 (0.0%)
12	L	0.42	0/1795	0.70	1/2420 (0.0%)
12	Z	0.41	0/1795	0.69	1/2420 (0.0%)
13	1	0.40	0/1855	0.67	1/2514 (0.0%)
13	M	0.40	0/1855	0.67	1/2514 (0.0%)
14	2	0.41	0/1541	0.67	1/2087 (0.0%)
14	N	0.43	0/1541	0.67	0/2087
All	All	0.39	0/50450	0.65	7/68192 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	95	LEU	N-CA-C	-5.53	96.07	111.00
13	M	95	LEU	N-CA-C	-5.39	96.43	111.00
14	2	22	THR	N-CA-C	-5.16	97.07	111.00
11	K	98	GLY	N-CA-C	-5.16	100.21	113.10
11	Y	98	GLY	N-CA-C	-5.14	100.25	113.10
12	L	145	TYR	CA-CB-CG	-5.09	103.73	113.40
12	Z	145	TYR	CA-CB-CG	-5.09	103.73	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	TYR	Sidechain

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	1915	0	1926	59	0
1	O	1915	0	1926	58	0
2	B	1905	0	1901	97	0
2	P	1905	0	1901	91	0
3	C	1891	0	1900	107	0
3	Q	1891	0	1900	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1862	0	1836	50	0
4	R	1862	0	1836	56	0
5	E	1795	0	1797	73	0
5	S	1795	0	1797	70	0
6	F	1897	0	1886	60	0
6	T	1897	0	1886	54	0
7	G	1921	0	1910	78	0
7	U	1921	0	1910	80	0
8	H	1685	0	1687	62	0
8	V	1685	0	1687	54	0
9	I	1581	0	1574	50	0
9	W	1581	0	1574	53	0
10	J	1585	0	1590	63	0
10	X	1585	0	1590	65	0
11	K	1644	0	1594	70	0
11	Y	1644	0	1594	71	0
12	L	1757	0	1711	52	0
12	Z	1757	0	1711	51	0
13	1	1824	0	1832	50	0
13	M	1824	0	1832	52	0
14	2	1512	0	1480	53	0
14	N	1512	0	1480	49	0
15	2	39	0	50	6	0
15	H	39	0	50	3	0
15	K	39	0	50	0	0
15	N	39	0	50	7	0
15	V	39	0	50	3	0
15	Y	39	0	50	0	0
16	1	74	0	0	4	0
16	2	59	0	0	1	0
16	A	55	0	0	4	0
16	B	36	0	0	1	0
16	C	46	0	0	1	0
16	D	42	0	0	2	0
16	E	23	0	0	1	0
16	F	46	0	0	2	0
16	G	62	0	0	3	0
16	H	51	0	0	3	0
16	I	66	0	0	2	0
16	J	53	0	0	3	0
16	K	42	0	0	6	0
16	L	56	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	M	68	0	0	6	0
16	N	59	0	0	2	0
16	O	35	0	0	0	0
16	P	29	0	0	2	0
16	Q	26	0	0	2	0
16	R	31	0	0	3	0
16	S	20	0	0	1	0
16	T	39	0	0	2	0
16	U	61	0	0	6	0
16	V	48	0	0	3	0
16	W	59	0	0	1	0
16	X	46	0	0	6	0
16	Y	48	0	0	13	0
16	Z	52	0	0	3	0
All	All	51114	0	49548	1656	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 17.

All (1656) 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)
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.10	1.16
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.33	1.10
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.33	1.10
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.10	1.09
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.11	1.09
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.10	1.06
4:D:175:GLU:HG2	4:D:196:ILE:HD12	1.36	1.06
7:U:9:ASP:HA	7:U:14:ILE:HD11	1.40	1.04
4:R:175:GLU:HG2	4:R:196:ILE:HD12	1.38	1.01
11:K:208:ASN:HD22	9:W:29:ASN:HD21	1.04	1.01
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.23	1.01
2:B:15:PHE:H	3:C:23:GLN:HE22	1.07	1.01
10:J:133:TYR:HD1	16:Y:232:HOH:O	1.44	1.00
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.10	0.99
7:G:9:ASP:HA	7:G:14:ILE:HD11	1.41	0.99
4:R:68:VAL:HG21	4:R:89:ILE:HD12	1.45	0.98
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.25	0.98
10:J:133:TYR:HE1	16:X:225:HOH:O	1.45	0.97
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.80	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:H	2:B:23:GLN:HE22	1.11	0.96
3:C:163:GLN:NE2	3:C:164:THR:H	1.63	0.96
4:D:68:VAL:HG21	4:D:89:ILE:HD12	1.47	0.96
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.79	0.96
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.27	0.96
2:P:202:THR:HG22	2:P:204:SER:H	1.29	0.95
7:U:96:ALA:HA	7:U:107:MET:HE2	1.44	0.95
2:B:202:THR:HG22	2:B:204:SER:H	1.31	0.95
11:K:207:ASN:ND2	10:X:144:PRO:HG3	1.82	0.95
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.64	0.95
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.49	0.95
3:C:163:GLN:HE21	3:C:164:THR:N	1.66	0.94
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	1.68	0.93
7:G:96:ALA:HA	7:G:107:MET:HE2	1.48	0.93
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.67	0.93
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.32	0.92
1:O:15:PHE:H	2:P:23:GLN:HE22	1.03	0.92
9:I:29:ASN:HD21	11:Y:208:ASN:HD22	1.01	0.92
3:C:185:THR:HB	3:C:188:GLU:HG2	1.50	0.92
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.13	0.92
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	1.85	0.92
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.35	0.91
12:L:123:GLN:HG3	12:L:145:TYR:OH	1.67	0.91
9:I:29:ASN:HD21	11:Y:208:ASN:ND2	1.69	0.91
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.52	0.91
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.53	0.91
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.11	0.90
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.37	0.90
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.51	0.90
11:Y:67:GLU:OE1	11:Y:73:ARG:HA	1.71	0.90
11:K:67:GLU:OE1	11:K:73:ARG:HA	1.72	0.89
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.15	0.89
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.54	0.89
3:C:15:PHE:H	4:D:23:GLN:HE22	1.16	0.89
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.19	0.88
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.15	0.88
3:Q:201:VAL:CG2	3:Q:210:ILE:HD11	2.03	0.88
11:K:99:THR:HG22	11:K:113:VAL:O	1.74	0.88
11:K:208:ASN:ND2	9:W:29:ASN:HD21	1.71	0.87
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.22	0.87
5:S:207:LEU:HD23	5:S:207:LEU:H	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.87	0.86
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.57	0.86
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.57	0.86
5:E:207:LEU:HD23	5:E:207:LEU:H	1.39	0.86
5:S:15:PHE:H	6:T:23:GLN:HE22	1.24	0.86
10:X:59:ILE:HD13	10:X:83:VAL:HG22	1.57	0.85
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.42	0.85
10:J:59:ILE:HD13	10:J:83:VAL:HG22	1.58	0.85
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.57	0.84
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.75	0.84
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.19	0.84
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.22	0.84
10:J:-1:MET:HG2	10:J:1:ASP:H	1.43	0.83
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.74	0.83
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.58	0.83
11:Y:210:ILE:HB	16:Y:248:HOH:O	1.78	0.83
3:C:201:VAL:CG2	3:C:210:ILE:HD11	2.03	0.83
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.43	0.83
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.44	0.83
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.44	0.82
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.44	0.82
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.79	0.82
4:D:175:GLU:HG2	4:D:196:ILE:CD1	2.10	0.82
7:G:96:ALA:HA	7:G:107:MET:CE	2.08	0.82
7:U:96:ALA:HA	7:U:107:MET:CE	2.08	0.82
9:I:29:ASN:ND2	11:Y:208:ASN:HD22	1.77	0.81
5:E:15:PHE:H	6:F:23:GLN:HE22	1.28	0.81
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.46	0.81
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.62	0.80
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.45	0.80
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.77	0.80
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.94	0.80
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.63	0.80
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.65	0.79
3:C:185:THR:HG22	3:C:187:GLU:H	1.46	0.79
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.80	0.79
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.65	0.79
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.96	0.79
2:P:202:THR:HG22	2:P:204:SER:N	1.98	0.79
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.64	0.79
10:X:-1:MET:HG2	10:X:1:ASP:H	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:208:ASN:HD22	9:W:29:ASN:ND2	1.80	0.79
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.63	0.78
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.64	0.78
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.95	0.78
8:H:41:ILE:HD12	8:H:76:VAL:HG22	1.66	0.78
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.66	0.78
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.84	0.78
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.81	0.77
2:B:186:VAL:HG11	2:B:216:ARG:HD3	1.67	0.77
2:P:186:VAL:HG11	2:P:216:ARG:HD3	1.65	0.77
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.66	0.77
4:R:175:GLU:HG2	4:R:196:ILE:CD1	2.14	0.77
9:I:29:ASN:ND2	11:Y:208:ASN:ND2	2.32	0.77
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.99	0.77
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.85	0.76
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.67	0.76
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.68	0.76
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.00	0.76
5:S:18(D):ILE:HD13	5:S:18(D):ILE:O	1.86	0.76
2:B:202:THR:HG22	2:B:204:SER:N	1.99	0.76
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.21	0.76
6:F:192:GLN:O	6:F:196:ILE:HG12	1.85	0.76
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.66	0.76
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.67	0.75
12:L:166:HIS:HD2	12:L:168:GLN:H	1.33	0.75
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.21	0.75
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.85	0.75
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.32	0.75
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.67	0.75
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.33	0.75
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.68	0.75
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.50	0.74
4:R:185:THR:OG1	4:R:188:GLU:HG3	1.87	0.74
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.68	0.74
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.68	0.74
13:1:42:VAL:HG23	13:1:178:ILE:HD11	1.70	0.74
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.23	0.74
11:K:208:ASN:ND2	9:W:29:ASN:ND2	2.35	0.74
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.88	0.74
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	1.96	0.74
6:F:35:THR:HG21	6:F:51:GLU:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.71	0.73
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.87	0.73
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.69	0.73
8:H:201:GLN:HG3	12:Z:153:LYS:HG2	1.71	0.73
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.90	0.73
11:K:143:LYS:O	11:K:146:LEU:HD13	1.89	0.73
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.70	0.73
6:T:192:GLN:O	6:T:196:ILE:HG12	1.87	0.73
7:G:77:VAL:HG12	7:G:137:THR:HB	1.71	0.73
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.03	0.73
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.70	0.73
2:B:185:LYS:HD3	2:B:186:VAL:N	2.04	0.72
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.71	0.72
6:T:237:GLN:O	6:T:240:ILE:HG22	1.89	0.72
8:V:172:ASN:HD22	8:V:193:THR:HA	1.54	0.72
8:H:165:ASN:HD22	13:1:139:ARG:NH1	1.87	0.72
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.02	0.72
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.71	0.72
8:H:172:ASN:HD22	8:H:193:THR:HA	1.55	0.72
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.03	0.72
6:T:35:THR:HG21	6:T:51:GLU:O	1.89	0.72
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.88	0.72
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.71	0.72
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.23	0.72
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.52	0.72
5:E:18(D):ILE:O	5:E:18(D):ILE:HD13	1.89	0.72
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.70	0.72
15:N:0:FEB:H14	15:N:0:FEB:H33	1.72	0.72
8:V:41:ILE:HD12	8:V:76:VAL:HG22	1.72	0.72
8:H:3:ILE:HD11	8:H:127:LEU:CB	2.18	0.72
4:D:185:THR:OG1	4:D:188:GLU:HG3	1.89	0.71
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.72	0.71
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.72	0.71
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.71	0.71
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.71	0.71
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.87	0.71
15:2:0:FEB:H14	15:2:0:FEB:H33	1.71	0.71
11:K:67:GLU:CD	11:K:73:ARG:HA	2.10	0.71
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.05	0.71
3:Q:163:GLN:HE21	3:Q:164:THR:H	0.82	0.71
12:L:153:LYS:HG2	8:V:201:GLN:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:3:ILE:HD11	8:V:127:LEU:CB	2.19	0.71
13:M:57:ARG:NE	16:M:244:HOH:O	2.23	0.71
14:N:22:THR:HG22	15:N:0:FEB:N25	2.06	0.70
2:P:185:LYS:HD3	2:P:186:VAL:N	2.06	0.70
6:F:237:GLN:O	6:F:240:ILE:HG22	1.91	0.70
14:2:22:THR:HG22	15:2:0:FEB:N25	2.06	0.70
3:C:185:THR:HG22	3:C:187:GLU:N	2.05	0.70
11:Y:67:GLU:CD	11:Y:73:ARG:HA	2.11	0.70
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.72	0.69
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.21	0.69
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.92	0.69
9:W:29:ASN:H	9:W:29:ASN:ND2	1.90	0.69
3:C:41:LYS:HG2	3:C:161:SER:O	1.91	0.69
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.74	0.69
5:E:207:LEU:CD2	5:E:207:LEU:H	2.06	0.69
10:J:146:MET:HE3	10:J:150:GLU:HB3	1.75	0.69
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.73	0.69
5:S:207:LEU:H	5:S:207:LEU:CD2	2.06	0.69
2:B:121:GLN:O	2:B:124:THR:HB	1.93	0.69
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.90	0.69
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.56	0.68
2:B:15:PHE:H	3:C:23:GLN:NE2	1.88	0.68
14:2:22:THR:CG2	15:2:0:FEB:N25	2.57	0.68
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.92	0.68
11:Y:38:ASN:ND2	16:Y:258:HOH:O	2.25	0.68
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.74	0.68
11:Y:181:ASP:N	16:Y:240:HOH:O	2.18	0.68
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.57	0.68
10:J:52:THR:HG22	10:J:53:VAL:N	2.09	0.67
4:R:192:LEU:O	4:R:196:ILE:HG12	1.95	0.67
7:U:77:VAL:HG12	7:U:137:THR:HB	1.75	0.67
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.04	0.67
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.77	0.67
9:I:2:ILE:HD13	9:I:159:LEU:CD1	2.24	0.67
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.41	0.67
9:I:6:MET:HE1	9:I:155:ILE:HA	1.76	0.67
13:M:139:ARG:NH1	8:V:165:ASN:HD22	1.91	0.67
10:J:112:GLN:NE2	16:J:234:HOH:O	2.26	0.67
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.23	0.67
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.77	0.67
2:B:149:TYR:OH	3:C:62(A):ILE:HB	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.43	0.67
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.41	0.67
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.75	0.67
14:2:20:THR:HG22	15:2:0:FEB:H8A	1.75	0.67
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.94	0.67
7:G:87:ASN:HD22	7:G:87:ASN:C	1.98	0.67
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.76	0.67
9:I:2:ILE:HD13	9:I:159:LEU:HD11	1.75	0.66
7:G:77:VAL:CG1	7:G:137:THR:HB	2.26	0.66
7:U:87:ASN:HD22	7:U:87:ASN:C	1.99	0.66
14:N:22:THR:CG2	15:N:0:FEB:N25	2.58	0.66
5:S:227:GLU:CD	5:S:227:GLU:H	1.98	0.66
13:1:40:ASN:HD22	13:1:40:ASN:H	1.42	0.66
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.78	0.66
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.77	0.66
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.91	0.66
14:2:18(A):ILE:HD13	14:2:18(B):PHE:N	2.11	0.66
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.95	0.66
12:L:135:MET:CE	9:W:165:ARG:NH2	2.58	0.66
10:X:52:THR:HG22	10:X:53:VAL:N	2.11	0.66
8:H:3:ILE:HD13	8:H:3:ILE:O	1.96	0.66
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.78	0.66
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.25	0.66
9:W:2:ILE:HD13	9:W:159:LEU:CD1	2.26	0.66
9:W:2:ILE:HD13	9:W:159:LEU:HD11	1.76	0.66
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.77	0.65
3:Q:197:LEU:O	3:Q:201:VAL:HG23	1.95	0.65
10:X:146:MET:HE3	10:X:150:GLU:HB3	1.77	0.65
13:M:40:ASN:HD22	13:M:40:ASN:H	1.43	0.65
9:I:29:ASN:H	9:I:29:ASN:ND2	1.93	0.65
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.12	0.65
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.45	0.65
8:V:3:ILE:O	8:V:3:ILE:HD13	1.97	0.65
11:K:73:ARG:NH2	11:K:104:TYR:O	2.30	0.65
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.26	0.65
5:E:227:GLU:CD	5:E:227:GLU:H	1.98	0.65
10:X:-1:MET:HG2	10:X:1:ASP:N	2.12	0.65
10:J:6:ILE:HD11	10:J:154:LEU:HD23	1.79	0.65
5:S:132:TYR:O	5:S:153:PRO:HB3	1.98	0.65
2:B:160:TRP:HA	3:C:59:GLN:HA	1.78	0.64
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.78	0.64
3:C:175:PHE:O	3:C:179:ASN:HB2	1.96	0.64
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.79	0.64
10:J:-1:MET:HG2	10:J:1:ASP:N	2.10	0.64
6:T:173:LYS:O	6:T:177:GLU:HG3	1.97	0.64
7:U:121:GLN:O	7:U:124:THR:HB	1.97	0.64
14:N:20:THR:HG22	15:N:0:FEB:H8A	1.77	0.64
2:P:121:GLN:O	2:P:124:THR:HB	1.96	0.64
2:P:181:LYS:O	2:P:184:MET:HG3	1.96	0.64
2:B:181:LYS:O	2:B:184:MET:HG3	1.98	0.64
7:G:198:ILE:HG23	7:G:203:THR:O	1.97	0.64
14:N:18(A):ILE:HD13	14:N:18(B):PHE:N	2.13	0.64
6:T:127:ASN:HD22	6:T:128:SER:N	1.96	0.64
12:Z:99:THR:HG23	16:Z:201:HOH:O	1.98	0.64
12:Z:109:ALA:HA	16:Z:205:HOH:O	1.97	0.64
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.28	0.64
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.80	0.64
6:F:127:ASN:HD22	6:F:128:SER:N	1.95	0.64
10:J:133:TYR:OH	10:X:24:ILE:O	2.16	0.64
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.78	0.64
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.79	0.63
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.79	0.63
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.29	0.63
7:G:55:PRO:HG2	7:G:56:ASP:H	1.63	0.63
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.64	0.63
7:U:55:PRO:HG2	7:U:56:ASP:H	1.64	0.63
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.28	0.63
3:C:41:LYS:HD3	3:C:161:SER:HA	1.80	0.63
3:Q:65:SER:HB2	16:Q:246:HOH:O	1.96	0.63
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.80	0.63
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.62	0.63
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.81	0.63
1:O:188:ASP:O	1:O:192:ILE:HG12	1.99	0.63
10:X:6:ILE:HD11	10:X:154:LEU:HD23	1.80	0.63
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.31	0.63
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.79	0.63
1:A:188:ASP:O	1:A:192:ILE:HG12	1.98	0.63
3:Q:175:PHE:O	3:Q:179:ASN:HB2	1.99	0.63
3:C:197:LEU:O	3:C:201:VAL:HG23	1.98	0.62
10:J:24:ILE:O	10:X:133:TYR:OH	2.17	0.62
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.95	0.62
7:U:77:VAL:CG1	7:U:137:THR:HB	2.28	0.62
11:Y:67:GLU:OE2	16:Y:255:HOH:O	2.16	0.62
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.79	0.62
5:E:226:GLY:O	5:E:229:VAL:HG22	2.00	0.62
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.95	0.62
3:Q:190:VAL:O	3:Q:194:VAL:HG23	1.99	0.62
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.34	0.62
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.14	0.62
3:C:190:VAL:O	3:C:194:VAL:HG23	2.00	0.62
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.29	0.62
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.30	0.62
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.81	0.62
6:F:173:LYS:O	6:F:177:GLU:HG3	1.99	0.62
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.82	0.62
9:I:2:ILE:CD1	9:I:159:LEU:HD11	2.30	0.62
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.47	0.62
11:K:181:ASP:N	16:K:239:HOH:O	2.32	0.62
5:S:207:LEU:N	5:S:207:LEU:HD23	2.14	0.62
4:D:192:LEU:O	4:D:196:ILE:HG12	2.00	0.62
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.00	0.62
13:1:12:VAL:HG21	13:1:102:ALA:HB1	1.82	0.61
1:A:110:LYS:HG2	16:A:245:HOH:O	2.00	0.61
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.00	0.61
11:Y:40:PHE:HB3	11:Y:73:ARG:HH21	1.64	0.61
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.00	0.61
11:K:40:PHE:HB3	11:K:73:ARG:HH21	1.65	0.61
4:R:237:LEU:HD22	4:R:241:GLU:HG3	1.82	0.61
11:K:44:THR:OG1	11:K:100:MET:HB2	2.00	0.61
10:X:156:LYS:O	10:X:160:GLN:HG3	2.01	0.61
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.81	0.61
10:J:55:PHE:CZ	10:J:59:ILE:HD11	2.36	0.61
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.82	0.61
7:U:198:ILE:HG23	7:U:203:THR:O	2.01	0.61
2:B:202:THR:CG2	2:B:204:SER:H	2.10	0.61
4:D:186:LEU:O	4:D:190:GLU:HG3	2.01	0.61
12:L:109:ALA:HA	16:L:233:HOH:O	1.99	0.61
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.49	0.61
10:J:178:VAL:HG22	10:J:184:ILE:HG12	1.83	0.61
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.66	0.61
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:LEU:HD23	5:E:207:LEU:N	2.14	0.61
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.82	0.61
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.82	0.61
5:E:132:TYR:O	5:E:153:PRO:HB3	1.99	0.61
13:1:148:VAL:HG23	16:1:228:HOH:O	2.01	0.61
2:B:163:ILE:HG12	2:B:164:SER:N	2.15	0.61
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.83	0.61
5:E:12:THR:HG21	5:E:124:THR:HA	1.83	0.61
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.01	0.61
5:E:198:SER:HA	5:E:201:LEU:HG	1.83	0.60
2:P:163:ILE:HG12	2:P:164:SER:N	2.15	0.60
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.83	0.60
10:X:6:ILE:CD1	10:X:154:LEU:HD23	2.31	0.60
7:G:121:GLN:O	7:G:124:THR:HB	2.00	0.60
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.00	0.60
10:J:146:MET:CE	10:J:150:GLU:HB3	2.31	0.60
10:J:6:ILE:CD1	10:J:154:LEU:HD23	2.31	0.60
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.01	0.60
16:P:250:HOH:O	3:Q:87:ILE:HD11	2.00	0.60
5:S:12:THR:HG21	5:S:124:THR:HA	1.83	0.60
4:D:112:LEU:C	4:D:112:LEU:HD13	2.21	0.60
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.83	0.60
2:P:202:THR:CG2	2:P:204:SER:H	2.10	0.60
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.82	0.60
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.84	0.60
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.84	0.60
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.83	0.60
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.83	0.60
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.84	0.60
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.83	0.60
6:F:179:LEU:HD21	6:F:192:GLN:HG2	1.83	0.60
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.32	0.60
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.82	0.60
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.37	0.60
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.83	0.60
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.83	0.60
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.84	0.60
3:C:46:VAL:O	3:C:215:VAL:HG12	2.02	0.60
3:Q:197:LEU:HD13	3:Q:210:ILE:HD12	1.82	0.60
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.02	0.59
7:U:67:ILE:CD1	7:U:211:GLU:HG2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:146:MET:CE	10:X:150:GLU:HB3	2.32	0.59
11:Y:104:TYR:CE1	11:Y:180:GLU:OE2	2.55	0.59
14:2:22:THR:HG22	15:2:0:FEB:HN25	1.67	0.59
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.38	0.59
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.68	0.59
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.83	0.59
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.84	0.59
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.00	0.59
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.33	0.59
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.84	0.59
9:W:2:ILE:CD1	9:W:159:LEU:HD11	2.32	0.59
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.67	0.59
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.37	0.59
3:C:197:LEU:HD13	3:C:210:ILE:HD12	1.83	0.59
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.95	0.59
6:T:186:ALA:O	6:T:190:VAL:HG23	2.02	0.59
9:W:48:LEU:HG	9:W:50:THR:HG22	1.84	0.59
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.02	0.59
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.37	0.59
10:J:-1:MET:N	16:J:246:HOH:O	2.32	0.59
5:S:226:GLY:O	5:S:229:VAL:HG22	2.03	0.59
2:P:186:VAL:HG11	2:P:216:ARG:CD	2.33	0.59
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.36	0.59
8:V:84:LYS:HG3	8:V:85:GLN:N	2.17	0.59
3:C:186:VAL:O	3:C:190:VAL:HG23	2.03	0.59
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.49	0.59
8:V:172:ASN:ND2	8:V:193:THR:HA	2.17	0.59
3:C:163:GLN:HE21	3:C:164:THR:H	0.80	0.58
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.33	0.58
8:H:128:GLY:O	8:H:131:SER:HB2	2.02	0.58
10:J:156:LYS:O	10:J:160:GLN:HG3	2.03	0.58
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.03	0.58
10:X:178:VAL:HG22	10:X:184:ILE:HG12	1.84	0.58
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.85	0.58
9:I:48:LEU:HG	9:I:50:THR:HG22	1.85	0.58
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.07	0.58
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.34	0.58
13:M:35:ILE:HG12	13:M:56:GLU:CG	2.34	0.58
5:S:221:PHE:CE1	5:S:223:ILE:HD11	2.39	0.58
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.04	0.58
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:198:SER:HA	5:S:201:LEU:HG	1.84	0.58
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.84	0.58
10:X:44:SER:OG	10:X:100:LEU:HB2	2.04	0.58
13:1:149:GLN:H	13:1:149:GLN:NE2	2.02	0.58
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.49	0.58
8:H:172:ASN:ND2	8:H:193:THR:HA	2.18	0.58
14:N:107:LYS:HG2	14:N:108:GLY:N	2.18	0.58
2:B:234:VAL:HA	2:B:239:THR:HA	1.85	0.58
14:N:22:THR:HG22	15:N:0:FEB:HN25	1.67	0.58
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.39	0.58
5:S:35:SER:HB3	5:S:66:LYS:HZ3	1.68	0.58
7:U:228:ASN:HB3	16:U:242:HOH:O	2.03	0.58
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.39	0.58
7:G:67:ILE:CD1	7:G:211:GLU:HG2	2.33	0.58
5:S:227:GLU:N	5:S:227:GLU:CD	2.57	0.58
3:C:57:LYS:O	3:C:58:LEU:HB2	2.02	0.58
4:D:85:ALA:O	4:D:89:ILE:HG12	2.03	0.58
6:F:186:ALA:O	6:F:190:VAL:HG23	2.04	0.58
10:J:44:SER:OG	10:J:100:LEU:HB2	2.04	0.58
11:K:104:TYR:CE1	11:K:180:GLU:OE2	2.57	0.58
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.04	0.58
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.39	0.58
1:O:86:ARG:NE	7:U:118:ASN:HD21	1.98	0.58
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.19	0.58
13:M:149:GLN:NE2	13:M:149:GLN:H	2.02	0.57
14:N:9:LYS:HA	14:N:145:ASN:HD22	1.69	0.57
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.04	0.57
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.04	0.57
2:B:71:ASN:ND2	2:B:72:ASP:H	2.02	0.57
3:C:227:GLU:OE1	3:C:227:GLU:N	2.37	0.57
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.85	0.57
1:O:21(L):ILE:N	1:O:21(L):ILE:HD12	2.19	0.57
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.14	0.57
2:B:15:PHE:N	3:C:23:GLN:HE22	1.89	0.57
5:E:221:PHE:CE1	5:E:223:ILE:HD11	2.40	0.57
7:G:212:VAL:HG23	7:G:229:ILE:HD13	1.85	0.57
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.85	0.57
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.70	0.57
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.86	0.57
11:Y:114:ASP:OD1	11:Y:116:ASP:HB2	2.04	0.57
5:E:227:GLU:CD	5:E:227:GLU:N	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:123:GLN:CG	12:L:145:TYR:OH	2.47	0.57
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.87	0.57
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.19	0.57
2:P:234:VAL:HA	2:P:239:THR:HA	1.85	0.57
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.86	0.57
12:L:166:HIS:CD2	12:L:168:GLN:H	2.20	0.57
4:R:112:LEU:C	4:R:112:LEU:HD13	2.25	0.57
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.70	0.57
7:G:233:LEU:O	7:G:236:ILE:HG13	2.05	0.57
2:P:75:ALA:HB2	2:P:221:GLN:NE2	2.20	0.57
14:2:107:LYS:HG2	14:2:108:GLY:N	2.19	0.57
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.04	0.57
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.85	0.57
8:H:41:ILE:CD1	8:H:76:VAL:HG22	2.34	0.57
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.87	0.57
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.87	0.57
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.70	0.57
8:H:200:LYS:HE3	9:I:140:SER:O	2.05	0.57
13:M:19:LEU:HD12	13:M:28:PHE:O	2.05	0.57
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.35	0.57
7:U:212:VAL:HG23	7:U:229:ILE:HD13	1.85	0.57
2:B:75:ALA:HB2	2:B:221:GLN:NE2	2.20	0.57
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.87	0.57
12:Z:123:GLN:CG	12:Z:145:TYR:OH	2.47	0.57
10:J:93:ARG:HH11	10:J:93:ARG:HG2	1.71	0.56
8:V:128:GLY:O	8:V:131:SER:HB2	2.04	0.56
5:E:167:ALA:HB3	16:E:253:HOH:O	2.06	0.56
5:E:36:VAL:HG13	5:E:197:ILE:HD11	1.87	0.56
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.34	0.56
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.20	0.56
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.41	0.56
2:P:71:ASN:ND2	2:P:72:ASP:H	2.02	0.56
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.69	0.56
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.87	0.56
13:I:35:ILE:HG12	13:I:56:GLU:CG	2.34	0.56
6:F:175:GLU:HB3	6:F:196:ILE:CD1	2.36	0.56
9:I:116:ILE:H	9:I:116:ILE:HD13	1.70	0.56
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.40	0.56
5:S:36:VAL:HG13	5:S:197:ILE:HD11	1.86	0.56
6:T:175:GLU:HB3	6:T:196:ILE:CD1	2.35	0.56
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:220:PRO:O	5:S:222:THR:HG23	2.06	0.56
8:V:200:LYS:HE3	9:W:140:SER:O	2.05	0.56
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.05	0.56
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.34	0.56
2:B:224:PHE:HD2	2:B:224:PHE:H	1.54	0.56
5:E:86:ARG:O	5:E:90:ASN:HB2	2.05	0.56
9:I:29:ASN:ND2	9:I:29:ASN:N	2.53	0.56
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.21	0.56
15:V:0:FEB:H26	9:W:115:LEU:HD21	1.88	0.56
9:W:29:ASN:ND2	9:W:29:ASN:N	2.51	0.56
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.70	0.56
3:C:35:THR:HB	3:C:51:GLU:HG3	1.87	0.56
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.35	0.56
8:H:84:LYS:HG3	8:H:85:GLN:N	2.18	0.56
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.86	0.56
10:X:55:PHE:CZ	10:X:59:ILE:HD11	2.39	0.56
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.41	0.56
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.40	0.56
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.06	0.56
4:R:186:LEU:O	4:R:190:GLU:HG3	2.06	0.56
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.88	0.56
14:2:9:LYS:HA	14:2:145:ASN:HD22	1.71	0.56
1:A:21(L):ILE:N	1:A:21(L):ILE:HD12	2.21	0.56
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.71	0.56
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.88	0.56
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.87	0.56
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.87	0.56
11:K:114:ASP:OD1	11:K:116:ASP:HB2	2.06	0.56
3:Q:224:LEU:N	3:Q:224:LEU:HD12	2.21	0.56
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.70	0.55
11:K:6:PHE:HA	11:K:123:ASP:O	2.05	0.55
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.06	0.55
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.06	0.55
5:S:73:HIS:HE1	5:S:107:LEU:O	1.87	0.55
5:S:86:ARG:O	5:S:90:ASN:HB2	2.06	0.55
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.35	0.55
13:1:113:VAL:HA	13:1:118:VAL:O	2.06	0.55
13:1:19:LEU:HD12	13:1:28:PHE:O	2.06	0.55
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.87	0.55
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.88	0.55
8:H:153:LYS:HD2	16:H:251:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:0:FEB:H26	9:I:115:LEU:HD21	1.89	0.55
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.06	0.55
4:R:85:ALA:O	4:R:89:ILE:HG12	2.07	0.55
8:V:34:LEU:HB2	16:V:238:HOH:O	2.07	0.55
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.70	0.55
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.37	0.55
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.87	0.55
1:O:57:PRO:HG3	7:U:177:GLU:CD	2.26	0.55
9:W:116:ILE:HD13	9:W:116:ILE:H	1.70	0.55
8:H:34:LEU:HB2	16:H:247:HOH:O	2.05	0.55
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.22	0.55
11:Y:41:LEU:HB2	16:Y:258:HOH:O	2.05	0.55
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.20	0.55
5:E:220:PRO:O	5:E:222:THR:HG23	2.07	0.55
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.88	0.55
11:K:142:TYR:O	11:K:143:LYS:HD2	2.07	0.55
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.40	0.55
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.70	0.55
4:D:12(F):GLY:HA3	16:D:267:HOH:O	2.07	0.55
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.22	0.55
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.88	0.55
14:N:163:ILE:O	16:N:188:HOH:O	2.18	0.55
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.20	0.55
3:C:15:PHE:CD1	3:C:21:ILE:HD11	2.42	0.55
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.88	0.55
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.87	0.55
2:P:160:TRP:CD2	2:P:163:ILE:HD12	2.42	0.55
5:S:15:PHE:H	6:T:23:GLN:NE2	1.98	0.55
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.88	0.55
13:M:157:ASN:ND2	16:M:279:HOH:O	2.39	0.55
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.37	0.55
10:X:113:ILE:HA	10:X:118:THR:O	2.07	0.55
11:Y:191:ASP:OD2	11:Y:193:GLY:N	2.40	0.55
5:E:73:HIS:HE1	5:E:107:LEU:O	1.89	0.55
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.88	0.55
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.10	0.55
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.89	0.55
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.42	0.55
2:B:186:VAL:HG11	2:B:216:ARG:CD	2.35	0.55
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.54	0.55
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.42	0.55
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.89	0.54
8:H:3:ILE:CD1	8:H:127:LEU:O	2.55	0.54
14:N:107:LYS:HG2	14:N:108:GLY:H	1.72	0.54
1:O:150:GLN:O	1:O:157:TYR:HA	2.07	0.54
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.90	0.54
2:P:223:ILE:HD12	2:P:223:ILE:N	2.22	0.54
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.89	0.54
16:L:199:HOH:O	9:W:192:ARG:HG3	2.07	0.54
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.89	0.54
2:B:160:TRP:CD2	2:B:163:ILE:HD12	2.41	0.54
2:B:223:ILE:N	2:B:223:ILE:HD12	2.22	0.54
6:F:179:LEU:HD21	6:F:192:GLN:CG	2.37	0.54
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.22	0.54
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.72	0.54
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.36	0.54
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.88	0.54
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.23	0.54
12:L:1:GLY:HA3	12:L:33:LYS:HZ2	1.72	0.54
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.89	0.54
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.42	0.54
2:P:239:THR:OXT	2:P:239:THR:HG22	2.07	0.54
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.36	0.54
16:I:224:HOH:O	10:J:122:LEU:HD13	2.06	0.54
11:K:191:ASP:OD2	11:K:193:GLY:N	2.40	0.54
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.20	0.54
1:O:141:HIS:HA	1:O:146:GLY:O	2.07	0.54
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.89	0.54
2:P:186:VAL:CG1	2:P:216:ARG:HD3	2.37	0.54
9:W:34:ILE:HB	16:W:215:HOH:O	2.08	0.54
13:M:113:VAL:HA	13:M:118:VAL:O	2.07	0.54
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.73	0.54
7:U:14:ILE:H	7:U:14:ILE:HD13	1.73	0.54
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.42	0.54
2:B:27:ALA:O	2:B:31:ILE:HG12	2.07	0.54
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.38	0.54
10:J:52:THR:CG2	10:J:53:VAL:N	2.71	0.54
2:P:224:PHE:H	2:P:224:PHE:HD2	1.54	0.54
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.89	0.54
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.89	0.54
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.89	0.54
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.90	0.54
5:S:160:LEU:HD13	5:S:163:THR:HB	1.90	0.54
9:W:29:ASN:H	9:W:29:ASN:HD22	1.55	0.54
4:R:40:ILE:HG13	4:R:193:VAL:CG2	2.37	0.53
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.90	0.53
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.89	0.53
10:J:52:THR:HG22	10:J:53:VAL:HG23	1.89	0.53
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.09	0.53
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.20	0.53
1:A:141:HIS:HA	1:A:146:GLY:O	2.09	0.53
1:A:69:LEU:HD23	1:A:69:LEU:C	2.28	0.53
2:B:239:THR:OXT	2:B:239:THR:HG22	2.09	0.53
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.72	0.53
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.21	0.53
1:O:69:LEU:HD23	1:O:69:LEU:C	2.29	0.53
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.91	0.53
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.39	0.53
5:E:35:SER:HB3	5:E:66:LYS:NZ	2.23	0.53
7:G:151:THR:HG22	7:G:157:TYR:CB	2.38	0.53
8:V:41:ILE:CD1	8:V:76:VAL:HG22	2.38	0.53
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.90	0.53
16:D:273:HOH:O	5:E:86:ARG:HD3	2.08	0.53
7:G:87:ASN:ND2	7:G:87:ASN:C	2.61	0.53
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.09	0.53
1:A:150:GLN:O	1:A:157:TYR:HA	2.08	0.53
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.90	0.53
5:S:67:ILE:HG21	5:S:223:ILE:HD12	1.90	0.53
7:U:9:ASP:HA	7:U:14:ILE:CD1	2.28	0.53
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.90	0.53
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.74	0.53
7:U:87:ASN:ND2	7:U:87:ASN:C	2.61	0.53
11:Y:38:ASN:O	11:Y:40:PHE:N	2.42	0.53
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.09	0.53
7:G:12:ILE:HD13	7:G:12:ILE:H	1.74	0.53
13:M:35:ILE:HG12	13:M:56:GLU:HG3	1.89	0.53
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.74	0.53
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.91	0.53
9:I:113:PHE:HA	9:I:118:CYS:O	2.08	0.53
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.23	0.53
8:V:35:HIS:CB	8:V:56:THR:HG21	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:170:GLU:N	4:D:170:GLU:OE1	2.41	0.53
5:E:15:PHE:H	6:F:23:GLN:NE2	2.03	0.53
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.38	0.53
3:Q:182:PRO:O	3:Q:184:ALA:N	2.42	0.53
4:R:205:GLU:OE2	4:R:205:GLU:HA	2.09	0.53
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.23	0.53
7:U:8:TYR:C	7:U:10:ARG:H	2.13	0.53
7:U:233:LEU:O	7:U:236:ILE:HG13	2.08	0.53
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.90	0.53
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.09	0.53
3:C:241:GLN:C	3:C:243:GLN:H	2.13	0.52
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.24	0.52
1:O:159:PRO:O	2:P:59:LEU:HD12	2.08	0.52
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.44	0.52
3:Q:241:GLN:C	3:Q:243:GLN:H	2.13	0.52
10:X:190:PHE:C	10:X:192:ALA:H	2.12	0.52
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.91	0.52
8:H:35:HIS:CB	8:H:56:THR:HG21	2.39	0.52
10:X:53:VAL:HB	16:Y:237:HOH:O	2.10	0.52
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.91	0.52
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.90	0.52
4:R:170:GLU:OE1	4:R:170:GLU:N	2.42	0.52
14:2:107:LYS:HG2	14:2:108:GLY:H	1.73	0.52
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.91	0.52
4:D:205:GLU:HA	4:D:205:GLU:OE2	2.08	0.52
7:U:186:TRP:O	7:U:190:VAL:HG23	2.09	0.52
2:B:186:VAL:CG1	2:B:216:ARG:HD3	2.38	0.52
3:C:224:LEU:N	3:C:224:LEU:HD12	2.24	0.52
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.45	0.52
10:X:93:ARG:HG2	10:X:93:ARG:HH11	1.73	0.52
15:2:0:FEB:HN25	15:2:0:FEB:HN18	1.57	0.52
3:C:182:PRO:O	3:C:184:ALA:N	2.42	0.52
6:F:28:VAL:O	6:F:32:GLU:HG3	2.10	0.52
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.92	0.52
10:J:113:ILE:HA	10:J:118:THR:O	2.09	0.52
11:K:99:THR:CG2	11:K:113:VAL:HB	2.39	0.52
15:N:0:FEB:HN18	15:N:0:FEB:HN25	1.58	0.52
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.91	0.52
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.90	0.52
11:K:184:TRP:O	11:K:185:ILE:HD13	2.08	0.52
13:M:184:LEU:HD23	13:M:184:LEU:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.10	0.52
9:W:113:PHE:HA	9:W:118:CYS:O	2.08	0.52
10:X:135:PHE:HZ	16:X:216:HOH:O	1.91	0.52
2:B:21(A):LYS:HE2	2:B:21(D):GLY:O	2.10	0.52
7:G:39:ALA:HB1	7:G:148:ILE:HD12	1.91	0.52
7:G:38:LEU:HD12	7:G:38:LEU:C	2.30	0.52
13:M:40:ASN:ND2	13:M:40:ASN:H	2.07	0.52
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.96	0.52
8:V:3:ILE:HD13	8:V:127:LEU:H	1.73	0.52
10:X:16:SER:HB2	16:X:233:HOH:O	2.08	0.52
7:G:186:TRP:O	7:G:190:VAL:HG23	2.10	0.52
7:G:172:ILE:HD13	7:G:197:MET:CE	2.40	0.52
11:K:161:ALA:HB1	10:X:136:SER:HB2	1.92	0.52
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.91	0.52
2:P:172:ALA:HB2	2:P:200:THR:HG21	1.91	0.52
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.25	0.52
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.09	0.52
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.90	0.52
10:X:52:THR:CG2	10:X:53:VAL:N	2.72	0.52
14:N:106:ASN:O	14:N:107:LYS:HB3	2.09	0.52
2:P:21(A):LYS:HE2	2:P:21(D):GLY:O	2.10	0.52
9:W:19:ARG:HB2	9:W:171:TRP:HB2	1.92	0.52
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.91	0.51
14:2:106:ASN:O	14:2:107:LYS:HB3	2.08	0.51
7:G:14:ILE:HD13	7:G:14:ILE:H	1.74	0.51
1:O:121:GLN:O	1:O:124:THR:HB	2.10	0.51
4:R:24:VAL:O	4:R:27:SER:HB3	2.10	0.51
3:C:36:CYS:N	3:C:51:GLU:HG2	2.25	0.51
7:G:8:TYR:C	7:G:10:ARG:H	2.12	0.51
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.75	0.51
11:K:143:LYS:HB2	11:K:146:LEU:HD11	1.92	0.51
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.10	0.51
2:P:27:ALA:O	2:P:31:ILE:HG12	2.09	0.51
3:Q:100:ARG:HH12	3:Q:106:PRO:HB3	1.70	0.51
5:S:35:SER:HB3	5:S:66:LYS:NZ	2.26	0.51
9:W:174:VAL:HG21	9:W:186:LYS:CE	2.41	0.51
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.91	0.51
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.92	0.51
5:E:160:LEU:HD13	5:E:163:THR:HB	1.92	0.51
3:Q:15:PHE:CD1	3:Q:21:ILE:HD11	2.45	0.51
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:40:ASN:HD22	13:1:40:ASN:N	2.05	0.51
6:F:91:ARG:O	6:F:95:GLU:HB2	2.10	0.51
7:G:12:ILE:HD11	7:G:14:ILE:HD12	1.92	0.51
8:H:3:ILE:HG12	8:H:100:ILE:HD12	1.92	0.51
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.93	0.51
11:Y:38:ASN:CG	16:Y:258:HOH:O	2.49	0.51
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.37	0.51
2:B:231:ASP:O	2:B:235:LYS:HG2	2.11	0.51
7:G:93:LYS:HD3	14:N:68:SER:HB3	1.90	0.51
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.92	0.51
8:H:3:ILE:HD13	8:H:127:LEU:H	1.76	0.51
11:K:38:ASN:O	11:K:40:PHE:N	2.43	0.51
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.20	0.51
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.93	0.51
10:J:190:PHE:C	10:J:192:ALA:H	2.13	0.51
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.41	0.51
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.46	0.51
10:J:143:ARG:HB2	10:J:146:MET:HG3	1.92	0.51
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.26	0.51
2:B:172:ALA:HB2	2:B:200:THR:HG21	1.91	0.51
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.45	0.51
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.75	0.51
15:V:0:FEB:H30A	9:W:92:PHE:HD2	1.76	0.51
14:2:3:ILE:HD13	14:2:46:SER:HB3	1.93	0.50
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.76	0.50
3:C:100:ARG:HH12	3:C:106:PRO:HB3	1.72	0.50
5:E:67:ILE:HG21	5:E:223:ILE:HD12	1.93	0.50
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.26	0.50
11:K:40:PHE:CB	11:K:73:ARG:NH2	2.74	0.50
7:U:38:LEU:C	7:U:38:LEU:HD12	2.32	0.50
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.93	0.50
11:Y:99:THR:CG2	11:Y:113:VAL:HB	2.41	0.50
13:1:184:LEU:C	13:1:184:LEU:HD23	2.31	0.50
3:C:173:ARG:O	3:C:177:GLU:HG3	2.11	0.50
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.92	0.50
6:T:91:ARG:O	6:T:95:GLU:HB2	2.11	0.50
7:U:39:ALA:HB1	7:U:148:ILE:HD12	1.92	0.50
9:W:89:GLU:O	9:W:90:ARG:NH1	2.45	0.50
10:X:52:THR:HG22	10:X:53:VAL:HG23	1.93	0.50
11:Y:143:LYS:HB2	11:Y:146:LEU:HD11	1.92	0.50
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.46	0.50
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.11	0.50
3:C:55:THR:O	3:C:56:LEU:HD22	2.12	0.50
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.50
13:1:40:ASN:ND2	13:1:40:ASN:H	2.06	0.50
3:C:211:GLU:C	3:C:212:ILE:HD12	2.32	0.50
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.37	0.50
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.46	0.50
11:K:142:TYR:C	11:K:143:LYS:HD2	2.31	0.50
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.93	0.50
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.93	0.50
8:V:148:LYS:HE3	8:V:177:VAL:HG11	1.92	0.50
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.32	0.50
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.12	0.50
2:B:186:VAL:CG2	2:B:216:ARG:HD3	2.42	0.50
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.93	0.50
9:I:89:GLU:O	9:I:90:ARG:NH1	2.45	0.50
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.47	0.50
10:J:135:PHE:HZ	16:J:234:HOH:O	1.93	0.50
14:N:20:THR:HG23	14:N:31:THR:OG1	2.12	0.50
9:W:27:VAL:HG13	16:X:216:HOH:O	2.12	0.50
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.46	0.50
11:Y:40:PHE:CB	11:Y:73:ARG:HH21	2.25	0.50
3:C:236:ILE:HA	3:C:239:GLU:HG2	1.93	0.50
7:G:172:ILE:CD1	7:G:197:MET:HE1	2.41	0.50
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.75	0.50
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.77	0.50
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.94	0.50
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.12	0.50
4:D:24:VAL:O	4:D:27:SER:HB3	2.12	0.50
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.12	0.50
7:G:9:ASP:HA	7:G:14:ILE:CD1	2.28	0.50
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.41	0.50
11:K:4:LEU:C	11:K:4:LEU:HD22	2.32	0.50
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.94	0.50
11:Y:40:PHE:CB	11:Y:73:ARG:NH2	2.74	0.50
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.46	0.50
10:X:143:ARG:HB2	10:X:146:MET:HG3	1.94	0.50
11:Y:157:ARG:HH11	11:Y:157:ARG:HG3	1.76	0.50
6:F:127:ASN:HD22	6:F:127:ASN:C	2.15	0.49
6:F:69:VAL:HG12	16:F:248:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:186:ARG:HD3	16:N:234:HOH:O	2.11	0.49
6:T:179:LEU:CD2	6:T:192:GLN:HG2	2.42	0.49
7:U:72:ARG:HG2	16:U:271:HOH:O	2.11	0.49
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.94	0.49
8:V:25:ILE:HD12	8:V:25:ILE:N	2.27	0.49
11:Y:184:TRP:O	11:Y:185:ILE:HD13	2.12	0.49
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.50	0.49
1:A:85:TYR:O	1:A:89:VAL:HG23	2.13	0.49
2:P:186:VAL:HG21	2:P:216:ARG:CD	2.40	0.49
1:A:5:THR:O	1:A:7:ARG:HG2	2.13	0.49
8:H:148:LYS:HE3	8:H:177:VAL:HG11	1.92	0.49
4:R:207:LEU:C	4:R:207:LEU:HD23	2.32	0.49
1:A:121:GLN:O	1:A:124:THR:HB	2.12	0.49
9:I:29:ASN:H	9:I:29:ASN:HD22	1.59	0.49
11:K:208:ASN:HB3	16:K:237:HOH:O	2.12	0.49
10:X:2:ILE:HD13	10:X:170:PHE:CG	2.47	0.49
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.93	0.49
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.95	0.49
2:B:90:ASN:O	2:B:94:ILE:HD12	2.12	0.49
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.78	0.49
9:I:174:VAL:HG21	9:I:186:LYS:CE	2.42	0.49
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.43	0.49
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.42	0.49
2:B:224:PHE:N	2:B:224:PHE:CD2	2.81	0.49
3:C:212:ILE:HG22	3:C:224:LEU:HD13	1.95	0.49
4:D:112:LEU:O	4:D:112:LEU:HD13	2.13	0.49
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.47	0.49
9:I:19:ARG:HB2	9:I:171:TRP:HB2	1.94	0.49
6:T:72:ARG:HD2	13:1:64:THR:OG1	2.13	0.49
7:U:12:ILE:H	7:U:12:ILE:HD13	1.76	0.49
13:1:35:ILE:HG12	13:1:56:GLU:HG3	1.93	0.49
6:F:136:THR:O	6:F:150:MET:HA	2.13	0.49
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.42	0.49
1:O:55:SER:O	1:O:56:SER:HB2	2.13	0.49
2:P:202:THR:CG2	2:P:204:SER:HB2	2.43	0.49
7:U:151:THR:HG22	7:U:157:TYR:CB	2.42	0.49
3:C:232:TYR:O	3:C:236:ILE:HG13	2.13	0.49
6:F:179:LEU:CD2	6:F:192:GLN:HG2	2.43	0.49
8:H:197:ARG:NH2	9:I:139:GLU:O	2.46	0.49
12:L:1(I):ASN:O	12:L:14(K):LYS:HG2	2.12	0.49
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:135:TYR:HB2	16:Y:232:HOH:O	2.12	0.49
2:P:231:ASP:O	2:P:235:LYS:HG2	2.12	0.49
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.48	0.49
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.48	0.49
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.95	0.49
10:X:190:PHE:HA	10:X:193:GLN:HB2	1.95	0.49
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.48	0.49
4:D:12(E):SER:O	5:E:123:ASN:OD1	2.31	0.49
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.95	0.49
10:J:190:PHE:HA	10:J:193:GLN:HB2	1.95	0.49
1:O:198:LYS:HE3	1:O:236:LEU:HD11	1.94	0.49
3:Q:14:ILE:C	3:Q:14:ILE:HD12	2.33	0.49
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.43	0.49
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.28	0.49
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.48	0.49
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.77	0.49
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.27	0.49
8:V:3:ILE:HG12	8:V:100:ILE:HD12	1.94	0.49
10:X:185:ARG:NH1	16:X:222:HOH:O	2.41	0.49
10:X:88:ALA:O	10:X:90(A):ILE:HG22	2.12	0.49
1:A:126:SER:HB3	16:A:253:HOH:O	2.12	0.48
3:C:163:GLN:HE22	3:C:173:ARG:NE	2.11	0.48
5:E:143:LYS:HB2	16:M:258:HOH:O	2.11	0.48
6:F:53:LEU:HD11	6:F:205:ASN:OD1	2.13	0.48
11:K:7:ARG:HD2	11:K:108:PRO:O	2.12	0.48
1:O:85:TYR:O	1:O:89:VAL:HG23	2.12	0.48
2:P:163:ILE:HG12	2:P:164:SER:H	1.78	0.48
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.66	0.48
6:F:20(B):GLU:CD	6:F:20(C):LYS:HE3	2.33	0.48
13:M:148:VAL:HG23	16:M:239:HOH:O	2.12	0.48
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.96	0.48
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.95	0.48
8:V:175:VAL:HG12	8:V:176:CYS:N	2.28	0.48
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.95	0.48
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.95	0.48
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.48	0.48
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.81	0.48
2:B:238:ILE:O	2:B:239:THR:O	2.31	0.48
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.49	0.48
10:J:45:PHE:CE1	10:J:52:THR:HG23	2.49	0.48
11:K:86:LEU:HD13	11:K:86:LEU:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:5:THR:O	1:O:7:ARG:HG2	2.14	0.48
3:Q:236:ILE:HA	3:Q:239:GLU:HG2	1.93	0.48
6:T:136:THR:O	6:T:150:MET:HA	2.12	0.48
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.34	0.48
11:K:38:ASN:OD1	11:K:38:ASN:C	2.51	0.48
12:L:145:TYR:CD1	12:L:146:LEU:N	2.80	0.48
6:T:28:VAL:O	6:T:32:GLU:HG3	2.14	0.48
12:Z:1(I):ASN:O	12:Z:14(K):LYS:HG2	2.14	0.48
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.14	0.48
3:C:169:SER:HA	3:C:172:VAL:CG1	2.43	0.48
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.48	0.48
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.48	0.48
4:D:177:LEU:CD2	5:E:58:LEU:HD13	2.41	0.48
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.28	0.48
7:G:131:PRO:HB3	16:G:243:HOH:O	2.13	0.48
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.77	0.48
1:O:47:VAL:HG23	1:O:212:LEU:HD21	1.94	0.48
2:P:224:PHE:N	2:P:224:PHE:CD2	2.81	0.48
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.47	0.48
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.34	0.48
12:Z:114:ASP:HB2	12:Z:118:SER:N	2.28	0.48
1:A:55:SER:O	1:A:56:SER:HB2	2.13	0.48
10:J:2:ILE:HD13	10:J:170:PHE:CG	2.49	0.48
10:J:52:THR:HG22	10:J:53:VAL:H	1.78	0.48
12:L:5:GLY:O	12:L:124:CYS:HA	2.13	0.48
2:P:88:LEU:HB3	2:P:116:LEU:HD21	1.96	0.48
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.56	0.48
6:T:20(B):GLU:CD	6:T:20(C):LYS:HE3	2.33	0.48
7:U:227:GLU:HG2	16:U:295:HOH:O	2.14	0.48
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.29	0.48
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.67	0.48
13:M:40:ASN:HD22	13:M:40:ASN:N	2.05	0.48
1:O:29:THR:O	1:O:33:GLN:HG2	2.14	0.48
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.14	0.48
8:V:3:ILE:CD1	8:V:127:LEU:O	2.61	0.48
8:H:25:ILE:N	8:H:25:ILE:HD12	2.28	0.48
11:K:10(B):LYS:CD	11:K:10(B):LYS:N	2.67	0.48
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.35	0.48
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.96	0.48
7:G:228:ASN:HB3	16:G:253:HOH:O	2.14	0.48
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:3:ILE:HD13	14:N:46:SER:HB3	1.96	0.48
5:S:15:PHE:N	6:T:23:GLN:HE22	2.02	0.48
3:Q:101:LEU:HD11	10:X:57:GLU:HB3	1.95	0.48
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.62	0.48
14:2:3:ILE:CD1	14:2:46:SER:HB3	2.43	0.47
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.40	0.47
8:H:26:VAL:HG11	8:H:29:LYS:HG2	1.94	0.47
3:Q:24:VAL:O	3:Q:27:ALA:HB3	2.13	0.47
10:X:52:THR:HG22	10:X:53:VAL:H	1.78	0.47
1:A:21(G):LEU:HG	1:A:21(I):TYR:CE1	2.49	0.47
4:D:40:ILE:HG13	4:D:193:VAL:HG22	1.95	0.47
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.12	0.47
13:M:3:VAL:O	13:M:126:ALA:HA	2.14	0.47
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.13	0.47
4:R:53:ARG:HD2	16:R:264:HOH:O	2.14	0.47
14:2:20:THR:HG23	14:2:31:THR:OG1	2.14	0.47
2:B:163:ILE:HG12	2:B:164:SER:H	1.79	0.47
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.27	0.47
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.96	0.47
7:G:212:VAL:HG23	7:G:229:ILE:CD1	2.45	0.47
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.96	0.47
12:Z:99:THR:CG2	16:Z:201:HOH:O	2.61	0.47
13:1:128:GLY:N	16:1:281:HOH:O	2.46	0.47
3:C:24:VAL:O	3:C:27:ALA:HB3	2.14	0.47
5:E:15:PHE:N	6:F:23:GLN:HE22	2.06	0.47
9:I:90:ARG:HD2	16:I:257:HOH:O	2.14	0.47
3:Q:211:GLU:C	3:Q:212:ILE:HD12	2.34	0.47
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.26	0.47
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.41	0.47
10:X:45:PHE:CE1	10:X:52:THR:HG23	2.50	0.47
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.11	0.47
15:H:0:FEB:H30A	9:I:92:PHE:HD2	1.80	0.47
12:L:114:ASP:HB2	12:L:118:SER:N	2.29	0.47
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.50	0.47
4:R:72:ARG:HG3	16:R:275:HOH:O	2.14	0.47
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.38	0.47
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.14	0.47
2:B:224:PHE:HD2	2:B:224:PHE:N	2.12	0.47
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.96	0.47
10:J:136:SER:HB2	11:Y:161:ALA:HB1	1.95	0.47
2:P:90:ASN:O	2:P:94:ILE:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.49	0.47
6:T:127:ASN:HD22	6:T:127:ASN:C	2.17	0.47
7:U:10:ARG:HG2	7:U:22:TYR:CD2	2.50	0.47
8:V:197:ARG:NH2	9:W:139:GLU:O	2.46	0.47
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.29	0.47
4:D:207:LEU:HD23	4:D:207:LEU:C	2.33	0.47
5:E:35:SER:HB3	5:E:66:LYS:HZ3	1.80	0.47
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.15	0.47
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.14	0.47
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.50	0.47
2:P:186:VAL:CG2	2:P:216:ARG:HD3	2.40	0.47
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.11	0.47
2:B:186:VAL:HG21	2:B:216:ARG:CD	2.42	0.47
3:C:14:ILE:HD12	3:C:14:ILE:C	2.35	0.47
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.96	0.47
10:J:45:PHE:CD1	10:J:52:THR:HG23	2.50	0.47
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.96	0.47
7:U:12:ILE:HD11	7:U:14:ILE:HD12	1.97	0.47
14:2:107:LYS:CG	14:2:108:GLY:H	2.28	0.47
1:A:198:LYS:HE3	1:A:236:LEU:CD1	2.45	0.47
1:A:38:LEU:HD12	1:A:38:LEU:O	2.15	0.47
2:B:202:THR:CG2	2:B:204:SER:HB2	2.45	0.47
3:C:36:CYS:H	3:C:51:GLU:HG2	1.80	0.47
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.44	0.47
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.30	0.47
4:R:40:ILE:HG13	4:R:193:VAL:HG22	1.96	0.47
6:T:114:ASP:O	6:T:118:GLN:HG2	2.15	0.47
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.44	0.47
4:D:12(E):SER:HB2	5:E:123:ASN:OD1	2.15	0.47
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.30	0.47
9:I:6:MET:CE	9:I:155:ILE:HA	2.44	0.47
3:Q:228:GLU:O	3:Q:232:TYR:HD1	1.97	0.47
8:V:37:ILE:HG23	8:V:60:GLY:HA2	1.97	0.47
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.80	0.47
13:I:41:THR:OG1	13:I:76:PRO:HG3	2.15	0.47
8:H:3:ILE:HD12	8:H:127:LEU:O	2.15	0.47
12:L:140:ASN:O	12:L:144:PHE:HA	2.15	0.47
2:P:224:PHE:N	2:P:224:PHE:HD2	2.12	0.47
3:Q:159:SER:O	4:R:59:LEU:HD22	2.15	0.47
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.15	0.47
15:V:0:FEB:H26A	9:W:116:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.12	0.46
11:K:67:GLU:OE2	16:K:241:HOH:O	2.19	0.46
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.96	0.46
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.15	0.46
8:H:175:VAL:HG12	8:H:176:CYS:N	2.31	0.46
10:J:168:MET:HE1	10:X:167:PRO:CB	2.45	0.46
2:P:229:ILE:O	2:P:233:LEU:HB2	2.15	0.46
7:U:74:ILE:HD13	16:U:287:HOH:O	2.15	0.46
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.50	0.46
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.96	0.46
8:H:38:SER:OG	8:H:41:ILE:HG12	2.16	0.46
10:J:93:ARG:HG2	10:J:93:ARG:NH1	2.30	0.46
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.98	0.46
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.80	0.46
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.97	0.46
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.75	0.46
7:U:59:LEU:O	7:U:61:PRO:HD3	2.15	0.46
12:L:93:PHE:N	12:L:94:PRO:HD3	2.30	0.46
1:O:40:ILE:HD12	1:O:193:ALA:HB2	1.96	0.46
3:Q:169:SER:HA	3:Q:172:VAL:HG12	1.98	0.46
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.77	0.46
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.30	0.46
3:C:16:SER:HB2	3:C:17:PRO:HD2	1.96	0.46
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.97	0.46
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.50	0.46
3:Q:159:SER:HB2	16:Q:264:HOH:O	2.16	0.46
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.46	0.46
9:W:6:MET:CE	9:W:155:ILE:HA	2.45	0.46
10:X:193:GLN:OXT	10:X:193:GLN:HG2	2.16	0.46
2:B:144:ARG:HG2	2:B:144:ARG:O	2.16	0.46
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.79	0.46
13:M:17:ASP:HA	13:M:173:PHE:CB	2.45	0.46
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.98	0.46
11:Y:135:TYR:CB	16:Y:232:HOH:O	2.63	0.46
16:T:273:HOH:O	14:2:70:TYR:HE2	1.98	0.46
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.96	0.46
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.15	0.46
3:Q:16:SER:HB2	3:Q:17:PRO:HD2	1.97	0.46
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.97	0.46
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.98	0.46
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:121:GLN:NE2	16:F:258:HOH:O	2.48	0.46
10:J:167:PRO:CB	10:X:168:MET:HE1	2.46	0.46
2:P:63:THR:HG22	2:P:63:THR:O	2.16	0.46
1:A:13:THR:O	2:B:130:ARG:HD3	2.16	0.46
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.45	0.46
14:N:14:LEU:O	14:N:175:MET:HA	2.16	0.46
7:U:212:VAL:HG23	7:U:229:ILE:CD1	2.46	0.46
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.16	0.46
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.51	0.46
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.97	0.46
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.96	0.46
12:L:1:GLY:N	16:L:224:HOH:O	2.49	0.46
14:N:3:ILE:CD1	14:N:46:SER:HB3	2.46	0.46
7:U:83:PRO:HG2	16:U:265:HOH:O	2.15	0.46
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.98	0.46
6:F:50:VAL:HG22	6:F:51:GLU:N	2.31	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.97	0.45
3:Q:141:PHE:CD1	3:Q:217:PRO:HG3	2.51	0.45
5:S:67:ILE:CG2	5:S:223:ILE:HD12	2.47	0.45
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.98	0.45
8:V:63:ILE:HA	8:V:63:ILE:HD13	1.85	0.45
2:B:229:ILE:O	2:B:233:LEU:HB2	2.15	0.45
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.99	0.45
3:C:163:GLN:HG3	3:C:164:THR:N	2.30	0.45
3:C:224:LEU:N	3:C:224:LEU:CD1	2.80	0.45
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.98	0.45
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.46	0.45
11:K:5:ALA:HA	11:K:13:ILE:O	2.17	0.45
2:P:144:ARG:O	2:P:144:ARG:HG2	2.16	0.45
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.31	0.45
6:T:78:TYR:CE1	6:T:85:GLY:HA3	2.51	0.45
7:U:171:GLU:OE1	7:U:171:GLU:N	2.47	0.45
1:A:29:THR:O	1:A:33:GLN:HG2	2.15	0.45
2:B:191:GLU:O	2:B:195:LYS:HG2	2.16	0.45
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.98	0.45
8:H:144:GLN:O	8:H:145:ASP:HB2	2.16	0.45
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.98	0.45
1:A:47:VAL:HG23	1:A:212:LEU:HD21	1.97	0.45
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.43	0.45
3:C:141:PHE:CD1	3:C:217:PRO:HG3	2.51	0.45
5:E:125:GLN:HE22	6:F:87:HIS:CD2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:203:GLU:C	6:F:205:ASN:H	2.19	0.45
7:G:96:ALA:CA	7:G:107:MET:CE	2.89	0.45
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.81	0.45
3:Q:57:LYS:HG2	3:Q:208:LYS:NZ	2.32	0.45
4:R:68:VAL:CG2	4:R:89:ILE:HD12	2.33	0.45
8:V:26:VAL:HG11	8:V:29:LYS:HG2	1.97	0.45
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.15	0.45
7:G:172:ILE:HD13	7:G:197:MET:HE1	1.98	0.45
7:G:218:ASP:O	7:G:220:LYS:HB2	2.16	0.45
10:J:88:ALA:O	10:J:90(A):ILE:HG22	2.16	0.45
6:T:203:GLU:C	6:T:205:ASN:H	2.19	0.45
7:U:146:PRO:HD2	16:U:299:HOH:O	2.16	0.45
7:U:47:VAL:HG12	7:U:49:ILE:CD1	2.47	0.45
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.99	0.45
1:A:21(L):ILE:HD11	8:H:186:TYR:CD2	2.52	0.45
5:E:64:GLN:NE2	5:E:82:ALA:HB2	2.32	0.45
8:H:37:ILE:HG23	8:H:60:GLY:HA2	1.98	0.45
12:L:4:LEU:HD23	12:L:159:PHE:CE1	2.52	0.45
1:O:21(G):LEU:HG	1:O:21(I):TYR:CE1	2.51	0.45
8:V:38:SER:OG	8:V:41:ILE:HG12	2.16	0.45
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.98	0.45
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.98	0.45
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.00	0.45
11:K:40:PHE:CB	11:K:73:ARG:HH21	2.25	0.45
11:K:74:ILE:HG13	11:K:75:SER:N	2.30	0.45
11:K:99:THR:HG22	11:K:113:VAL:HB	1.99	0.45
13:M:-3:VAL:HA	13:M:21:SER:O	2.17	0.45
8:V:196:VAL:HG23	16:V:242:HOH:O	2.16	0.45
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.12	0.45
5:E:197:ILE:HG23	5:E:198:SER:N	2.32	0.45
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.47	0.45
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.16	0.45
12:L:14(E):GLU:HB2	12:L:14(M):VAL:HB	1.98	0.45
13:1:146:THR:HA	16:1:233:HOH:O	2.17	0.45
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.46	0.45
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.98	0.45
3:C:57:LYS:HG2	3:C:208:LYS:NZ	2.32	0.45
6:F:43:ASN:HD22	6:F:44:ASP:N	2.15	0.45
13:M:57:ARG:CD	16:M:244:HOH:O	2.64	0.45
9:W:101:VAL:O	9:W:110:ILE:HA	2.17	0.45
10:X:112:GLN:NE2	10:X:126:ALA:H	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:45:PHE:CD1	10:X:52:THR:HG23	2.52	0.45
13:1:-3:VAL:HA	13:1:21:SER:O	2.17	0.45
3:C:228:GLU:O	3:C:232:TYR:HD1	1.99	0.45
7:G:151:THR:HG22	7:G:157:TYR:HB3	1.98	0.45
12:L:-2:ASN:HA	12:L:21:ILE:O	2.16	0.45
12:L:4:LEU:HD23	12:L:159:PHE:HE1	1.82	0.45
4:R:102:TYR:O	12:Z:81:ARG:HG3	2.16	0.45
4:R:112:LEU:O	4:R:112:LEU:HD13	2.16	0.45
5:S:111:ARG:NH1	5:S:111:ARG:HG2	2.32	0.45
8:V:144:GLN:O	8:V:145:ASP:HB2	2.16	0.45
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.52	0.45
11:Y:74:ILE:HG13	11:Y:75:SER:N	2.32	0.45
12:Z:14(E):GLU:HB2	12:Z:14(M):VAL:HB	1.99	0.45
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.98	0.44
14:2:116:GLY:HA3	16:2:191:HOH:O	2.15	0.44
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.32	0.44
1:A:38:LEU:HD12	1:A:38:LEU:C	2.37	0.44
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	1.99	0.44
10:J:-1:MET:CG	10:J:1:ASP:H	2.23	0.44
11:K:157:ARG:HH11	11:K:157:ARG:HG3	1.82	0.44
12:L:4:LEU:HD12	12:L:5:GLY:N	2.32	0.44
5:S:125:GLN:HE22	6:T:87:HIS:CD2	2.34	0.44
5:S:197:ILE:HG23	5:S:198:SER:N	2.31	0.44
7:U:218:ASP:O	7:U:220:LYS:HB2	2.17	0.44
12:Z:1:GLY:HA3	12:Z:33:LYS:NZ	2.32	0.44
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.46	0.44
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.16	0.44
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.51	0.44
6:F:78:TYR:CE1	6:F:85:GLY:HA3	2.52	0.44
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.18	0.44
2:P:87:ILE:O	2:P:91:THR:HG23	2.16	0.44
3:Q:14:ILE:O	3:Q:14:ILE:HD12	2.17	0.44
4:R:177:LEU:CD2	5:S:58:LEU:HD13	2.43	0.44
7:U:172:ILE:HD13	7:U:197:MET:CE	2.47	0.44
12:Z:114:ASP:HB2	12:Z:118:SER:H	1.83	0.44
12:Z:1:GLY:HA3	12:Z:33:LYS:HZ2	1.81	0.44
14:2:146:MET:HB3	14:2:150:GLU:HB2	1.98	0.44
3:C:43:LYS:O	3:C:43:LYS:HG2	2.17	0.44
10:J:112:GLN:NE2	10:J:126:ALA:H	2.15	0.44
13:M:19:LEU:HD12	13:M:20:GLY:H	1.83	0.44
1:O:198:LYS:HE3	1:O:236:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.46	0.44
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.17	0.44
7:G:136:LEU:O	7:G:150:LYS:HA	2.17	0.44
7:G:59:LEU:O	7:G:61:PRO:HD3	2.16	0.44
1:O:38:LEU:HD12	1:O:38:LEU:O	2.18	0.44
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.52	0.44
2:P:53:LYS:HG2	2:P:54:VAL:HG23	1.99	0.44
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	2.00	0.44
2:B:63:THR:HG22	2:B:63:THR:O	2.17	0.44
2:B:85:ALA:O	2:B:89:ILE:HG13	2.18	0.44
5:S:44:THR:HG23	5:S:183:ASP:HB3	2.00	0.44
11:Y:99:THR:HG22	11:Y:113:VAL:HB	1.99	0.44
3:C:169:SER:HA	3:C:172:VAL:HG12	1.97	0.44
3:C:33:ARG:HG2	3:C:33:ARG:O	2.17	0.44
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.88	0.44
2:P:191:GLU:O	2:P:195:LYS:HG2	2.16	0.44
6:T:50:VAL:HG22	6:T:51:GLU:N	2.32	0.44
10:X:93:ARG:NH1	10:X:93:ARG:HG2	2.33	0.44
13:1:17:ASP:HA	13:1:173:PHE:CB	2.47	0.44
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.52	0.44
2:B:6:ARG:HG2	3:C:10:ARG:NH2	2.33	0.44
4:D:122:ARG:NH1	4:D:122:ARG:HG2	2.32	0.44
11:K:4:LEU:HD11	11:K:15:ALA:HB3	2.00	0.44
14:N:107:LYS:CG	14:N:108:GLY:H	2.28	0.44
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.99	0.44
9:W:7:THR:HG23	9:W:110:ILE:HD13	2.00	0.44
9:W:2:ILE:HD11	9:W:17:ASP:HB3	2.00	0.44
11:Y:200:LYS:HE2	16:Y:239:HOH:O	2.17	0.44
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.52	0.44
1:A:21(I):TYR:HE2	1:A:21(L):ILE:HD13	1.83	0.44
2:B:171:ALA:O	2:B:175:LEU:HG	2.17	0.44
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.37	0.44
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.18	0.44
5:E:44:THR:HG23	5:E:183:ASP:HB3	2.00	0.44
7:G:12:ILE:HD13	7:G:12:ILE:N	2.33	0.44
7:G:17(C):LYS:HE3	7:G:17(C):LYS:HB2	1.75	0.44
10:J:133:TYR:HE2	10:J:166:MET:SD	2.41	0.44
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.98	0.44
11:K:67:GLU:HG2	11:K:72:GLU:O	2.18	0.44
1:O:58:LEU:HB3	7:U:162:ALA:O	2.16	0.44
2:P:186:VAL:CB	2:P:216:ARG:HD3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:109:ILE:HB	6:T:110:PRO:HD3	2.00	0.44
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.18	0.44
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	2.00	0.44
11:Y:208:ASN:O	11:Y:209:VAL:C	2.56	0.44
11:Y:40:PHE:CG	11:Y:73:ARG:NH2	2.86	0.44
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.18	0.44
14:2:14:LEU:O	14:2:175:MET:HA	2.18	0.43
2:B:112:LEU:C	2:B:112:LEU:HD23	2.39	0.43
2:B:126:HIS:HA	16:C:267:HOH:O	2.17	0.43
3:C:235:GLN:O	3:C:239:GLU:HG2	2.18	0.43
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.39	0.43
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.47	0.43
11:K:32:LYS:N	11:K:32:LYS:HD2	2.33	0.43
12:L:114:ASP:HB2	12:L:118:SER:H	1.83	0.43
2:P:95:HIS:CD2	2:P:115:ARG:HG2	2.53	0.43
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.99	0.43
13:1:40:ASN:ND2	13:1:40:ASN:N	2.65	0.43
7:G:188:LYS:HA	7:G:188:LYS:HD3	1.87	0.43
15:H:0:FEB:H26A	9:I:116:ILE:HD12	1.99	0.43
9:I:1:GLY:HA2	9:I:17:ASP:OD1	2.18	0.43
1:O:38:LEU:HD12	1:O:38:LEU:C	2.38	0.43
3:Q:163:GLN:HE22	3:Q:173:ARG:NE	2.12	0.43
1:O:86:ARG:NE	7:U:118:ASN:ND2	2.55	0.43
13:1:3:VAL:O	13:1:126:ALA:HA	2.18	0.43
14:2:59:VAL:HG11	14:2:83:PHE:CE2	2.54	0.43
5:E:4:PHE:CG	5:E:5:ARG:N	2.86	0.43
9:I:160:LEU:HD12	9:I:191:MET:HE3	2.00	0.43
10:J:138:LEU:HD21	10:J:158:CYS:SG	2.59	0.43
4:R:128:MET:HE3	4:R:130:ARG:O	2.19	0.43
6:T:172:ALA:O	6:T:176:LEU:HD23	2.18	0.43
6:T:210:LEU:HD21	6:T:212:ILE:HD11	2.00	0.43
8:V:22:GLN:CG	8:V:27:ALA:HB2	2.48	0.43
11:Y:32:LYS:HD2	11:Y:32:LYS:N	2.32	0.43
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.18	0.43
13:1:12:VAL:CG2	13:1:102:ALA:HB1	2.48	0.43
3:C:57:LYS:HG2	3:C:208:LYS:HZ3	1.83	0.43
8:H:18:THR:HB	8:H:30:ASN:HD22	1.84	0.43
9:I:7:THR:HG23	9:I:110:ILE:HD13	2.00	0.43
9:I:2:ILE:HD11	9:I:17:ASP:HB3	2.00	0.43
13:M:165:ARG:HA	14:2:26:ILE:HB	2.00	0.43
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:33:ARG:HG2	3:Q:33:ARG:O	2.17	0.43
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.76	0.43
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.54	0.43
6:T:18:ASP:N	6:T:18:ASP:OD2	2.43	0.43
6:T:37:SER:HB3	6:T:50:VAL:HG23	2.00	0.43
16:V:264:HOH:O	9:W:150:ASP:HA	2.19	0.43
13:1:148:VAL:CG2	16:1:228:HOH:O	2.62	0.43
14:2:105:ASP:OD2	14:2:106:ASN:N	2.45	0.43
1:A:170:VAL:HB	16:A:252:HOH:O	2.19	0.43
2:B:184:MET:HE2	2:B:188:ASP:HB3	1.99	0.43
3:C:194:VAL:O	3:C:198:LEU:HG	2.17	0.43
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.32	0.43
2:P:112:LEU:HD23	2:P:112:LEU:C	2.39	0.43
2:P:122:GLY:C	2:P:124:THR:H	2.22	0.43
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.39	0.43
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.88	0.43
7:U:136:LEU:O	7:U:150:LYS:HA	2.17	0.43
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.31	0.43
12:Z:4:LEU:HD23	12:Z:159:PHE:HE1	1.82	0.43
2:B:184:MET:CE	2:B:188:ASP:HB3	2.49	0.43
6:F:90:ASN:O	6:F:94:GLU:HG3	2.19	0.43
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.18	0.43
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.39	0.43
14:N:19:ARG:CZ	14:N:26:ILE:HD11	2.48	0.43
2:P:238:ILE:O	2:P:239:THR:O	2.37	0.43
2:P:68:TYR:CG	2:P:89:ILE:HD12	2.52	0.43
5:S:199:GLN:CA	5:S:199:GLN:HE21	2.32	0.43
5:S:5:ARG:HG3	5:S:22:PHE:CZ	2.54	0.43
9:W:123:ASP:OD1	9:W:124:PHE:N	2.46	0.43
12:Z:4:LEU:HD12	12:Z:5:GLY:N	2.33	0.43
14:2:146:MET:CE	14:2:150:GLU:HB3	2.49	0.43
2:B:227:GLN:OE1	2:B:230:LYS:HD3	2.19	0.43
3:C:152:GLU:HB2	3:C:153:PRO:HD2	2.00	0.43
6:F:37:SER:HB3	6:F:50:VAL:HG23	2.00	0.43
10:J:133:TYR:CD1	16:Y:232:HOH:O	2.34	0.43
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.49	0.43
10:X:138:LEU:HD21	10:X:158:CYS:SG	2.58	0.43
2:B:87:ILE:O	2:B:91:THR:HG23	2.18	0.43
9:I:101:VAL:O	9:I:110:ILE:HA	2.19	0.43
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.53	0.43
11:K:4:LEU:CD1	11:K:159:ILE:CD1	2.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:136:PHE:O	2:P:150:THR:HA	2.19	0.43
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.54	0.43
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.82	0.43
5:S:4:PHE:CG	5:S:5:ARG:N	2.86	0.43
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.17	0.43
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	2.01	0.43
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.83	0.43
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.99	0.43
2:B:95:HIS:CD2	2:B:115:ARG:HG2	2.53	0.43
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.19	0.43
7:G:12:ILE:CD1	7:G:14:ILE:HD12	2.49	0.43
11:K:184:TRP:C	11:K:185:ILE:HD13	2.38	0.43
11:K:208:ASN:O	11:K:209:VAL:C	2.57	0.43
11:K:40:PHE:CG	11:K:73:ARG:NH2	2.87	0.43
14:N:146:MET:CE	14:N:150:GLU:HB3	2.49	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.54	0.43
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.18	0.43
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.19	0.43
8:H:201:GLN:HG2	12:Z:153:LYS:HA	2.00	0.43
12:Z:4:LEU:HD23	12:Z:159:PHE:CE1	2.53	0.43
3:C:195:ARG:CG	3:C:236:ILE:HD13	2.46	0.43
7:G:8:TYR:C	7:G:10:ARG:N	2.73	0.43
1:O:77:VAL:HG12	1:O:137:LEU:HB2	2.00	0.43
3:Q:43:LYS:HG2	3:Q:43:LYS:O	2.19	0.43
7:U:96:ALA:CA	7:U:107:MET:CE	2.89	0.43
14:2:36:ARG:HG3	14:2:42:TRP:NE1	2.33	0.42
3:C:206:GLY:HA3	3:C:209:ASN:HD22	1.84	0.42
8:H:22:GLN:CG	8:H:27:ALA:HB2	2.48	0.42
11:K:67:GLU:CB	16:K:241:HOH:O	2.67	0.42
12:L:17:ASP:HA	12:L:172:GLY:O	2.19	0.42
14:N:59:VAL:HG11	14:N:83:PHE:CE2	2.54	0.42
1:O:21(I):TYR:HE2	1:O:21(L):ILE:HD13	1.84	0.42
2:P:184:MET:CE	2:P:188:ASP:HB3	2.49	0.42
11:Y:40:PHE:CG	11:Y:73:ARG:CZ	3.02	0.42
14:2:147:SER:OG	14:2:150:GLU:HG3	2.19	0.42
2:B:40:ILE:HD12	2:B:193:ALA:HB2	2.01	0.42
3:C:58:LEU:HA	3:C:58:LEU:HD12	1.77	0.42
6:F:31:VAL:HG22	6:F:134:VAL:HA	2.01	0.42
11:K:111:TYR:CE1	11:K:121:LYS:HB2	2.55	0.42
12:L:185:ARG:NH1	16:L:242:HOH:O	2.51	0.42
14:N:147:SER:OG	14:N:150:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:15:PHE:H	2:P:23:GLN:NE2	1.88	0.42
2:P:227:GLN:OE1	2:P:230:LYS:HD3	2.18	0.42
2:P:41:MET:HE2	16:P:244:HOH:O	2.19	0.42
3:Q:76:LEU:HD23	3:Q:76:LEU:C	2.40	0.42
7:U:12:ILE:N	7:U:12:ILE:HD13	2.33	0.42
7:U:39:ALA:CB	7:U:148:ILE:HD12	2.49	0.42
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.50	0.42
1:A:90:ASP:OD1	16:A:244:HOH:O	2.22	0.42
4:D:128:MET:HE3	4:D:130:ARG:O	2.19	0.42
4:D:148:LEU:HB3	4:D:160:TYR:O	2.19	0.42
5:E:5:ARG:HG3	5:E:22:PHE:CZ	2.54	0.42
7:G:191:GLU:HG3	7:G:232:ARG:HG3	2.01	0.42
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.16	0.42
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.54	0.42
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.61	0.42
14:N:107:LYS:NZ	14:N:145:ASN:HD21	2.17	0.42
4:R:121:LEU:HA	4:R:123:PHE:HE1	1.84	0.42
7:U:18(D):ILE:O	7:U:18(G):GLU:N	2.50	0.42
7:U:225:SER:O	7:U:229:ILE:HG13	2.19	0.42
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.49	0.42
5:E:67:ILE:CG2	5:E:223:ILE:HD12	2.49	0.42
7:G:74:ILE:HD13	16:G:246:HOH:O	2.20	0.42
14:N:146:MET:HB3	14:N:150:GLU:HB2	2.00	0.42
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.55	0.42
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.55	0.42
5:S:52:LYS:HB3	5:S:63:TYR:HB3	2.02	0.42
6:T:157:TYR:CD1	6:T:157:TYR:C	2.92	0.42
6:T:43:ASN:HD22	6:T:44:ASP:N	2.17	0.42
11:Y:39:PRO:HG3	16:Y:256:HOH:O	2.19	0.42
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.83	0.42
1:A:130:ARG:HG2	7:G:125:GLN:HG3	2.02	0.42
1:O:142:ASP:OD1	1:O:145:ASN:HB2	2.20	0.42
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.19	0.42
6:T:172:ALA:O	6:T:176:LEU:CD2	2.68	0.42
7:U:191:GLU:HG3	7:U:232:ARG:HG3	2.02	0.42
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.20	0.42
1:A:40:ILE:HD12	1:A:193:ALA:HB2	2.01	0.42
4:D:68:VAL:CG2	4:D:89:ILE:HD12	2.35	0.42
5:E:199:GLN:CA	5:E:199:GLN:HE21	2.32	0.42
12:L:21:ILE:HD12	12:L:21:ILE:C	2.40	0.42
13:M:12:VAL:CG2	13:M:102:ALA:HB1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.20	0.42
8:V:206:PHE:CZ	9:W:157:GLN:HG3	2.55	0.42
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.54	0.42
10:X:3:ILE:HD13	10:X:3:ILE:HA	1.90	0.42
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	2.14	0.42
5:E:111:ARG:NH1	5:E:111:ARG:HG2	2.33	0.42
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.19	0.42
1:A:97:HIS:HD2	8:H:61:SER:OG	2.03	0.42
9:I:123:ASP:OD1	9:I:124:PHE:N	2.50	0.42
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.55	0.42
4:D:102:TYR:O	12:L:81:ARG:HG3	2.20	0.42
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	2.00	0.42
3:Q:224:LEU:H	3:Q:224:LEU:CD1	2.32	0.42
4:R:59:LEU:HD13	4:R:59:LEU:C	2.40	0.42
12:Z:14(I):THR:HB	12:Z:14(M):VAL:HG23	2.01	0.42
7:U:93:LYS:HD3	14:2:68:SER:HB3	2.01	0.42
2:B:213:ALA:HA	2:B:222:LYS:O	2.20	0.42
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.55	0.42
8:H:206:PHE:CZ	9:I:157:GLN:HG3	2.55	0.42
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.02	0.42
1:O:49:ALA:HB2	1:O:212:LEU:HG	2.00	0.42
4:R:17:PRO:HA	5:S:26:TYR:CD1	2.54	0.42
6:T:31:VAL:HG22	6:T:134:VAL:HA	2.02	0.42
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.20	0.42
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.85	0.42
12:L:1:GLY:HA3	12:L:33:LYS:NZ	2.34	0.42
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.85	0.42
3:Q:194:VAL:O	3:Q:198:LEU:HG	2.19	0.42
3:Q:212:ILE:HG22	3:Q:224:LEU:HD13	2.00	0.42
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.20	0.42
8:V:18:THR:HB	8:V:30:ASN:HD22	1.85	0.42
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.85	0.42
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.55	0.42
2:B:184:MET:HE2	2:B:188:ASP:CB	2.50	0.42
2:B:186:VAL:CB	2:B:216:ARG:HD3	2.50	0.42
3:C:76:LEU:HD23	3:C:76:LEU:C	2.40	0.42
5:E:44:THR:CG2	5:E:183:ASP:HB3	2.50	0.42
7:G:158:VAL:HG22	7:G:159:GLY:N	2.35	0.42
9:I:28:SER:HB2	10:J:120:VAL:HG21	2.01	0.42
10:J:190:PHE:C	10:J:192:ALA:N	2.74	0.42
13:M:14(G):ILE:HB	13:M:144:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:55:ILE:O	14:N:59:VAL:HG23	2.20	0.42
1:O:13:THR:O	2:P:130:ARG:HD3	2.19	0.42
1:O:32:LYS:HE2	1:O:32:LYS:HA	2.01	0.42
2:P:213:ALA:HA	2:P:222:LYS:O	2.20	0.42
5:S:7:ASN:HA	5:S:7:ASN:HD22	1.64	0.42
7:U:18(H):GLU:H	7:U:18(H):GLU:CD	2.23	0.42
14:2:113:ILE:HG12	14:2:119:VAL:HG13	2.01	0.41
14:2:19:ARG:CZ	14:2:26:ILE:HD11	2.50	0.41
2:B:141:TYR:CE2	2:B:145:GLY:HA2	2.54	0.41
3:C:159:SER:O	4:D:59:LEU:HD22	2.20	0.41
7:G:225:SER:O	7:G:229:ILE:HG13	2.20	0.41
2:P:149:TYR:OH	3:Q:62(A):ILE:HB	2.20	0.41
5:S:118:ASP:HA	16:S:234:HOH:O	2.20	0.41
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.49	0.41
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.84	0.41
9:W:28:SER:HB2	10:X:120:VAL:HG21	2.02	0.41
1:A:212:LEU:HD23	1:A:213:ALA:N	2.35	0.41
2:B:68:TYR:CG	2:B:89:ILE:HD12	2.55	0.41
3:C:55:THR:C	3:C:56:LEU:HD22	2.41	0.41
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.56	0.41
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.55	0.41
7:U:212:VAL:CG2	7:U:229:ILE:HD13	2.49	0.41
11:Y:143:LYS:HB2	11:Y:146:LEU:HD12	2.01	0.41
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.55	0.41
12:Z:21:ILE:HD12	12:Z:21:ILE:C	2.41	0.41
1:A:212:LEU:HD23	1:A:212:LEU:C	2.41	0.41
2:B:225:LYS:N	2:B:228:GLU:OE1	2.48	0.41
3:C:52:ARG:HD2	3:C:208:LYS:O	2.20	0.41
4:D:59:LEU:C	4:D:59:LEU:HD13	2.40	0.41
5:E:214:ILE:HG12	5:E:215:VAL:N	2.35	0.41
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.73	0.41
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.51	0.41
7:G:39:ALA:CB	7:G:148:ILE:HD12	2.49	0.41
8:H:40:LYS:HB2	16:H:238:HOH:O	2.20	0.41
8:H:52:THR:O	8:H:56:THR:HB	2.20	0.41
12:L:35:PHE:O	12:L:42:VAL:HA	2.20	0.41
4:R:122:ARG:HG2	4:R:122:ARG:NH1	2.35	0.41
5:S:194:VAL:O	5:S:197:ILE:HG22	2.20	0.41
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.49	0.41
10:X:190:PHE:C	10:X:192:ALA:N	2.73	0.41
10:X:98:ASN:HB3	10:X:127:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:112:TYR:CE1	13:1:127:THR:HG22	2.55	0.41
2:B:20:ARG:HG2	2:B:20:ARG:NH1	2.35	0.41
2:B:71:ASN:HD22	2:B:72:ASP:H	1.69	0.41
6:F:157:TYR:C	6:F:157:TYR:CD1	2.92	0.41
5:E:125:GLN:HE22	6:F:87:HIS:HD2	1.68	0.41
7:G:212:VAL:CG2	7:G:229:ILE:HD13	2.50	0.41
7:G:55:PRO:HG2	7:G:56:ASP:N	2.33	0.41
9:I:165:ARG:NH2	12:Z:135:MET:HE2	2.35	0.41
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	2.02	0.41
4:R:148:LEU:HB3	4:R:160:TYR:O	2.21	0.41
5:S:38:VAL:HG12	5:S:39:GLY:N	2.35	0.41
7:U:39:ALA:HA	7:U:47:VAL:O	2.21	0.41
14:2:172:VAL:HB	14:2:18(A):ILE:HD11	2.02	0.41
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.85	0.41
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.50	0.41
2:B:14(A):TYR:HB2	2:B:147:GLN:NE2	2.36	0.41
6:F:18:ASP:N	6:F:18:ASP:OD2	2.46	0.41
6:F:35:THR:CG2	6:F:51:GLU:O	2.63	0.41
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.50	0.41
10:J:154:LEU:HA	10:J:154:LEU:HD12	1.89	0.41
12:L:14:LEU:HD13	12:L:34:VAL:CG1	2.44	0.41
4:R:85:ALA:O	4:R:89:ILE:CG1	2.68	0.41
5:S:214:ILE:HG12	5:S:215:VAL:N	2.34	0.41
13:1:122:SER:HB3	13:1:124:THR:O	2.20	0.41
14:2:107:LYS:CG	14:2:108:GLY:N	2.82	0.41
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.55	0.41
3:C:14:ILE:HD12	3:C:14:ILE:O	2.19	0.41
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.60	0.41
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.84	0.41
11:K:200:LYS:HE2	16:K:244:HOH:O	2.21	0.41
14:N:26:ILE:HB	13:1:165:ARG:HA	2.01	0.41
1:O:136:LEU:O	1:O:150:GLN:HA	2.21	0.41
3:Q:208:LYS:HD2	3:Q:208:LYS:O	2.21	0.41
7:U:192:PHE:CD1	7:U:192:PHE:C	2.93	0.41
7:U:172:ILE:CD1	7:U:197:MET:HE1	2.50	0.41
5:E:160:LEU:HD23	6:F:59:LEU:HA	2.03	0.41
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.86	0.41
11:K:40:PHE:CG	11:K:73:ARG:CZ	3.04	0.41
13:M:112:TYR:C	13:M:112:TYR:CD2	2.94	0.41
13:M:69(C):LEU:HD13	13:M:71(B):GLU:HB2	2.03	0.41
2:P:40:ILE:HD12	2:P:193:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:225:LYS:N	2:P:228:GLU:OE1	2.49	0.41
9:W:61:TYR:C	9:W:61:TYR:CD1	2.94	0.41
1:A:49:ALA:HB2	1:A:212:LEU:HG	2.03	0.41
1:A:77:VAL:HG12	1:A:137:LEU:HB2	2.02	0.41
3:C:175:PHE:CZ	3:C:195:ARG:HB3	2.56	0.41
3:C:215:VAL:HG13	3:C:215:VAL:O	2.20	0.41
3:C:238:GLN:O	3:C:242:GLU:HG3	2.21	0.41
6:F:179:LEU:HD11	6:F:192:GLN:HG3	2.02	0.41
6:F:65:VAL:HA	6:F:211:GLU:OE2	2.20	0.41
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.51	0.41
8:H:34:LEU:HD22	8:H:174:ASP:HB3	2.03	0.41
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.20	0.41
10:J:3:ILE:HD12	10:J:44:SER:HB2	2.01	0.41
11:K:156:LYS:HD3	11:K:195:LEU:HD11	2.03	0.41
3:Q:125:GLN:NE2	16:R:263:HOH:O	2.54	0.41
7:U:203:THR:HG22	7:U:204:GLU:O	2.21	0.41
8:V:34:LEU:HD22	8:V:174:ASP:HB3	2.02	0.41
11:Y:111:TYR:CE1	11:Y:121:LYS:HB2	2.55	0.41
14:2:107:LYS:NZ	14:2:145:ASN:HD21	2.18	0.41
1:A:195:LEU:HD23	1:A:236:LEU:HD21	2.03	0.41
2:B:10:SER:HB2	16:B:248:HOH:O	2.21	0.41
3:C:158:SER:CB	4:D:59:LEU:HD21	2.51	0.41
3:C:57:LYS:HD2	3:C:58:LEU:N	2.35	0.41
5:E:38:VAL:HG12	5:E:39:GLY:N	2.35	0.41
7:G:47:VAL:CG1	7:G:49:ILE:CD1	2.99	0.41
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.21	0.41
11:K:12:ILE:HB	11:K:178:VAL:HB	2.03	0.41
13:M:40:ASN:ND2	13:M:40:ASN:N	2.64	0.41
14:N:36:ARG:HG3	14:N:42:TRP:NE1	2.34	0.41
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.60	0.41
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.18	0.41
7:G:10:ARG:HG2	7:G:22:TYR:CD2	2.55	0.41
12:L:14(I):THR:HB	12:L:14(M):VAL:HG23	2.02	0.41
3:Q:215:VAL:O	3:Q:215:VAL:HG13	2.20	0.41
6:T:103:TYR:O	6:T:104:LYS:HB3	2.21	0.41
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.51	0.41
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.03	0.41
9:W:160:LEU:HD12	9:W:191:MET:HE3	2.03	0.41
1:A:136:LEU:O	1:A:150:GLN:HA	2.21	0.41
3:C:120:GLN:O	3:C:124:THR:HG23	2.21	0.41
2:B:149:TYR:CZ	3:C:62(A):ILE:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:171:GLU:OE1	7:G:171:GLU:N	2.47	0.41
8:H:63:ILE:HD13	8:H:63:ILE:HA	1.83	0.41
13:M:9:ASP:OD1	13:M:10:ASN:N	2.54	0.41
1:O:77:VAL:CG1	1:O:137:LEU:HB2	2.51	0.41
1:O:26:TYR:CD1	1:O:26:TYR:N	2.88	0.41
2:P:14(A):TYR:HB2	2:P:147:GLN:NE2	2.36	0.41
3:Q:76:LEU:HD22	3:Q:89:ILE:HG12	2.03	0.41
4:R:121:LEU:HD13	5:S:130:ARG:HH21	1.86	0.41
9:W:45:ILE:HB	9:W:52:VAL:HG13	2.03	0.41
10:X:3:ILE:O	10:X:126:ALA:HA	2.20	0.41
10:X:136:SER:HA	10:X:139:ASP:HB2	2.03	0.41
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.56	0.41
12:Z:35:PHE:O	12:Z:42:VAL:HA	2.21	0.41
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.56	0.40
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.69	0.40
1:A:77:VAL:CG1	1:A:137:LEU:HB2	2.52	0.40
1:A:32:LYS:HE2	1:A:32:LYS:HA	2.03	0.40
2:B:174:THR:O	2:B:178:MET:HB2	2.21	0.40
2:B:20:ARG:NH2	3:C:33:ARG:HE	2.19	0.40
4:D:121:LEU:HA	4:D:123:PHE:HE1	1.83	0.40
7:G:192:PHE:CD1	7:G:192:PHE:C	2.94	0.40
12:L:134:ILE:HD11	12:L:162:ALA:HB2	2.03	0.40
13:M:-1:GLY:HA2	16:M:214:HOH:O	2.20	0.40
2:P:176:LEU:C	2:P:178:MET:H	2.24	0.40
2:P:39:GLY:O	2:P:148:LEU:HD21	2.21	0.40
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.36	0.40
3:Q:66:LYS:HE2	3:Q:78:PHE:CZ	2.57	0.40
9:W:6:MET:HE1	9:W:155:ILE:HA	2.03	0.40
14:2:13:ILE:HD12	14:2:151:THR:CG2	2.52	0.40
4:D:123:PHE:CZ	4:D:131:PRO:HG3	2.56	0.40
5:E:221:PHE:HE1	5:E:223:ILE:HD11	1.84	0.40
9:I:2:ILE:O	9:I:2:ILE:HD12	2.21	0.40
11:K:180:GLU:N	16:K:239:HOH:O	2.53	0.40
14:N:20:THR:HA	15:N:0:FEB:O12	2.21	0.40
2:P:44:ASP:N	2:P:44:ASP:OD2	2.54	0.40
16:T:244:HOH:O	7:U:86:ARG:HD2	2.19	0.40
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.36	0.40
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	2.02	0.40
2:B:159:GLY:O	3:C:59:GLN:HB3	2.21	0.40
13:M:35:ILE:HA	13:M:36:PRO:HD3	1.93	0.40
14:N:172:VAL:HB	14:N:18(A):ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:206:PHE:CE1	1:O:210:ILE:HD11	2.57	0.40
2:P:71:ASN:HD22	2:P:72:ASP:H	1.69	0.40
3:Q:195:ARG:CG	3:Q:236:ILE:HD13	2.47	0.40
4:R:123:PHE:CZ	4:R:131:PRO:HG3	2.56	0.40
5:S:44:THR:CG2	5:S:183:ASP:HB3	2.50	0.40
10:X:166:MET:HA	10:X:167:PRO:HD3	1.79	0.40
10:X:3:ILE:HD12	10:X:44:SER:HB2	2.02	0.40
5:E:76:LEU:HB2	5:E:137:LEU:O	2.21	0.40
6:F:114:ASP:O	6:F:118:GLN:HG2	2.21	0.40
7:G:54:VAL:HA	7:G:55:PRO:HD2	1.96	0.40
8:H:3:ILE:CD1	8:H:3:ILE:H	2.35	0.40
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.84	0.40
11:K:143:LYS:HB2	11:K:146:LEU:HD12	2.03	0.40
14:N:105:ASP:OD2	14:N:106:ASN:N	2.46	0.40
1:O:195:LEU:HD23	1:O:236:LEU:HD21	2.03	0.40
2:P:171:ALA:O	2:P:175:LEU:HG	2.20	0.40
2:P:67:LEU:HD23	2:P:213:ALA:HB2	2.03	0.40
4:R:121:LEU:HD23	4:R:123:PHE:HE1	1.87	0.40
4:R:12(E):SER:O	5:S:123:ASN:OD1	2.39	0.40
1:O:21(L):ILE:HD11	8:V:186:TYR:CD2	2.57	0.40
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.51	0.40
10:X:3:ILE:HB	16:X:234:HOH:O	2.20	0.40
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.57	0.40
13:1:130:GLY:O	13:1:134:ALA:HB3	2.22	0.40
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.17	0.40
2:B:67:LEU:HD23	2:B:213:ALA:HB2	2.02	0.40
6:F:179:LEU:HD11	6:F:192:GLN:HG2	2.04	0.40
8:H:24:PRO:HG2	8:H:25:ILE:CD1	2.50	0.40
8:H:84:LYS:HE2	8:H:119:THR:CG2	2.51	0.40
10:J:105:ASP:O	10:J:106:ASN:N	2.55	0.40
10:J:136:SER:HA	10:J:139:ASP:HB2	2.04	0.40
12:L:43:MET:CB	12:L:101:ILE:HG22	2.51	0.40
2:P:163:ILE:CG1	2:P:164:SER:N	2.82	0.40
2:P:185:LYS:O	2:P:188:ASP:HB2	2.22	0.40
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.37	0.40
3:Q:175:PHE:CZ	3:Q:195:ARG:HB3	2.56	0.40
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.49	0.40
9:W:143:GLU:HA	9:W:144:PRO:HD3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	231 (93%)	15 (6%)	2 (1%)	19	39
1	O	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	13	27
2	B	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	9	18
2	P	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	9	18
3	C	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	12	24
3	Q	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	12	24
4	D	240/242 (99%)	221 (92%)	12 (5%)	7 (3%)	4	7
4	R	240/242 (99%)	221 (92%)	13 (5%)	6 (2%)	5	9
5	E	231/233 (99%)	214 (93%)	13 (6%)	4 (2%)	9	18
5	S	231/233 (99%)	213 (92%)	16 (7%)	2 (1%)	17	35
6	F	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	13	27
6	T	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	13	27
7	G	241/243 (99%)	229 (95%)	12 (5%)	0	100	100
7	U	241/243 (99%)	229 (95%)	11 (5%)	1 (0%)	34	57
8	H	220/222 (99%)	210 (96%)	8 (4%)	2 (1%)	17	35
8	V	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	29	52
9	I	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
10	J	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	29	52
10	X	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	29	52
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	29	52
11	Y	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	29	52
12	L	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	29	52
12	Z	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	29	52
13	1	231/233 (99%)	217 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6312/6368 (99%)	5948 (94%)	310 (5%)	54 (1%)	17	35

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	56	SER
3	C	58	LEU
4	D	12(G)	GLU
10	J	192	ALA
1	O	5	THR
1	O	56	SER
3	Q	58	LEU
4	R	12(G)	GLU
10	X	192	ALA
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
4	D	18(D)	SER
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	18(D)	SER
4	D	12(F)	GLY
5	E	202	ARG
6	F	206	LYS
11	K	39	PRO
2	P	6	ARG
4	R	12(F)	GLY
5	S	202	ARG
6	T	206	LYS
11	Y	39	PRO
2	B	6	ARG
5	E	231	LYS

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Mol	Chain	Res	Type
6	F	205	ASN
5	S	231	LYS
6	T	205	ASN
4	D	60	GLU
4	D	61	SER
4	R	60	GLU
4	R	61	SER
4	D	12(C)	GLY
4	D	128	MET
5	E	180	LEU
5	E	217	LYS
6	F	13	SER
1	O	167	LYS
4	R	12(C)	GLY
6	T	13	SER
8	V	96	GLY
8	H	180	ILE
12	L	14(H)	GLY
8	H	96	GLY
7	U	55	PRO
12	Z	14(H)	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	204 (98%)	5 (2%)	49	74
1	O	209/209 (100%)	204 (98%)	5 (2%)	49	74
2	B	203/203 (100%)	195 (96%)	8 (4%)	32	58
2	P	203/203 (100%)	195 (96%)	8 (4%)	32	58
3	C	213/213 (100%)	204 (96%)	9 (4%)	30	55
3	Q	213/213 (100%)	204 (96%)	9 (4%)	30	55
4	D	198/198 (100%)	187 (94%)	11 (6%)	21	42
4	R	198/198 (100%)	187 (94%)	11 (6%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	192/192 (100%)	171 (89%)	21 (11%)	6	11
5	S	192/192 (100%)	171 (89%)	21 (11%)	6	11
6	F	201/201 (100%)	186 (92%)	15 (8%)	13	27
6	T	201/201 (100%)	185 (92%)	16 (8%)	12	24
7	G	207/207 (100%)	193 (93%)	14 (7%)	16	32
7	U	207/207 (100%)	192 (93%)	15 (7%)	14	29
8	H	181/181 (100%)	173 (96%)	8 (4%)	28	53
8	V	181/181 (100%)	174 (96%)	7 (4%)	32	58
9	I	172/172 (100%)	168 (98%)	4 (2%)	50	75
9	W	172/172 (100%)	168 (98%)	4 (2%)	50	75
10	J	175/175 (100%)	168 (96%)	7 (4%)	31	57
10	X	175/175 (100%)	168 (96%)	7 (4%)	31	57
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	56
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	50
12	L	185/185 (100%)	174 (94%)	11 (6%)	19	39
12	Z	185/185 (100%)	173 (94%)	12 (6%)	17	34
13	1	199/199 (100%)	189 (95%)	10 (5%)	24	47
13	M	199/199 (100%)	190 (96%)	9 (4%)	27	52
14	2	162/162 (100%)	152 (94%)	10 (6%)	18	37
14	N	162/162 (100%)	152 (94%)	10 (6%)	18	37
All	All	5332/5332 (100%)	5050 (95%)	282 (5%)	22	45

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
2	B	58	LEU
2	B	71	ASN
2	B	89	ILE
2	B	121	GLN
2	B	150	THR

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Mol	Chain	Res	Type
2	B	192	LEU
2	B	218	ASN
2	B	224	PHE
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	174	GLU
3	C	208	LYS
3	C	227	GLU
4	D	28	LEU
4	D	40	ILE
4	D	110	GLU
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
4	D	244	GLU
5	E	12	THR
5	E	13	VAL
5	E	32	LYS
5	E	56	ASP
5	E	57	GLU
5	E	76	LEU
5	E	90	ASN
5	E	97	ASN
5	E	104	ASN
5	E	111	ARG
5	E	121	GLN
5	E	18(D)	ILE
5	E	185	ASN
5	E	189	LEU
5	E	197	ILE
5	E	199	GLN
5	E	207	LEU
5	E	2(C)	VAL
5	E	2(E)	ASN

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Mol	Chain	Res	Type
5	E	227	GLU
5	E	231	LYS
6	F	35	THR
6	F	43	ASN
6	F	56	SER
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	21(C)	ASN
7	G	12	ILE
7	G	14	ILE
7	G	35	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	184	ASN
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	3	ILE
8	H	30	ASN
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	99	LEU
8	H	144	GLN
8	H	197	ARG
9	I	29	ASN
9	I	116	ILE
9	I	160	LEU

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Mol	Chain	Res	Type
9	I	171	TRP
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	121	GLU
10	J	137	LEU
10	J	168	MET
11	K	4	LEU
11	K	9	GLN
11	K	38	ASN
11	K	65	LEU
11	K	87	VAL
11	K	104	TYR
11	K	10(B)	LYS
12	L	-7	ASN
12	L	4	LEU
12	L	14	LEU
12	L	25	SER
12	L	58	ARG
12	L	70(A)	ASN
12	L	99	THR
12	L	123	GLN
12	L	134	ILE
12	L	1(I)	ASN
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	112	TYR
13	M	129	PHE
13	M	14(C)	ARG
13	M	149	GLN
13	M	204	LYS
13	M	211	ILE
14	N	70	TYR
14	N	84	LYS
14	N	89	GLU
14	N	10(A)	ASP
14	N	115	LEU
14	N	119	VAL
14	N	149	GLU

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Mol	Chain	Res	Type
14	N	178	LEU
14	N	18(A)	ILE
14	N	18(I)	GLN
1	O	33	GLN
1	O	64	LEU
1	O	135	SER
1	O	158	PHE
1	O	179	ARG
2	P	58	LEU
2	P	71	ASN
2	P	89	ILE
2	P	121	GLN
2	P	150	THR
2	P	192	LEU
2	P	218	ASN
2	P	224	PHE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	174	GLU
3	Q	208	LYS
3	Q	227	GLU
4	R	28	LEU
4	R	40	ILE
4	R	110	GLU
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
4	R	244	GLU
5	S	12	THR
5	S	13	VAL
5	S	32	LYS
5	S	56	ASP
5	S	57	GLU
5	S	76	LEU

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Mol	Chain	Res	Type
5	S	90	ASN
5	S	97	ASN
5	S	104	ASN
5	S	111	ARG
5	S	121	GLN
5	S	18(D)	ILE
5	S	185	ASN
5	S	189	LEU
5	S	197	ILE
5	S	199	GLN
5	S	207	LEU
5	S	2(C)	VAL
5	S	2(E)	ASN
5	S	227	GLU
5	S	231	LYS
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	56	SER
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
7	U	12	ILE
7	U	14	ILE
7	U	35	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	169	GLN
7	U	184	ASN
7	U	197	MET

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Mol	Chain	Res	Type
7	U	217	LYS
7	U	229	ILE
7	U	232	ARG
7	U	233	LEU
8	V	3	ILE
8	V	30	ASN
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	144	GLN
8	V	197	ARG
9	W	29	ASN
9	W	116	ILE
9	W	160	LEU
9	W	171	TRP
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
10	X	137	LEU
10	X	168	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	38	ASN
11	Y	65	LEU
11	Y	87	VAL
11	Y	99	THR
11	Y	104	TYR
11	Y	10(B)	LYS
12	Z	-7	ASN
12	Z	4	LEU
12	Z	14	LEU
12	Z	25	SER
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	99	THR
12	Z	114	ASP
12	Z	123	GLN
12	Z	134	ILE
12	Z	1(I)	ASN
12	Z	145	TYR

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Mol	Chain	Res	Type
13	1	39	ASP
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	14(C)	ARG
13	1	149	GLN
13	1	204	LYS
13	1	211	ILE
14	2	70	TYR
14	2	84	LYS
14	2	89	GLU
14	2	10(A)	ASP
14	2	115	LEU
14	2	119	VAL
14	2	149	GLU
14	2	178	LEU
14	2	18(A)	ILE
14	2	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (194) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	243	GLN

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Mol	Chain	Res	Type
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	10	ASN
8	H	30	ASN
8	H	66	HIS
8	H	91	GLN
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN

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Mol	Chain	Res	Type
9	I	29	ASN
9	I	81	GLN
10	J	36	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	53	GLN
11	K	66	HIS
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	1(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	69	GLN
14	N	145	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
2	P	121	GLN

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Mol	Chain	Res	Type
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	185	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	170	GLN

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Mol	Chain	Res	Type
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	91	GLN
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	81	GLN
10	X	36	GLN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	53	GLN
11	Y	66	HIS
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	85	HIS
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN

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Mol	Chain	Res	Type
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	69	GLN
14	2	141	ASN
14	2	145	ASN
14	2	161	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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	FEB	Y	0	11	38,38,38	0.89	1 (2%)	46,47,47	0.78	0
15	FEB	H	0	8	38,38,38	0.83	0	46,47,47	0.89	1 (2%)
15	FEB	N	0	14	38,38,38	1.48	5 (13%)	46,47,47	1.16	5 (10%)
15	FEB	K	0	11	38,38,38	0.89	1 (2%)	46,47,47	0.80	0
15	FEB	V	0	8	38,38,38	0.81	0	46,47,47	0.91	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	FEB	2	0	14	38,38,38	1.52	6 (15%)	46,47,47	1.20	4 (8%)

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
15	FEB	Y	0	11	-	5/48/48/48	-
15	FEB	H	0	8	-	4/48/48/48	-
15	FEB	N	0	14	-	10/48/48/48	-
15	FEB	K	0	11	-	5/48/48/48	-
15	FEB	V	0	8	-	4/48/48/48	-
15	FEB	2	0	14	-	10/48/48/48	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	0	FEB	C19-N18	5.80	1.58	1.45
15	N	0	FEB	C19-N18	5.69	1.57	1.45
15	N	0	FEB	C36-C27	3.13	1.61	1.52
15	2	0	FEB	C36-C27	3.12	1.61	1.52
15	2	0	FEB	O21-C20	2.47	1.28	1.23
15	2	0	FEB	C3-C2	2.36	1.56	1.52
15	K	0	FEB	C19-N18	2.30	1.50	1.45
15	2	0	FEB	C19-C20	2.28	1.58	1.52
15	N	0	FEB	O21-C20	2.26	1.27	1.23
15	Y	0	FEB	C19-N18	2.14	1.50	1.45
15	N	0	FEB	C10-C11	2.09	1.58	1.52
15	2	0	FEB	C29-C26	2.06	1.61	1.52
15	N	0	FEB	C29-C26	2.02	1.60	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	0	FEB	C19-N18-C38	3.11	129.65	121.65
15	N	0	FEB	C19-N18-C38	2.92	129.16	121.65
15	2	0	FEB	C2-N1-C11	2.87	127.77	123.20
15	N	0	FEB	C2-N1-C11	2.68	127.47	123.20
15	2	0	FEB	C10-N9-C20	2.67	127.40	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	0	FEB	C10-N9-C20	2.61	127.27	121.67
15	2	0	FEB	C20-C19-N18	2.55	118.09	111.16
15	N	0	FEB	C20-C19-N18	2.35	117.55	111.16
15	H	0	FEB	C19-C22-C23	2.18	116.58	112.24
15	N	0	FEB	C19-C20-N9	-2.11	112.06	116.70
15	V	0	FEB	C19-C22-C23	2.04	116.30	112.24

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	N	0	FEB	C20-C19-N18-C38
15	N	0	FEB	C36-C38-N18-C19
15	N	0	FEB	O49-C38-N18-C19
15	N	0	FEB	C26-C27-C36-C38
15	N	0	FEB	O37-C27-C36-C38
15	2	0	FEB	C20-C19-N18-C38
15	2	0	FEB	C36-C38-N18-C19
15	2	0	FEB	O49-C38-N18-C19
15	2	0	FEB	C26-C27-C36-C38
15	2	0	FEB	O37-C27-C36-C38
15	K	0	FEB	C29-C26-C27-O37
15	Y	0	FEB	C31-C32-C33-C34
15	K	0	FEB	C31-C32-C33-C34
15	Y	0	FEB	C29-C26-C27-O37
15	V	0	FEB	C30-C31-C32-C33
15	H	0	FEB	C30-C31-C32-C33
15	Y	0	FEB	C29-C26-C27-C36
15	K	0	FEB	C29-C26-C27-C36
15	Y	0	FEB	C30-C31-C32-C33
15	K	0	FEB	C30-C31-C32-C33
15	V	0	FEB	C32-C33-C34-C35
15	H	0	FEB	C32-C33-C34-C35
15	Y	0	FEB	C32-C33-C34-C35
15	K	0	FEB	C32-C33-C34-C35
15	N	0	FEB	C19-C22-C23-O24
15	N	0	FEB	C19-C22-C23-N25
15	2	0	FEB	C19-C22-C23-O24
15	2	0	FEB	C19-C22-C23-N25
15	N	0	FEB	C27-C26-C29-C28
15	2	0	FEB	C27-C26-C29-C28
15	H	0	FEB	C27-C36-C38-O49

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Mol	Chain	Res	Type	Atoms
15	V	0	FEB	C27-C36-C38-O49
15	H	0	FEB	C27-C36-C38-N18
15	N	0	FEB	C13-C14-C15-N17
15	V	0	FEB	C10-C13-C14-C15
15	N	0	FEB	C13-C14-C15-O16
15	2	0	FEB	C13-C14-C15-O16
15	2	0	FEB	C13-C14-C15-N17

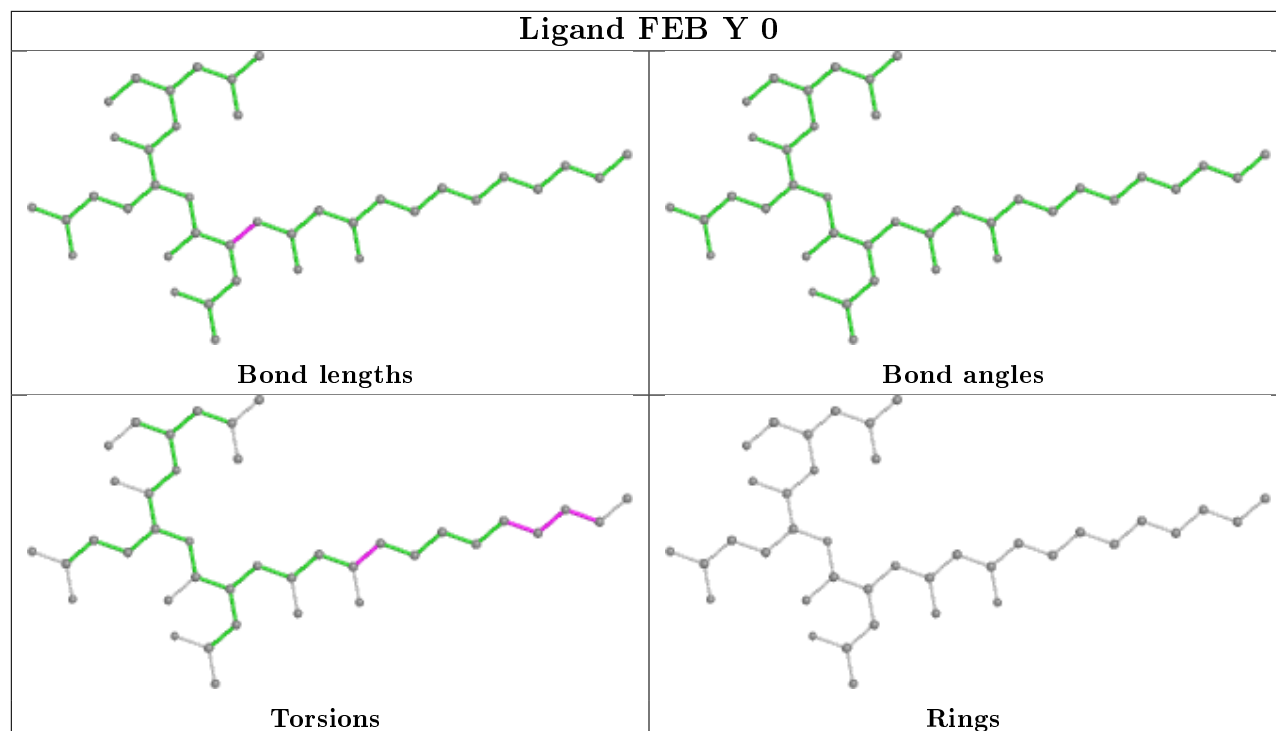
There are no ring outliers.

4 monomers are involved in 19 short contacts:

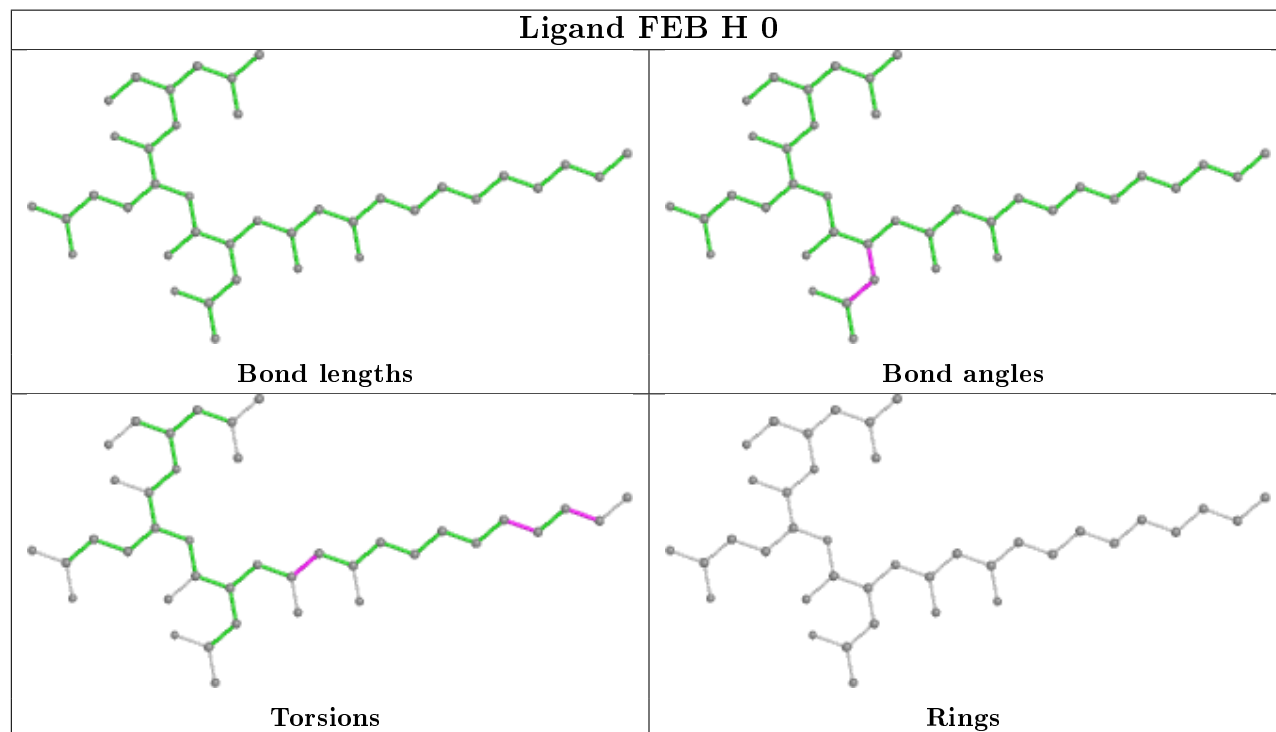
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	0	FEB	3	0
15	N	0	FEB	7	0
15	V	0	FEB	3	0
15	2	0	FEB	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

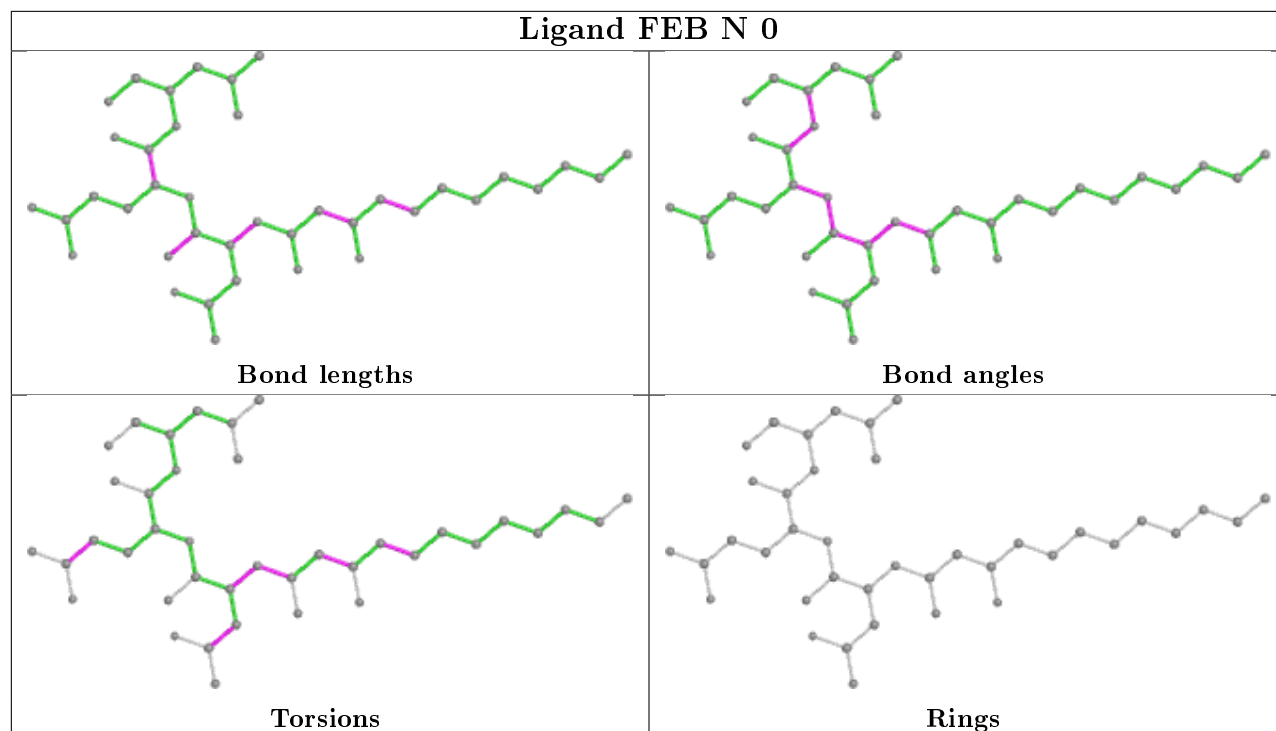
Ligand FEB Y 0



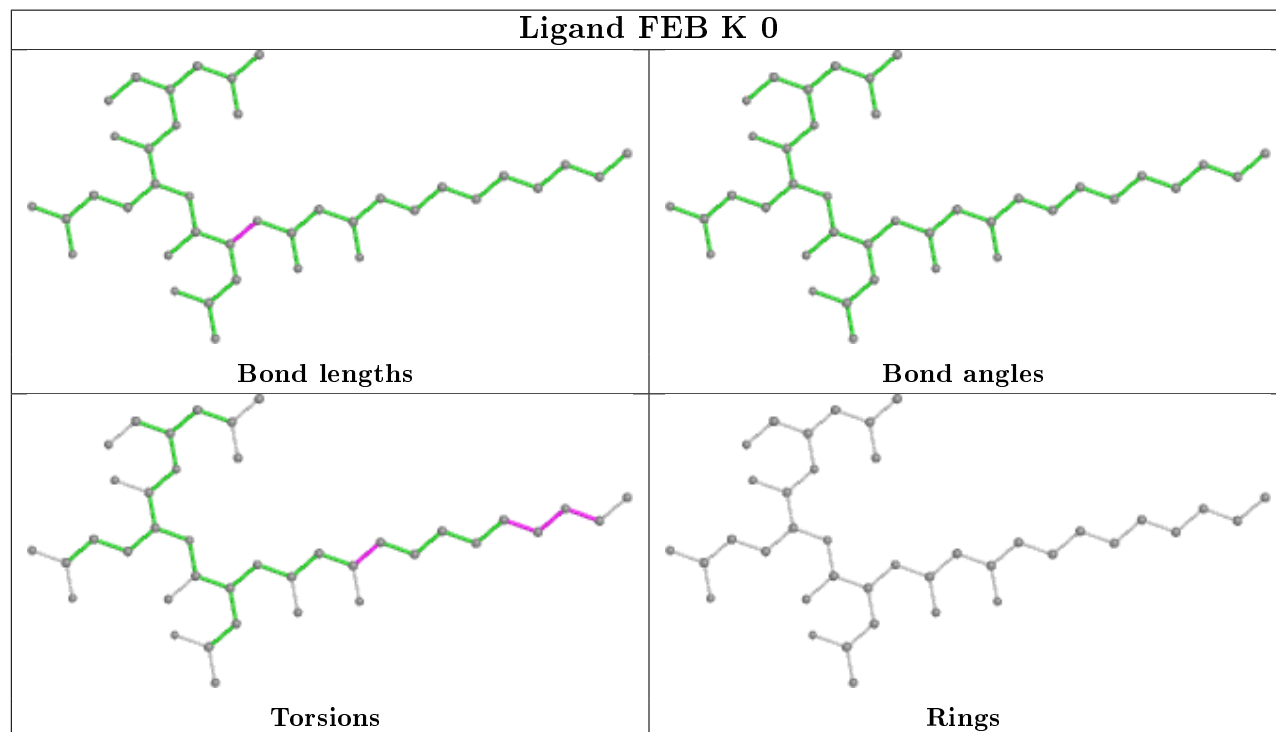
Ligand FEB H 0

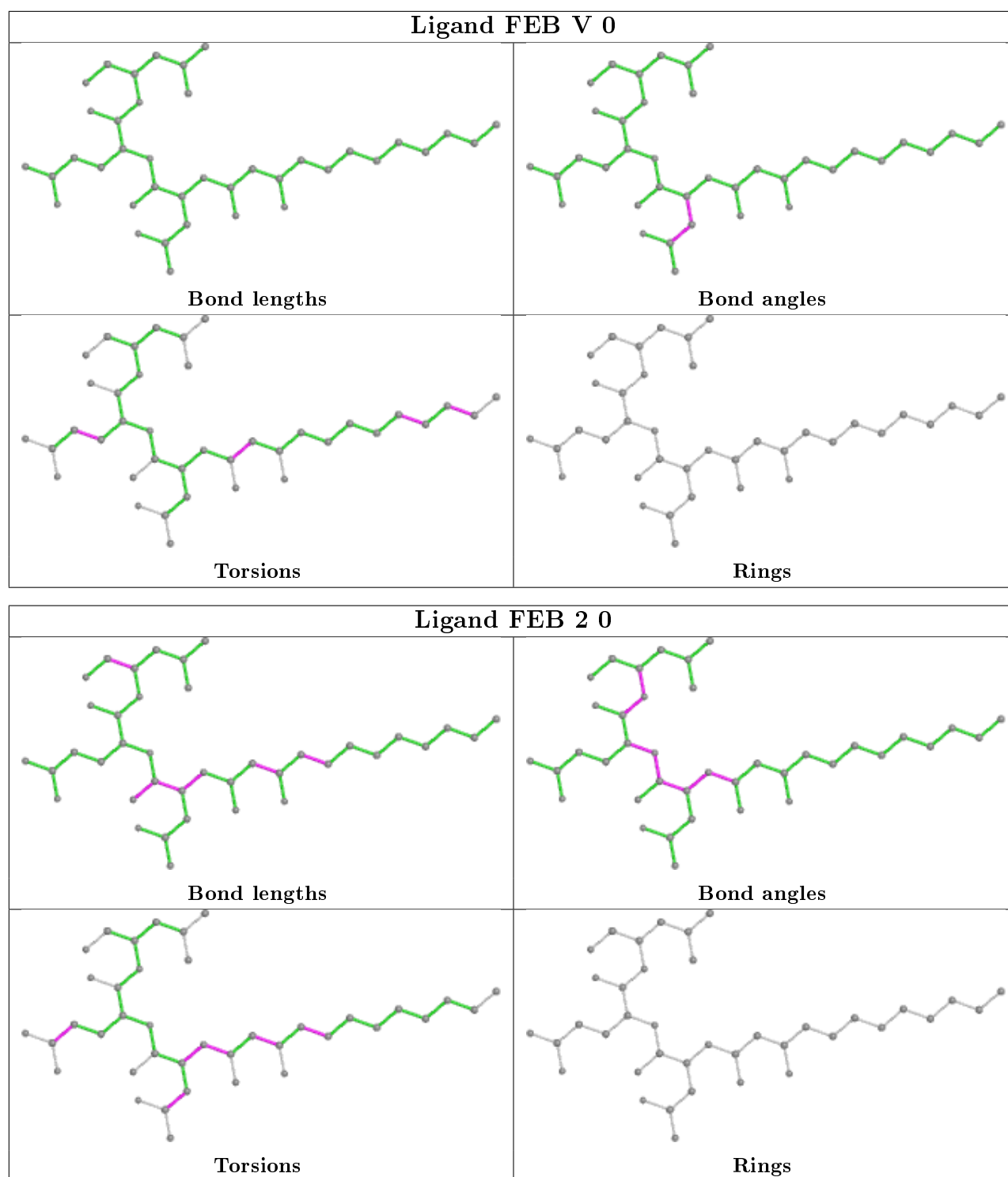


Ligand FEB N 0



Ligand FEB K 0





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.09	9 (3%)	42	35	34, 52, 85, 106	0
1	O	250/250 (100%)	-0.01	14 (5%)	24	19	35, 54, 85, 105	0
2	B	244/244 (100%)	0.18	14 (5%)	23	18	37, 56, 89, 116	0
2	P	244/244 (100%)	0.19	15 (6%)	21	16	40, 56, 89, 116	0
3	C	241/241 (100%)	0.41	26 (10%)	5	3	39, 61, 110, 124	0
3	Q	241/241 (100%)	0.54	37 (15%)	2	1	41, 62, 110, 124	0
4	D	242/242 (100%)	0.22	17 (7%)	16	12	43, 58, 94, 121	0
4	R	242/242 (100%)	0.29	17 (7%)	16	12	44, 59, 95, 122	0
5	E	233/233 (100%)	0.02	9 (3%)	39	32	42, 55, 82, 109	0
5	S	233/233 (100%)	-0.03	8 (3%)	45	38	41, 54, 82, 109	0
6	F	244/244 (100%)	-0.17	9 (3%)	41	34	36, 50, 89, 106	0
6	T	244/244 (100%)	-0.18	7 (2%)	51	45	34, 50, 89, 106	0
7	G	243/243 (100%)	-0.18	9 (3%)	41	34	33, 47, 75, 112	0
7	U	243/243 (100%)	-0.12	8 (3%)	46	39	33, 47, 75, 111	0
8	H	222/222 (100%)	-0.36	3 (1%)	75	71	30, 44, 62, 100	0
8	V	222/222 (100%)	-0.41	3 (1%)	75	71	29, 45, 63, 100	0
9	I	204/204 (100%)	-0.37	4 (1%)	65	60	35, 45, 63, 80	0
9	W	204/204 (100%)	-0.35	3 (1%)	73	70	36, 46, 64, 80	0
10	J	198/198 (100%)	-0.09	8 (4%)	38	31	38, 49, 69, 122	0
10	X	198/198 (100%)	-0.10	6 (3%)	50	43	38, 49, 69, 122	0
11	K	212/212 (100%)	-0.12	10 (4%)	31	25	34, 47, 72, 86	0
11	Y	212/212 (100%)	-0.15	11 (5%)	27	21	35, 47, 74, 86	0
12	L	222/222 (100%)	-0.18	6 (2%)	54	48	33, 48, 74, 89	0
12	Z	222/222 (100%)	-0.23	10 (4%)	33	26	34, 47, 74, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.47	1 (0%) 92 91	31, 43, 57, 61	0
13	M	233/233 (100%)	-0.40	2 (0%) 84 82	32, 43, 57, 63	0
14	2	196/196 (100%)	-0.40	2 (1%) 82 80	31, 41, 61, 81	0
14	N	196/196 (100%)	-0.40	1 (0%) 91 89	31, 40, 60, 81	0
All	All	6368/6368 (100%)	-0.10	269 (4%) 36 29	29, 50, 84, 124	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(C)	GLY	13.2
3	C	55	THR	12.6
4	R	12(E)	SER	11.7
4	D	12(E)	SER	10.0
10	X	192	ALA	9.8
7	U	240	ASP	9.8
4	R	12(C)	GLY	9.6
4	R	12(F)	GLY	9.2
4	D	12(D)	ALA	9.0
10	J	192	ALA	8.9
4	R	12(D)	ALA	8.4
3	Q	55	THR	7.9
2	B	217	ALA	7.7
7	G	240	ASP	7.4
2	B	54	VAL	7.3
2	B	218	ASN	7.3
3	C	56	LEU	7.0
6	F	5	GLY	6.9
4	D	12(F)	GLY	6.7
10	X	193	GLN	6.7
10	J	191	GLN	6.6
7	U	6	ALA	6.5
7	G	6	ALA	6.5
3	Q	240	LYS	6.4
1	A	5	THR	6.3
2	P	218	ASN	6.2
1	O	5	THR	6.2
10	X	191	GLN	6.2
1	O	4	MET	6.1
11	Y	208	ASN	6.0
2	P	21(A)	LYS	6.0
1	A	4	MET	6.0

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Mol	Chain	Res	Type	RSRZ
12	L	145	TYR	5.9
10	J	193	GLN	5.9
2	P	54	VAL	5.8
11	K	208	ASN	5.7
2	P	217	ALA	5.6
12	Z	145	TYR	5.6
4	R	126	ARG	5.5
5	S	203	ASP	5.4
3	C	240	LYS	5.3
3	Q	242	GLU	5.3
2	P	219	GLU	5.2
5	E	203	ASP	5.2
3	Q	203	THR	5.2
3	Q	243	GLN	5.1
5	E	4	PHE	5.0
2	P	21(C)	ASP	4.9
3	Q	56	LEU	4.9
8	H	223	ASP	4.9
4	D	125	GLU	4.8
8	V	223	ASP	4.7
9	W	-8	SER	4.7
2	B	21(A)	LYS	4.7
3	Q	54	SER	4.7
4	R	242	ALA	4.6
12	L	14(P)	PRO	4.6
5	S	5	ARG	4.6
3	C	241	GLN	4.5
5	S	4	PHE	4.5
1	O	53	LYS	4.4
3	Q	241	GLN	4.4
4	R	243	ALA	4.3
1	A	236	LEU	4.3
6	T	240	ILE	4.3
4	R	127	LEU	4.3
1	O	21(P)	LYS	4.2
9	I	-8	SER	4.2
3	Q	64	PRO	4.2
4	R	125	GLU	4.2
4	D	127	LEU	4.1
3	Q	207	ALA	4.1
3	Q	236	ILE	4.0
2	B	21(B)	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
4	D	126	ARG	4.0
5	E	5	ARG	4.0
11	K	207	ASN	3.9
13	1	-8	THR	3.9
8	V	222	CYS	3.9
2	B	219	GLU	3.9
7	G	239	GLN	3.9
11	K	210	ILE	3.9
12	L	14(H)	GLY	3.8
11	Y	104	TYR	3.8
5	S	178	ARG	3.8
3	Q	63	THR	3.7
6	F	204	ASP	3.7
3	C	43	LYS	3.7
6	F	241	ASN	3.7
11	K	104	TYR	3.7
12	L	14(M)	VAL	3.7
11	K	143	LYS	3.6
4	D	244	GLU	3.6
2	P	21(B)	GLY	3.6
11	Y	210	ILE	3.6
1	O	235	ALA	3.6
3	C	243	GLN	3.6
3	Q	18(C)	LYS	3.6
6	F	20(B)	GLU	3.6
11	Y	10(A)	ARG	3.6
10	J	92	ARG	3.5
12	Z	14(W)	LYS	3.5
7	U	8	TYR	3.4
5	S	217	LYS	3.4
8	H	220	ASN	3.4
11	Y	207	ASN	3.4
1	A	203	GLU	3.4
6	T	241	ASN	3.4
5	S	127	TYR	3.4
2	P	239	THR	3.3
2	P	53	LYS	3.3
3	Q	53	ARG	3.3
4	R	12(G)	GLU	3.3
3	Q	7	GLY	3.3
13	M	-8	THR	3.3
3	Q	202	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
8	H	222	CYS	3.3
2	B	21(C)	ASP	3.3
3	C	33	ARG	3.3
11	Y	67	GLU	3.3
14	N	18(I)	GLN	3.3
7	G	8	TYR	3.3
8	V	220	ASN	3.3
1	O	236	LEU	3.3
2	P	185	LYS	3.2
7	U	7	GLY	3.2
6	F	240	ILE	3.2
11	Y	181	ASP	3.2
14	2	18(I)	GLN	3.2
2	B	20(B)	ALA	3.2
7	G	7	GLY	3.2
10	J	-1	MET	3.2
2	B	239	THR	3.2
3	Q	178	LYS	3.2
4	D	243	ALA	3.2
3	Q	208	LYS	3.2
4	D	12(G)	GLU	3.2
11	K	40	PHE	3.1
12	L	14(W)	LYS	3.1
3	Q	239	GLU	3.1
3	Q	223	ALA	3.1
3	Q	222	VAL	3.1
6	T	6	THR	3.0
5	E	127	TYR	3.0
12	Z	-9	GLN	3.0
2	P	220	TYR	3.0
10	X	92	ARG	3.0
9	W	182	ASP	3.0
3	C	203	THR	3.0
11	K	10(A)	ARG	3.0
6	F	6	THR	3.0
3	Q	206	GLY	3.0
3	C	52	ARG	2.9
5	E	233	ILE	2.9
7	G	218	ASP	2.9
12	Z	14(P)	PRO	2.9
7	G	18(A)	ILE	2.9
11	K	73	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	21(F)	LEU	2.9
2	P	183	ASP	2.9
9	I	181	LYS	2.8
6	T	18(E)	GLU	2.8
3	Q	62	ARG	2.8
1	O	43	THR	2.8
3	Q	62(A)	ILE	2.8
4	R	9	ASP	2.8
6	F	18(E)	GLU	2.8
3	Q	238	GLN	2.8
5	S	204	GLU	2.8
12	Z	14(H)	GLY	2.8
3	C	238	GLN	2.7
11	Y	180	GLU	2.7
7	G	18(H)	GLU	2.7
3	C	194	VAL	2.7
7	U	218	ASP	2.7
11	K	181	ASP	2.7
4	D	218	GLN	2.7
3	C	237	GLU	2.7
3	Q	14(B)	ASP	2.7
3	Q	18(D)	GLU	2.7
2	P	21(D)	GLY	2.7
6	F	206	LYS	2.7
12	L	70(A)	ASN	2.7
3	Q	187	GLU	2.7
4	R	244	GLU	2.7
2	B	237	GLY	2.6
2	P	20(A)	SER	2.6
3	C	53	ARG	2.6
12	Z	14(M)	VAL	2.6
2	P	181	LYS	2.6
4	D	9	ASP	2.6
3	Q	234	THR	2.6
11	Y	73	ARG	2.6
3	C	233	VAL	2.5
7	U	239	GLN	2.5
5	E	217	LYS	2.5
5	S	233	ILE	2.5
3	Q	33	ARG	2.5
5	E	204	GLU	2.5
1	O	143	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	20(A)	SER	2.5
4	D	10	ARG	2.5
3	C	227	GLU	2.4
4	R	241	GLU	2.4
11	K	180	GLU	2.4
10	X	188	ASP	2.4
1	A	21(P)	LYS	2.4
3	C	208	LYS	2.4
6	T	20(C)	LYS	2.4
4	R	12(B)	GLU	2.4
2	B	183	ASP	2.4
1	A	21(N)	THR	2.3
3	C	234	THR	2.3
2	B	21(D)	GLY	2.3
1	O	55	SER	2.3
4	D	18(D)	SER	2.3
10	J	188	ASP	2.3
1	O	178	LYS	2.3
1	A	234	GLU	2.3
1	O	234	GLU	2.3
3	Q	14(A)	ARG	2.3
3	Q	18(B)	ARG	2.3
3	C	54	SER	2.2
3	C	202	GLN	2.2
7	G	238	GLU	2.2
9	I	182	ASP	2.2
4	R	10	ARG	2.2
3	Q	233	VAL	2.2
7	U	17(E)	LYS	2.2
3	Q	58	LEU	2.2
6	T	238	LYS	2.2
9	W	12(A)	LYS	2.2
4	D	205	GLU	2.2
13	M	211	ILE	2.2
1	O	203	GLU	2.2
1	A	204	GLY	2.2
1	O	21(M)	PRO	2.2
4	D	122	ARG	2.2
7	U	72	ARG	2.2
3	Q	227	GLU	2.1
4	D	202	GLU	2.1
12	Z	70(A)	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
12	Z	120	GLU	2.1
3	C	235	GLN	2.1
3	Q	52	ARG	2.1
11	Y	40	PHE	2.1
1	A	21(E)	ASP	2.1
2	B	185	LYS	2.1
5	E	178	ARG	2.1
10	J	144	PRO	2.1
5	E	18(E)	LYS	2.1
3	C	236	ILE	2.1
4	R	231	GLU	2.1
6	F	18(B)	HIS	2.1
6	T	18(D)	PRO	2.1
10	X	168	MET	2.1
12	Z	1(I)	ASN	2.1
3	C	178	LYS	2.1
4	R	240	LYS	2.1
3	C	59	GLN	2.0
3	C	187	GLU	2.0
10	J	145	ASP	2.0
14	2	107	LYS	2.0
3	C	18(C)	LYS	2.0
9	I	107	LYS	2.0
12	Z	180	LYS	2.0
3	C	7	GLY	2.0
3	Q	18	ASP	2.0
11	Y	143	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

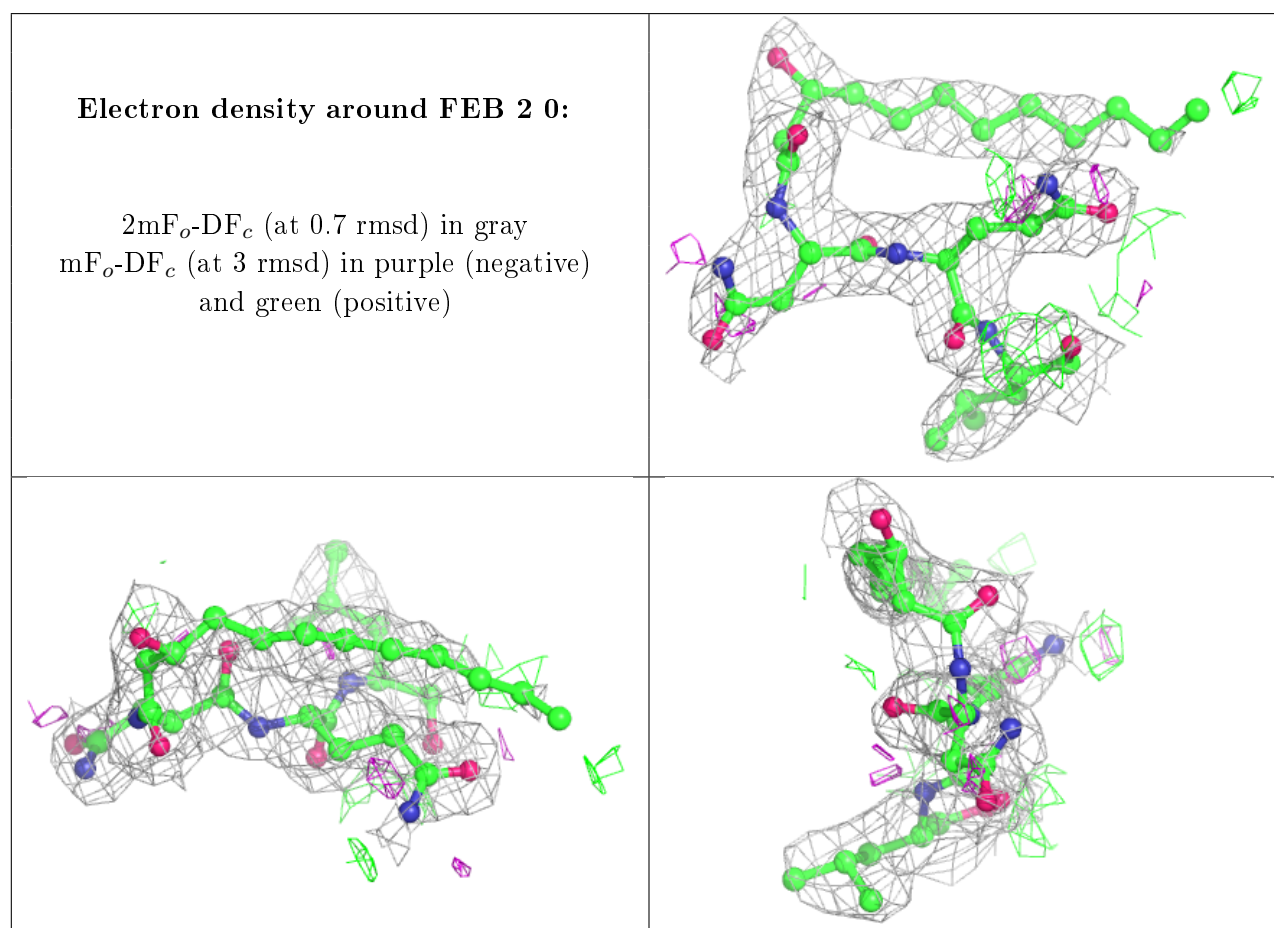
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

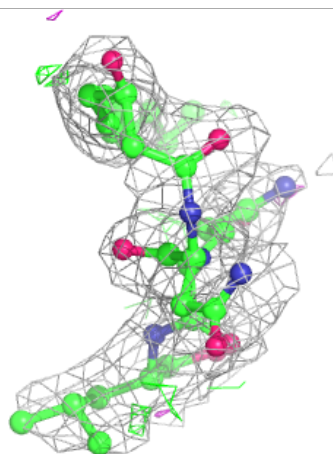
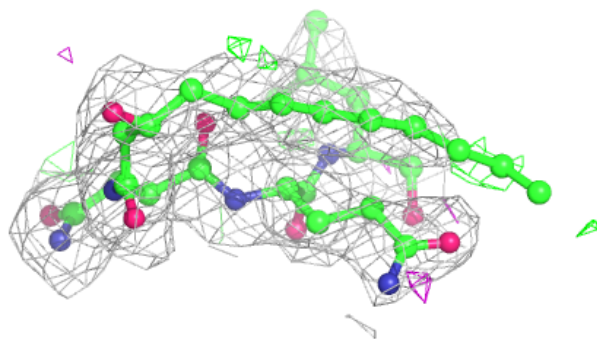
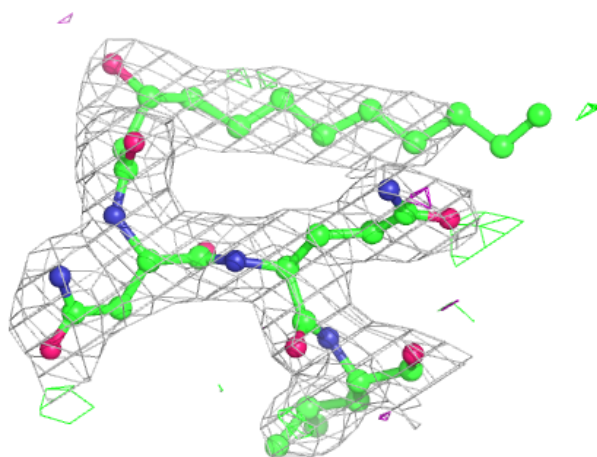
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	FEB	2	0	39/39	0.88	0.27	39,50,60,65	0
15	FEB	N	0	39/39	0.90	0.22	40,49,60,61	0
15	FEB	V	0	39/39	0.91	0.20	39,45,58,63	0
15	FEB	Y	0	39/39	0.91	0.20	34,43,56,58	0
15	FEB	K	0	39/39	0.92	0.18	32,40,55,56	0
15	FEB	H	0	39/39	0.93	0.17	38,45,58,63	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



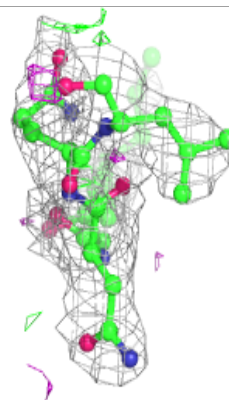
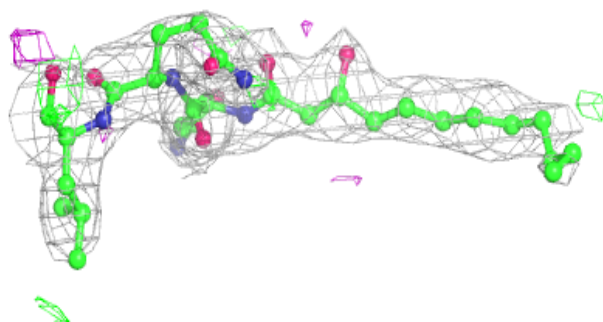
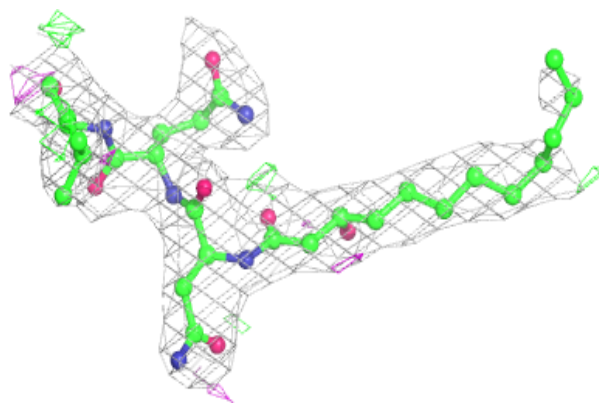
Electron density around FEB N 0:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

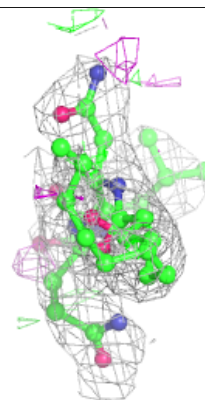
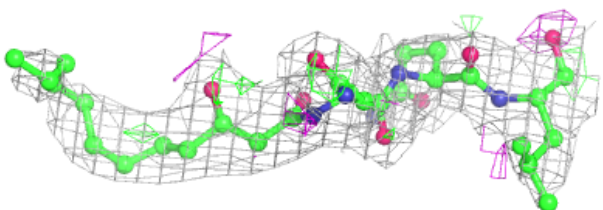
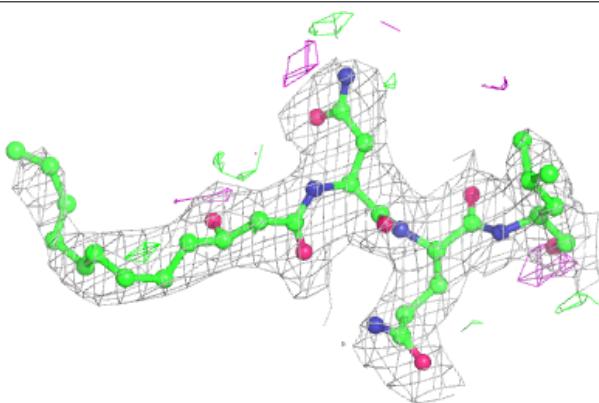


Electron density around FEB V 0:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

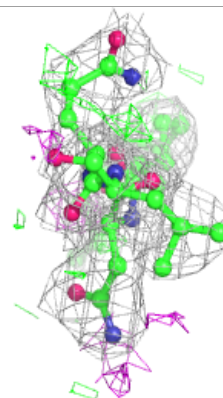
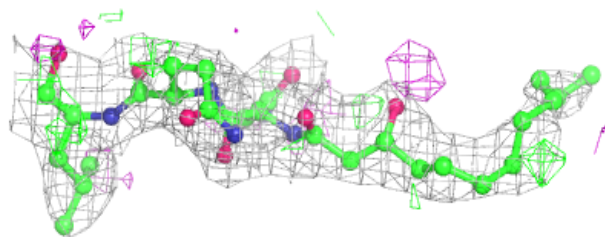
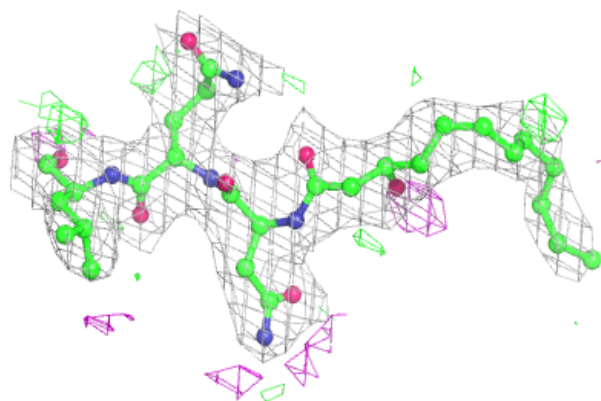
**Electron density around FEB Y 0:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

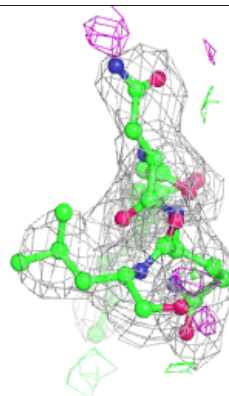
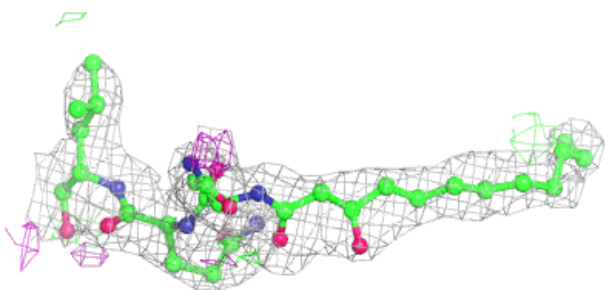
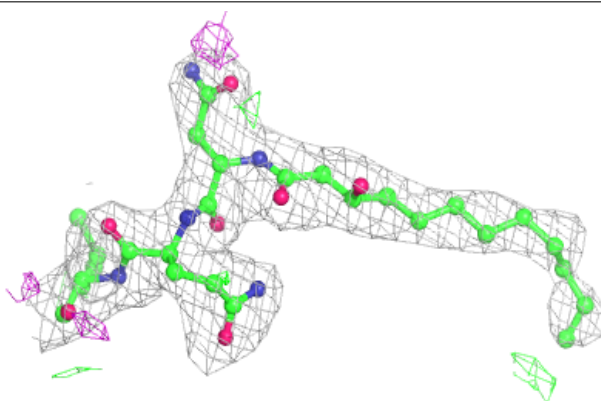


Electron density around FEB K 0:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FEB H 0:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.