



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:56 am BST

PDB ID : 3F5P
Title : Complex Structure of Insulin-like Growth Factor Receptor and 3-Cyanoquinoline Inhibitor
Authors : Xu, W.; Miller, L.M.; Mayer, S.C.; Berger, D.M.; Boschelli, D.H.; Boschelli, F.
Deposited on : 2008-11-04
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<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:

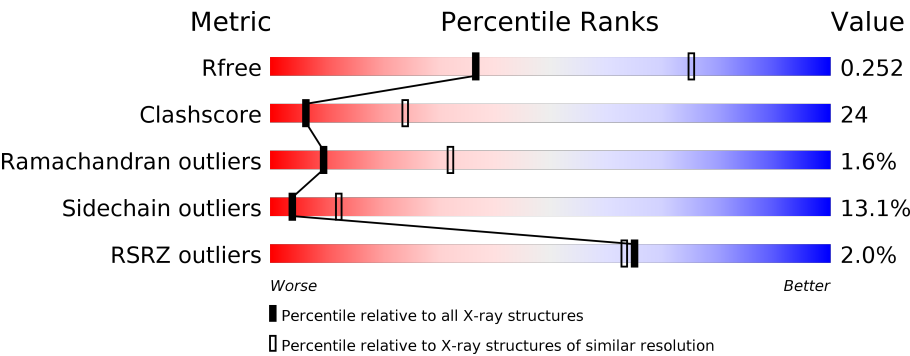
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	308	<div><div>2%</div><div><div></div><div>56%</div><div>35%</div><div>7%</div><div></div></div><div></div></div>
1	B	308	<div><div>%</div><div><div></div><div>53%</div><div>39%</div><div>6%</div><div></div></div><div></div></div>
1	C	308	<div><div>3%</div><div><div></div><div>50%</div><div>40%</div><div>8%</div><div></div></div><div></div></div>
1	D	308	<div><div>2%</div><div><div></div><div>58%</div><div>33%</div><div>6%</div><div></div></div><div></div></div>
1	E	308	<div><div>4%</div><div><div></div><div>55%</div><div>36%</div><div>8%</div><div></div></div><div></div></div>
1	F	308	<div><div>4%</div><div><div></div><div>59%</div><div>32%</div><div>6%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	308	
1	H	308	
1	I	308	
1	J	308	
1	K	308	
1	L	308	
1	M	308	
1	R	308	
1	S	308	
1	T	308	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PTR	M	1166	-	-	X	-
1	PTR	S	1161	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39086 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.

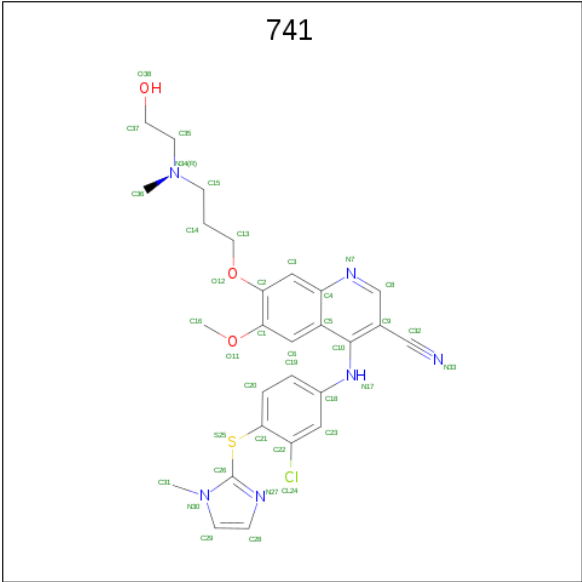
- Molecule 1 is a protein called Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	P	S	0	0	0
			2420	1530	400	464	3	23			
1	B	301	Total	C	N	O	P	S	0	0	0
			2408	1525	399	460	2	22			
1	C	304	Total	C	N	O	P	S	0	0	0
			2420	1531	402	463	2	22			
1	D	300	Total	C	N	O	P	S	0	0	0
			2399	1520	398	457	2	22			
1	E	302	Total	C	N	O	P	S	0	0	0
			2405	1522	399	460	2	22			
1	F	302	Total	C	N	O	P	S	0	0	0
			2412	1529	399	460	2	22			
1	G	302	Total	C	N	O	P	S	0	0	0
			2416	1532	400	460	2	22			
1	H	302	Total	C	N	O	P	S	0	0	0
			2416	1530	400	461	2	23			
1	I	297	Total	C	N	O	P	S	0	0	0
			2380	1508	395	453	2	22			
1	J	296	Total	C	N	O	P	S	0	0	0
			2369	1500	393	452	2	22			
1	K	296	Total	C	N	O	P	S	0	0	0
			2369	1500	393	452	2	22			
1	M	298	Total	C	N	O	P	S	0	0	0
			2381	1508	395	454	2	22			
1	L	296	Total	C	N	O	P	S	0	0	0
			2369	1500	393	452	2	22			
1	R	297	Total	C	N	O	P	S	0	0	0
			2376	1505	394	453	2	22			
1	S	298	Total	C	N	O	P	S	0	0	0
			2386	1511	396	455	2	22			
1	T	298	Total	C	N	O	P	S	0	0	0
			2386	1511	396	455	2	22			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	979	GLY	-	EXPRESSION TAG	UNP P08069
A	980	SER	-	EXPRESSION TAG	UNP P08069
B	979	GLY	-	EXPRESSION TAG	UNP P08069
B	980	SER	-	EXPRESSION TAG	UNP P08069
C	979	GLY	-	EXPRESSION TAG	UNP P08069
C	980	SER	-	EXPRESSION TAG	UNP P08069
D	979	GLY	-	EXPRESSION TAG	UNP P08069
D	980	SER	-	EXPRESSION TAG	UNP P08069
E	979	GLY	-	EXPRESSION TAG	UNP P08069
E	980	SER	-	EXPRESSION TAG	UNP P08069
F	979	GLY	-	EXPRESSION TAG	UNP P08069
F	980	SER	-	EXPRESSION TAG	UNP P08069
G	979	GLY	-	EXPRESSION TAG	UNP P08069
G	980	SER	-	EXPRESSION TAG	UNP P08069
H	979	GLY	-	EXPRESSION TAG	UNP P08069
H	980	SER	-	EXPRESSION TAG	UNP P08069
I	979	GLY	-	EXPRESSION TAG	UNP P08069
I	980	SER	-	EXPRESSION TAG	UNP P08069
J	979	GLY	-	EXPRESSION TAG	UNP P08069
J	980	SER	-	EXPRESSION TAG	UNP P08069
K	979	GLY	-	EXPRESSION TAG	UNP P08069
K	980	SER	-	EXPRESSION TAG	UNP P08069
M	979	GLY	-	EXPRESSION TAG	UNP P08069
M	980	SER	-	EXPRESSION TAG	UNP P08069
L	979	GLY	-	EXPRESSION TAG	UNP P08069
L	980	SER	-	EXPRESSION TAG	UNP P08069
R	979	GLY	-	EXPRESSION TAG	UNP P08069
R	980	SER	-	EXPRESSION TAG	UNP P08069
S	979	GLY	-	EXPRESSION TAG	UNP P08069
S	980	SER	-	EXPRESSION TAG	UNP P08069
T	979	GLY	-	EXPRESSION TAG	UNP P08069
T	980	SER	-	EXPRESSION TAG	UNP P08069

- Molecule 2 is 4-[[3-chloro-4-(1-methylimidazol-2-yl)sulfanyl-phenyl]amino]-7-[3-(2-hydroxy ethyl-methyl-amino)propoxy]-6-methoxy-quinoline-3-carbonitrile (three-letter code: 741) (formula: C₂₇H₂₉ClN₆O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	B	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	C	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	D	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	E	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	F	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	G	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	H	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	I	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	J	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	K	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	M	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	L	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	R	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	S	1	Total	C	Cl	N	O	S	
			38	27	1	6	3	1	0
2	T	1	Total	C	Cl	N	O	S	
			38	27	1	6	3	1	0

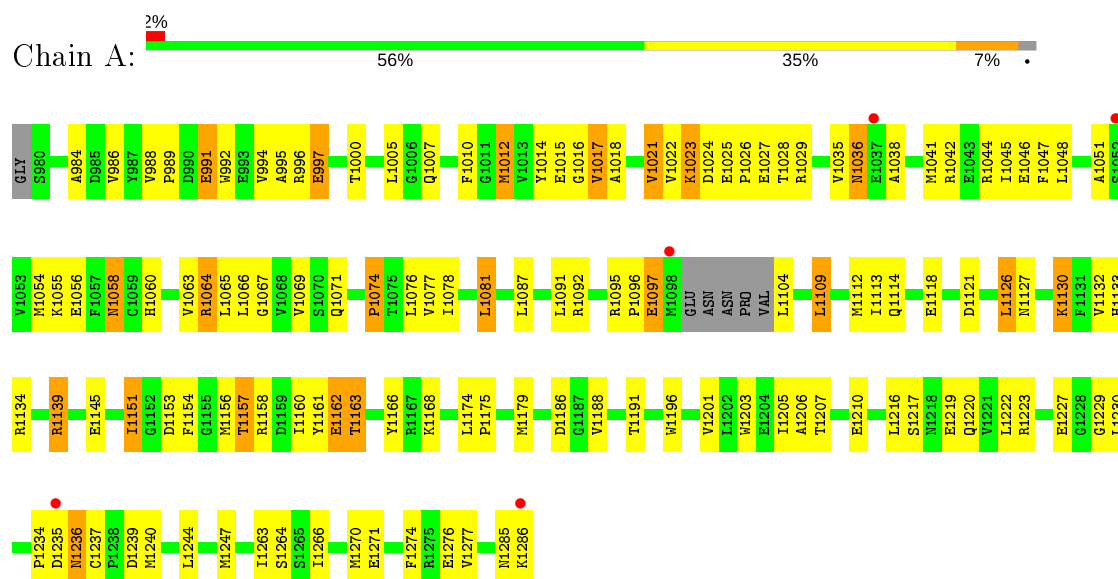
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O		
			5	5	0	0
3	B	19	Total	O		
			19	19	0	0
3	C	18	Total	O		
			18	18	0	0
3	D	7	Total	O		
			7	7	0	0
3	E	1	Total	O		
			1	1	0	0
3	F	4	Total	O		
			4	4	0	0
3	G	14	Total	O		
			14	14	0	0
3	H	19	Total	O		
			19	19	0	0
3	I	19	Total	O		
			19	19	0	0
3	J	29	Total	O		
			29	29	0	0
3	K	1	Total	O		
			1	1	0	0
3	M	1	Total	O		
			1	1	0	0
3	L	6	Total	O		
			6	6	0	0
3	R	16	Total	O		
			16	16	0	0
3	S	6	Total	O		
			6	6	0	0
3	T	1	Total	O		
			1	1	0	0

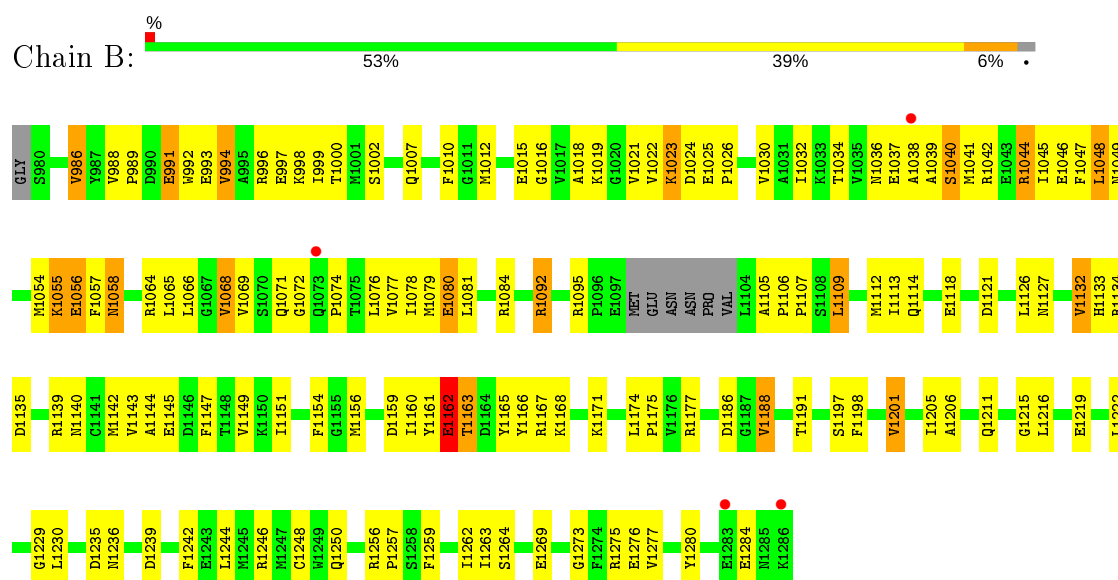
3 Residue-property plots

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

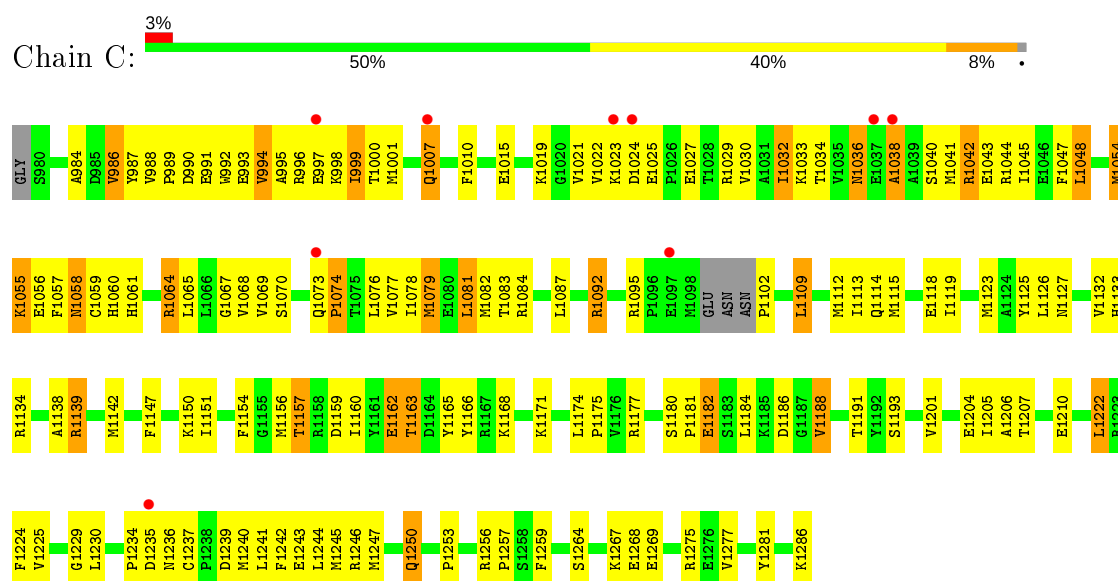
- Molecule 1: Insulin-like growth factor 1 receptor



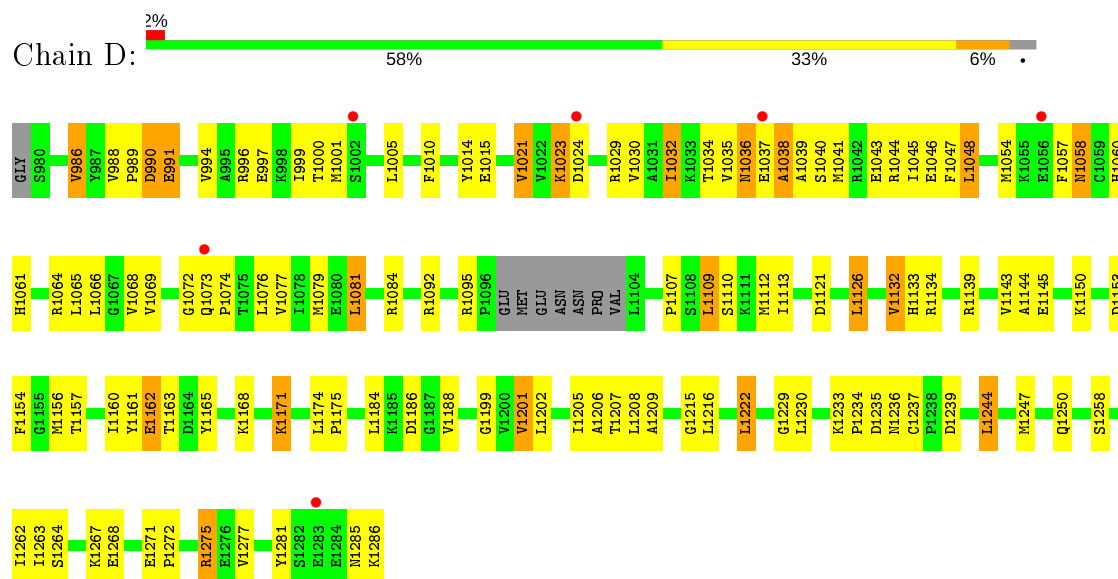
- Molecule 1: Insulin-like growth factor 1 receptor



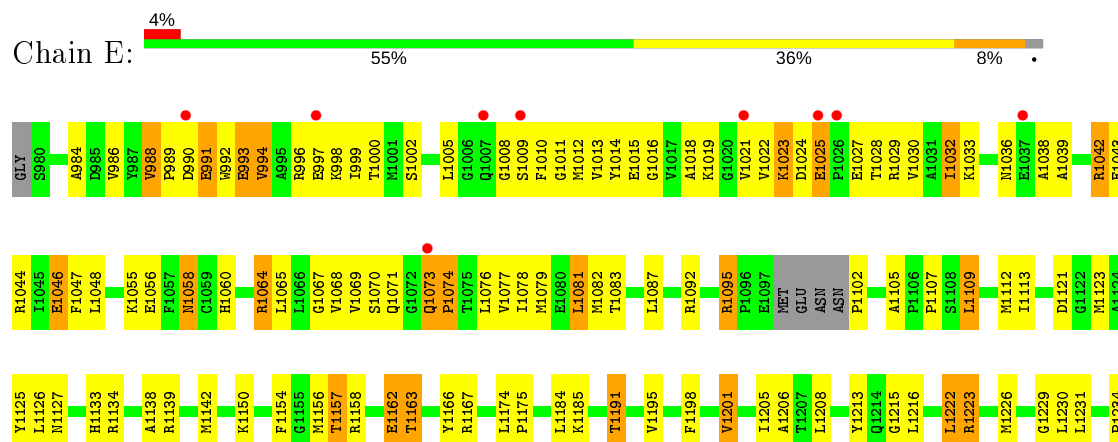
- Molecule 1: Insulin-like growth factor 1 receptor



• Molecule 1: Insulin-like growth factor 1 receptor

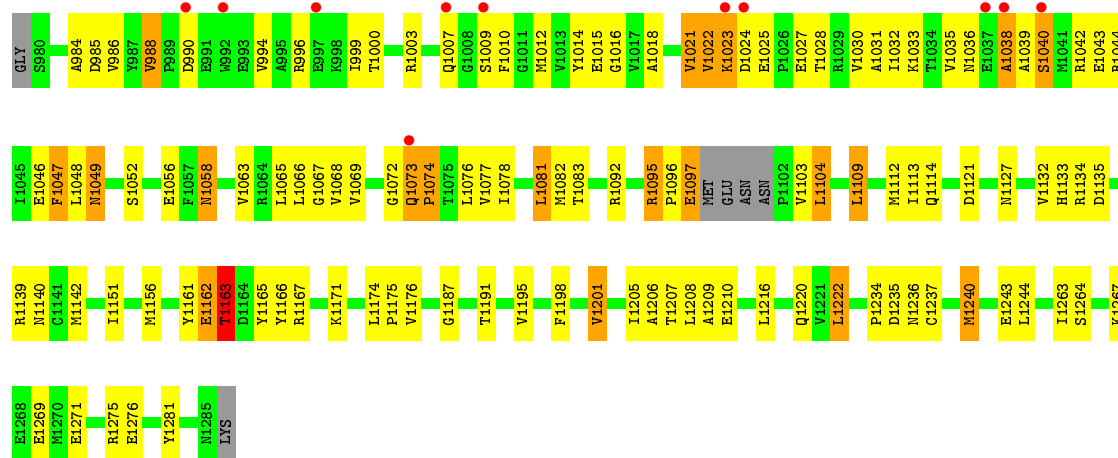


• Molecule 1: Insulin-like growth factor 1 receptor

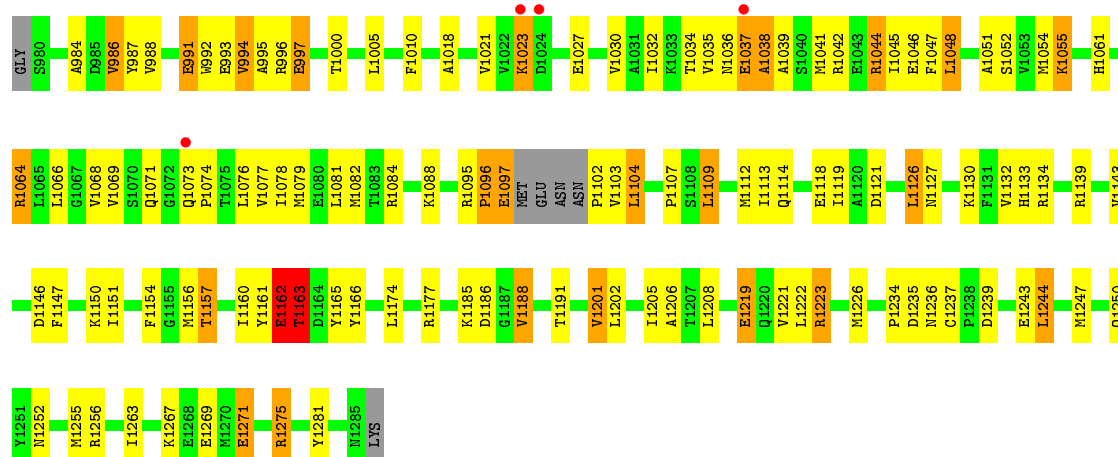




• Molecule 1: Insulin-like growth factor 1 receptor

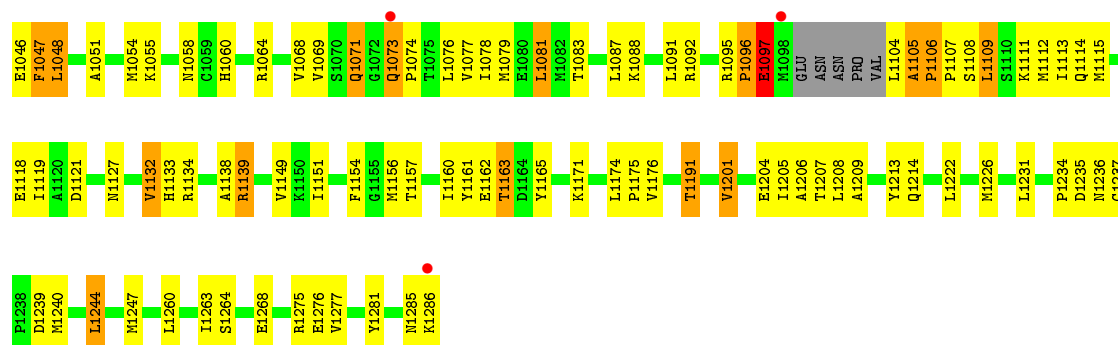


• Molecule 1: Insulin-like growth factor 1 receptor

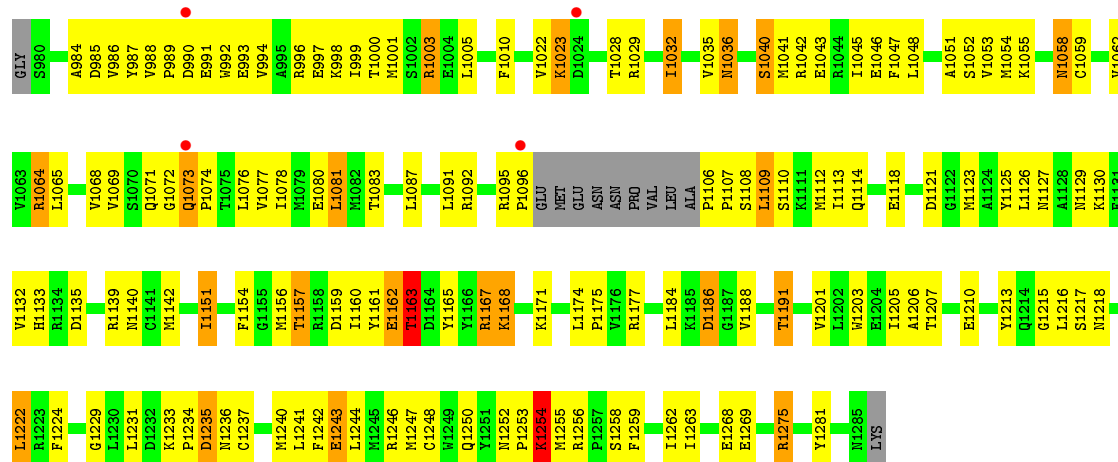


• Molecule 1: Insulin-like growth factor 1 receptor

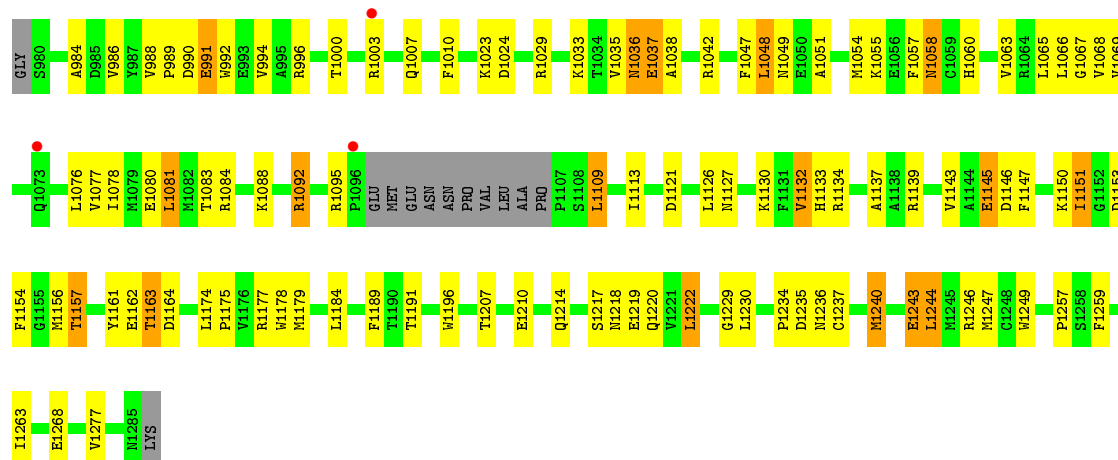




• Molecule 1: Insulin-like growth factor 1 receptor

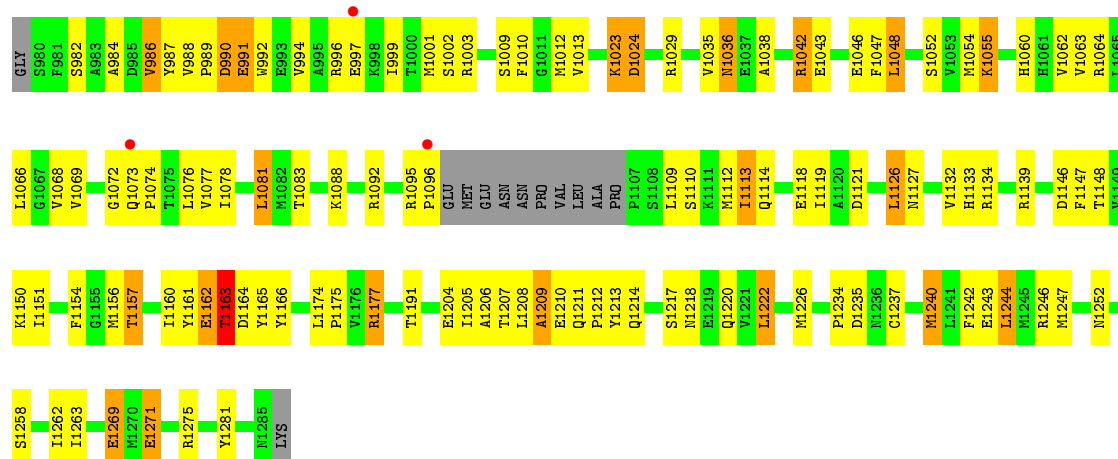


• Molecule 1: Insulin-like growth factor 1 receptor

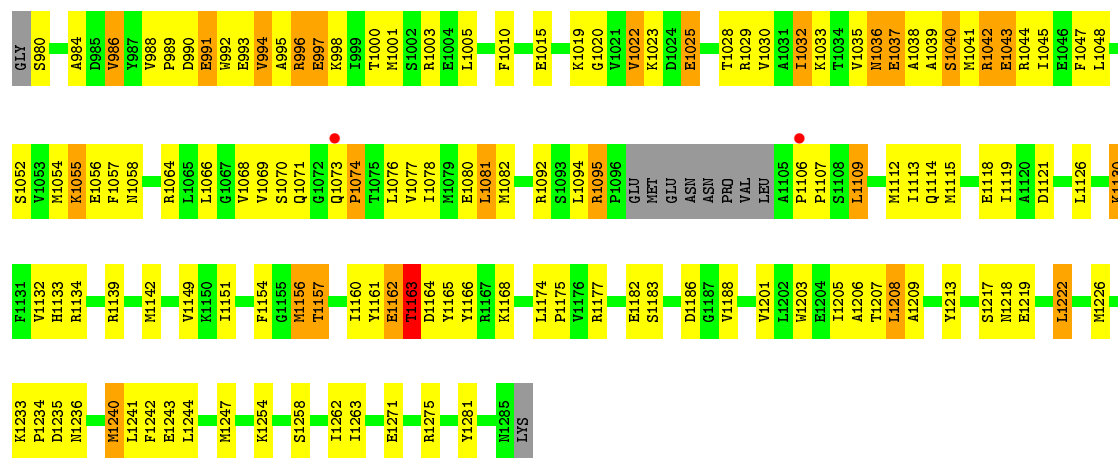


• Molecule 1: Insulin-like growth factor 1 receptor

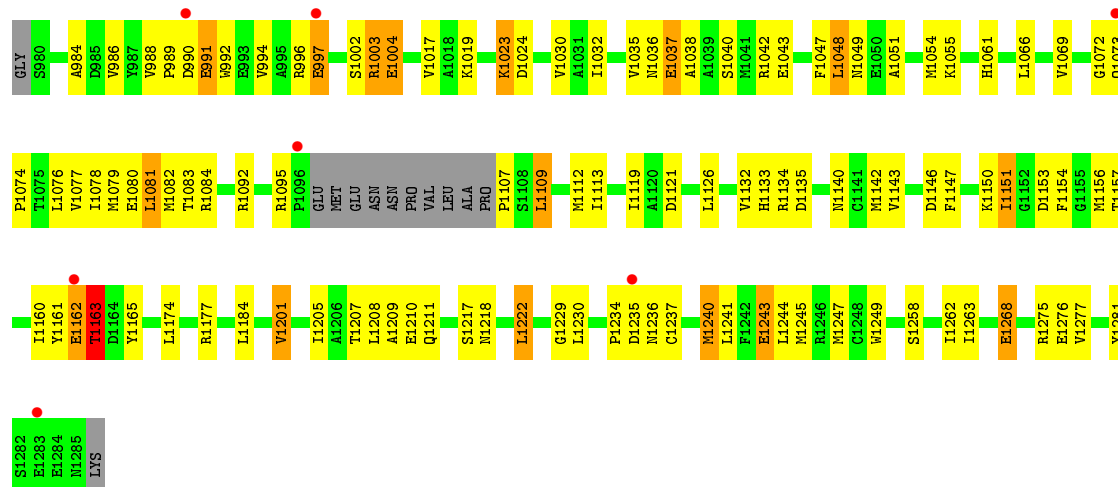




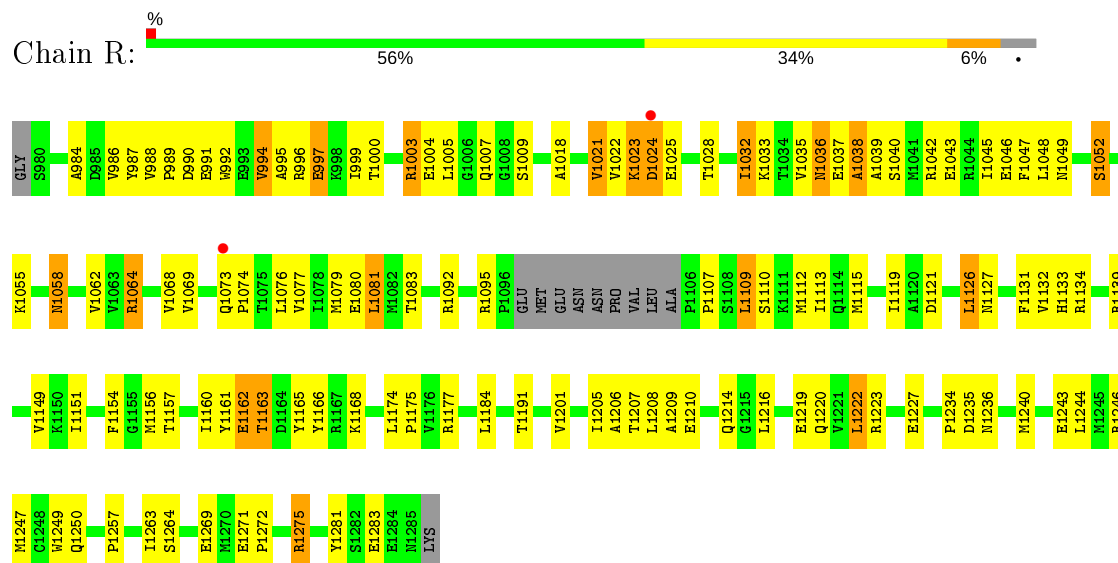
• Molecule 1: Insulin-like growth factor 1 receptor



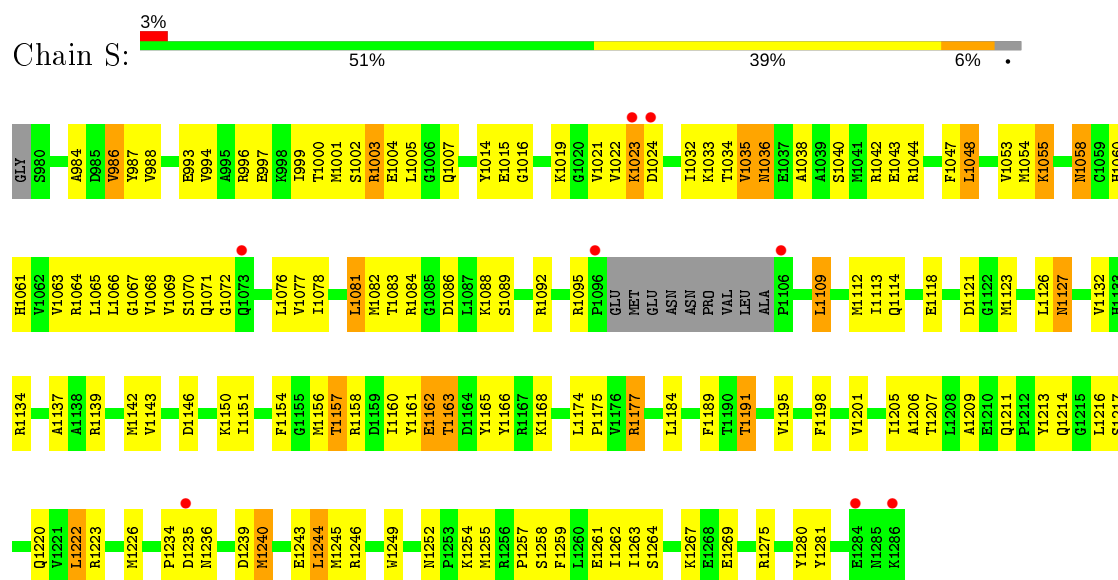
• Molecule 1: Insulin-like growth factor 1 receptor



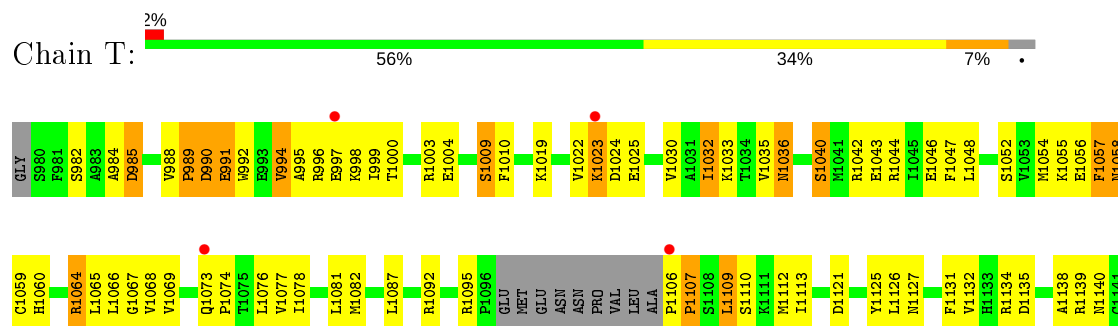
- Molecule 1: Insulin-like growth factor 1 receptor

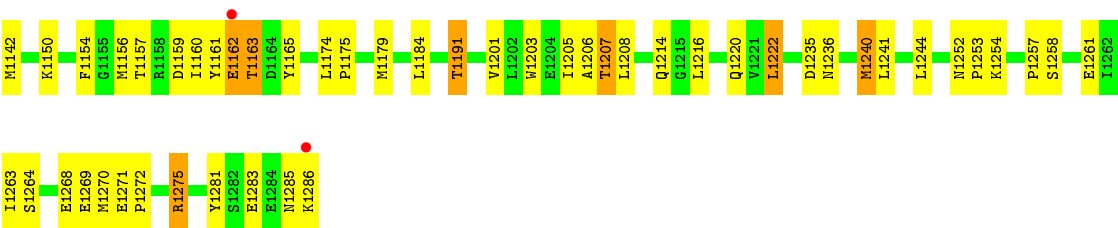


- Molecule 1: Insulin-like growth factor 1 receptor



- Molecule 1: Insulin-like growth factor 1 receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.34Å 137.02Å 178.99Å 90.00° 110.36° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.99-2.90) 97.1 (19.99-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.258 0.206 , 0.252	Depositor DCC
R_{free} test set	6715 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	39086	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1640e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 741, PTR

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	0.40	0/2418	0.57	0/3255
1	B	0.39	0/2410	0.55	0/3245
1	C	0.39	0/2422	0.56	1/3262 (0.0%)
1	D	0.39	0/2401	0.55	1/3233 (0.0%)
1	E	0.39	0/2407	0.58	1/3244 (0.0%)
1	F	0.39	0/2415	0.57	0/3255
1	G	0.37	0/2419	0.53	0/3259
1	H	0.37	0/2418	0.55	0/3255
1	I	0.46	1/2382 (0.0%)	0.59	0/3207
1	J	0.39	0/2370	0.55	0/3191
1	K	0.41	0/2370	0.56	0/3191
1	L	0.38	0/2370	0.54	0/3191
1	M	0.40	0/2383	0.56	0/3211
1	R	0.39	0/2378	0.55	0/3203
1	S	0.39	0/2388	0.56	0/3214
1	T	0.42	0/2388	0.58	0/3214
All	All	0.40	1/38339 (0.0%)	0.56	3/51630 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1254	LYS	CE-NZ	-5.91	1.34	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1102	PRO	N-CA-CB	6.57	111.19	103.30
1	C	1102	PRO	N-CA-CB	6.10	110.62	103.30
1	D	1048	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2420	0	2358	111	0
1	B	2408	0	2349	110	0
1	C	2420	0	2346	145	0
1	D	2399	0	2343	112	0
1	E	2405	0	2331	125	0
1	F	2412	0	2353	112	0
1	G	2416	0	2364	118	0
1	H	2416	0	2358	112	0
1	I	2380	0	2326	139	0
1	J	2369	0	2308	104	0
1	K	2369	0	2308	102	0
1	L	2369	0	2308	87	0
1	M	2381	0	2319	126	0
1	R	2376	0	2315	114	0
1	S	2386	0	2328	118	0
1	T	2386	0	2328	114	0
2	A	38	0	29	5	0
2	B	38	0	29	3	0
2	C	38	0	29	2	0
2	D	38	0	29	1	0
2	E	38	0	29	5	0
2	F	38	0	29	5	0
2	G	38	0	29	2	0
2	H	38	0	29	4	0
2	I	38	0	29	9	0
2	J	38	0	29	2	0
2	K	38	0	29	2	0
2	L	38	0	29	3	0
2	M	38	0	29	1	0
2	R	38	0	29	6	0
2	S	38	0	29	4	0
2	T	38	0	29	3	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	0	0	1	0
3	C	18	0	0	2	0
3	D	7	0	0	3	0
3	E	1	0	0	1	0
3	F	4	0	0	1	0
3	G	14	0	0	0	0
3	H	19	0	0	1	0
3	I	19	0	0	0	0
3	J	29	0	0	7	0
3	K	1	0	0	0	0
3	L	6	0	0	0	0
3	M	1	0	0	0	0
3	R	16	0	0	3	0
3	S	6	0	0	0	0
3	T	1	0	0	0	0
All	All	39086	0	37806	1849	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 24.

All (1849) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1254:LYS:HE3	1:I:1254:LYS:N	1.61	1.13
1:C:1092:ARG:HG3	1:C:1092:ARG:HH11	0.99	1.13
1:K:989:PRO:HG2	1:K:992:TRP:HD1	1.09	1.11
1:H:1023:LYS:H	1:H:1023:LYS:HD2	1.17	1.09
1:M:996:ARG:HH12	1:M:1074:PRO:HD2	0.93	1.09
1:L:1023:LYS:H	1:L:1023:LYS:HD2	1.11	1.08
1:M:996:ARG:NH1	1:M:1074:PRO:HD2	1.72	1.05
1:J:1036:ASN:ND2	1:J:1038:ALA:H	1.54	1.04
1:T:996:ARG:HH12	1:T:1074:PRO:HD2	1.18	1.01
1:M:1058:ASN:HD21	1:M:1064:ARG:NH2	1.58	1.01
1:I:1023:LYS:HD3	1:I:1023:LYS:N	1.74	1.01
1:A:1023:LYS:HD3	1:A:1023:LYS:H	1.25	1.00
1:E:1105:ALA:H	1:S:1007:GLN:NE2	1.58	1.00
1:E:1042:ARG:HG2	1:E:1042:ARG:HH11	1.19	1.00
1:T:1058:ASN:ND2	1:T:1064:ARG:HH12	1.60	1.00
1:H:1112:MET:CE	1:H:1206:ALA:HA	1.93	0.99
1:K:989:PRO:HG2	1:K:992:TRP:CD1	1.99	0.98
1:B:1114:GLN:O	1:B:1118:GLU:HG3	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1023:LYS:HD2	1:S:1023:LYS:H	1.29	0.98
1:F:1069:VAL:HB	1:F:1076:LEU:HB2	1.46	0.96
1:M:1161:PTR:HD1	1:M:1162:GLU:N	1.80	0.95
1:M:996:ARG:HH12	1:M:1074:PRO:CD	1.79	0.95
1:G:996:ARG:HB3	1:G:1069:VAL:HG11	1.44	0.95
1:S:1023:LYS:CD	1:S:1023:LYS:H	1.78	0.94
1:C:1092:ARG:CG	1:C:1092:ARG:HH11	1.80	0.94
1:D:1084:ARG:HH11	1:D:1084:ARG:HG2	1.32	0.94
1:I:1023:LYS:H	1:I:1023:LYS:HD3	1.27	0.94
1:C:1092:ARG:HG3	1:C:1092:ARG:NH1	1.77	0.94
1:R:1042:ARG:HH11	1:R:1042:ARG:HG2	1.31	0.94
1:J:1036:ASN:HD21	1:J:1038:ALA:H	1.08	0.93
1:C:1133:HIS:HA	1:C:1157:THR:HG22	1.51	0.93
1:D:1044:ARG:O	1:D:1048:LEU:HD22	1.67	0.93
1:A:1036:ASN:HD22	1:A:1036:ASN:H	0.94	0.92
1:F:1092:ARG:HD3	1:F:1209:ALA:HB3	1.50	0.92
1:I:1161:PTR:HD1	1:I:1162:GLU:N	1.84	0.92
1:M:1163:THR:HG22	1:M:1165:PTR:CE1	2.00	0.92
1:M:1162:GLU:O	1:M:1163:THR:OG1	1.85	0.92
1:C:1044:ARG:HB2	1:C:1044:ARG:NH1	1.84	0.91
1:C:1044:ARG:HB2	1:C:1044:ARG:HH11	1.32	0.91
1:M:1058:ASN:HD21	1:M:1064:ARG:CZ	1.82	0.91
1:D:996:ARG:NH1	1:D:1074:PRO:HD2	1.85	0.91
1:B:1044:ARG:HH11	1:B:1044:ARG:HG3	1.36	0.91
1:G:992:TRP:CZ2	1:G:1055:LYS:HB2	2.06	0.90
1:F:1023:LYS:HD3	1:F:1023:LYS:H	1.37	0.90
1:G:1112:MET:CE	1:G:1206:ALA:HA	2.01	0.90
1:A:1156:MET:HG2	1:A:1174:LEU:HD21	1.52	0.90
1:K:1042:ARG:HH11	1:K:1042:ARG:CG	1.85	0.90
1:R:1156:MET:HG2	1:R:1174:LEU:HD21	1.53	0.89
1:A:1036:ASN:H	1:A:1036:ASN:ND2	1.70	0.89
1:H:996:ARG:NH1	1:H:1074:PRO:HD2	1.88	0.89
1:L:996:ARG:HB3	1:L:1069:VAL:HG11	1.52	0.89
1:M:994:VAL:HG22	1:M:1069:VAL:HG22	1.53	0.89
1:R:989:PRO:HG2	1:R:992:TRP:HD1	1.34	0.89
1:C:1182:GLU:OE1	1:C:1253:PRO:HG3	1.73	0.89
1:G:1163:THR:HG22	1:G:1165:PTR:CE1	2.02	0.88
1:I:996:ARG:HB3	1:I:1069:VAL:HG11	1.53	0.88
1:L:1132:VAL:HG23	1:L:1160:ILE:HD13	1.54	0.88
1:B:1112:MET:CE	1:B:1206:ALA:HA	2.03	0.88
1:G:1163:THR:HG22	1:G:1165:PTR:CD1	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1163:THR:HG22	1:L:1165:PTR:CE1	2.02	0.87
1:A:1112:MET:CE	1:A:1206:ALA:HA	2.03	0.87
1:M:1022:VAL:HG13	1:M:1025:GLU:HB3	1.57	0.86
1:J:1036:ASN:O	1:J:1037:GLU:HB2	1.75	0.86
1:E:1010:PHE:CD1	1:E:1047:PHE:HD1	1.92	0.86
1:M:998:LYS:HA	1:M:1019:LYS:HD3	1.56	0.86
1:B:1010:PHE:CD1	1:B:1047:PHE:HD1	1.93	0.86
1:G:1223:ARG:HG3	1:G:1223:ARG:HH11	1.41	0.86
1:D:1112:MET:CE	1:D:1206:ALA:HA	2.06	0.86
1:M:996:ARG:NH2	1:M:1074:PRO:O	2.09	0.85
1:M:1092:ARG:O	1:M:1095:ARG:HG3	1.76	0.85
1:F:1112:MET:CE	1:F:1206:ALA:HA	2.06	0.85
1:E:1023:LYS:O	1:E:1024:ASP:HB2	1.75	0.85
1:D:1060:HIS:CD2	1:D:1277:VAL:HB	2.12	0.85
1:R:1047:PHE:CZ	1:R:1077:VAL:HG21	2.11	0.85
1:A:1036:ASN:HD22	1:A:1036:ASN:N	1.75	0.85
1:C:1010:PHE:CD1	1:C:1047:PHE:HD1	1.94	0.85
1:K:1036:ASN:C	1:K:1036:ASN:HD22	1.79	0.85
1:B:1066:LEU:HB2	1:B:1078:ILE:HG22	1.58	0.84
1:M:1042:ARG:HH11	1:M:1042:ARG:HG2	1.41	0.84
1:D:1010:PHE:CD1	1:D:1047:PHE:HD1	1.95	0.84
1:B:1163:THR:HG22	1:B:1165:PTR:CE1	2.07	0.84
1:I:1254:LYS:HZ2	1:I:1255:MET:HG2	1.38	0.84
1:C:996:ARG:NH1	1:C:1074:PRO:HD2	1.93	0.84
1:J:1092:ARG:O	1:J:1095:ARG:HG3	1.78	0.83
1:L:1040:SER:OG	1:L:1043:GLU:HG3	1.77	0.83
1:E:1023:LYS:H	1:E:1023:LYS:HD2	1.41	0.83
1:I:1252:ASN:CG	1:I:1254:LYS:HE2	1.98	0.83
1:R:1133:HIS:HA	1:R:1157:THR:HG22	1.61	0.83
1:G:1156:MET:HG2	1:G:1174:LEU:HD21	1.58	0.83
1:T:1203:TRP:O	1:T:1207:THR:HG23	1.79	0.83
1:F:1156:MET:HG2	1:F:1174:LEU:HD21	1.60	0.83
1:M:1036:ASN:H	1:M:1036:ASN:HD22	1.25	0.83
1:S:1058:ASN:ND2	1:S:1064:ARG:HH22	1.76	0.82
1:T:989:PRO:HB2	1:T:992:TRP:CD1	2.14	0.82
1:T:1165:PTR:C	1:T:1165:PTR:HD2	2.08	0.82
1:B:1132:VAL:HG22	1:B:1160:ILE:HD13	1.60	0.82
1:M:1042:ARG:CG	1:M:1042:ARG:HH11	1.91	0.82
1:E:1092:ARG:O	1:E:1095:ARG:HG3	1.80	0.81
1:E:1112:MET:CE	1:E:1206:ALA:HA	2.09	0.81
1:F:1073:GLN:HE21	1:F:1073:GLN:HA	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1156:MET:HG2	1:I:1174:LEU:HD21	1.61	0.81
1:F:1092:ARG:O	1:F:1095:ARG:HG3	1.79	0.81
1:A:1235:ASP:O	1:A:1236:ASN:HB2	1.81	0.81
1:S:1156:MET:HG2	1:S:1174:LEU:HD21	1.60	0.81
1:G:1044:ARG:HB2	1:G:1044:ARG:HH11	1.45	0.81
2:I:9:741:H36	2:I:9:741:O38	1.80	0.81
1:L:1073:GLN:HB3	1:L:1074:PRO:HD3	1.62	0.81
1:M:1166:PTR:HE2	1:M:1168:LYS:HD3	1.63	0.81
1:C:1058:ASN:HD22	1:C:1058:ASN:C	1.84	0.81
1:D:1156:MET:HG2	1:D:1174:LEU:HD21	1.63	0.81
1:I:1186:ASP:HB2	1:I:1188:VAL:HG23	1.59	0.81
1:H:1112:MET:HE2	1:H:1206:ALA:HA	1.62	0.80
1:D:1250:GLN:HE21	1:D:1250:GLN:HA	1.44	0.80
1:L:1023:LYS:H	1:L:1023:LYS:CD	1.88	0.80
1:R:1040:SER:OG	1:R:1043:GLU:HG2	1.82	0.80
1:G:1052:SER:O	1:G:1055:LYS:HG3	1.81	0.80
1:B:1018:ALA:HB1	1:B:1021:VAL:HG11	1.64	0.80
1:S:1139:ARG:HH22	1:S:1175:PRO:HG3	1.47	0.80
1:I:1163:THR:HG22	1:I:1165:PTR:CD1	2.11	0.80
1:E:1047:PHE:HZ	1:E:1077:VAL:HG21	1.47	0.79
1:A:1023:LYS:CD	1:A:1023:LYS:H	1.92	0.79
1:T:1127:ASN:CG	1:T:1191:THR:HG22	2.03	0.79
1:E:1042:ARG:NH1	1:E:1042:ARG:HG2	1.90	0.78
1:J:1092:ARG:CG	1:J:1092:ARG:HH11	1.96	0.78
1:T:1044:ARG:O	1:T:1048:LEU:HD23	1.82	0.78
1:L:1023:LYS:N	1:L:1023:LYS:HD2	1.95	0.78
1:T:996:ARG:NH2	1:T:1074:PRO:O	2.16	0.78
1:H:1019:LYS:HG2	1:H:1027:GLU:HG2	1.63	0.78
1:D:1250:GLN:NE2	1:D:1250:GLN:HA	1.98	0.78
1:H:1036:ASN:HD22	1:H:1036:ASN:C	1.86	0.78
1:H:1112:MET:HE1	1:H:1206:ALA:HA	1.63	0.78
1:A:1066:LEU:HB2	1:A:1078:ILE:HG22	1.66	0.78
1:A:1217:SER:OG	1:A:1220:GLN:HG3	1.83	0.78
1:C:1073:GLN:HB2	1:C:1074:PRO:HD3	1.65	0.78
1:E:1112:MET:HE1	1:E:1206:ALA:HA	1.66	0.78
1:E:1025:GLU:HG2	1:E:1027:GLU:O	1.84	0.78
1:M:1114:GLN:OE1	1:M:1271:GLU:HG2	1.84	0.78
1:H:1047:PHE:CZ	1:H:1077:VAL:HG21	2.18	0.77
1:E:1275:ARG:HA	1:E:1281:TYR:HD1	1.49	0.77
1:I:1036:ASN:HD22	1:I:1036:ASN:C	1.86	0.77
1:K:1162:GLU:O	1:K:1163:THR:OG1	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1127:ASN:OD1	1:K:1191:THR:HB	1.83	0.77
1:C:1044:ARG:CB	1:C:1044:ARG:HH11	1.96	0.77
1:F:1267:LYS:HD2	1:F:1281:TYR:OH	1.84	0.77
1:T:996:ARG:NH1	1:T:1074:PRO:HD2	1.96	0.77
1:K:996:ARG:HG2	1:K:1069:VAL:HG11	1.66	0.77
1:R:1023:LYS:HZ3	1:R:1023:LYS:H	1.32	0.77
1:I:1254:LYS:HE3	1:I:1254:LYS:H	1.45	0.77
1:E:1156:MET:HG2	1:E:1174:LEU:HD21	1.67	0.77
1:H:1023:LYS:H	1:H:1023:LYS:CD	1.93	0.77
1:R:996:ARG:HB2	1:R:1069:VAL:HG11	1.65	0.77
1:R:1023:LYS:NZ	1:R:1023:LYS:H	1.82	0.77
1:T:1156:MET:HG2	1:T:1174:LEU:HD21	1.67	0.77
1:K:1042:ARG:HG2	1:K:1042:ARG:HH11	1.48	0.76
1:A:1276:GLU:OE1	1:R:1283:GLU:HG3	1.83	0.76
1:E:1223:ARG:HG3	1:E:1223:ARG:HH11	1.51	0.76
1:J:1127:ASN:OD1	1:J:1191:THR:HB	1.86	0.76
1:L:1234:PRO:HB2	1:L:1237:CYS:HB2	1.67	0.76
1:I:1161:PTR:HD1	1:I:1161:PTR:C	2.15	0.76
1:H:1047:PHE:HZ	1:H:1077:VAL:HG21	1.49	0.76
1:E:1127:ASN:OD1	1:E:1191:THR:HB	1.86	0.76
1:A:1127:ASN:OD1	1:A:1191:THR:HB	1.85	0.76
1:C:984:ALA:O	1:C:988:VAL:HG12	1.86	0.76
1:C:1234:PRO:HB2	1:C:1237:CYS:HB2	1.68	0.76
1:G:1223:ARG:NH1	1:G:1223:ARG:HG3	1.95	0.76
1:I:1163:THR:HG22	1:I:1165:PTR:CE1	2.16	0.76
1:R:1036:ASN:H	1:R:1036:ASN:HD22	1.32	0.76
1:E:1107:PRO:HD3	1:E:1208:LEU:HD21	1.67	0.76
1:H:984:ALA:O	1:H:988:VAL:HG22	1.86	0.75
1:C:1010:PHE:CG	1:C:1047:PHE:HD1	2.03	0.75
1:I:1073:GLN:HB3	1:I:1074:PRO:HD3	1.68	0.75
1:M:1161:PTR:HD1	1:M:1161:PTR:C	2.16	0.75
1:C:1036:ASN:HD21	1:C:1038:ALA:HB3	1.51	0.75
1:S:1127:ASN:N	1:S:1127:ASN:HD22	1.83	0.75
1:D:1161:PTR:O	1:D:1162:GLU:HB3	1.86	0.75
1:G:1166:PTR:O3P	1:G:1166:PTR:HE1	1.85	0.75
1:E:996:ARG:HH12	1:E:1074:PRO:HG2	1.52	0.75
1:E:1107:PRO:HD2	1:E:1112:MET:HE3	1.68	0.75
1:E:1021:VAL:HG23	1:E:1022:VAL:HG23	1.69	0.75
1:S:1092:ARG:O	1:S:1095:ARG:HG3	1.86	0.75
1:A:1023:LYS:N	1:A:1023:LYS:HD3	2.01	0.74
1:C:999:ILE:HG12	1:C:1078:ILE:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:984:ALA:O	1:K:988:VAL:HG22	1.87	0.74
1:K:1073:GLN:HB2	1:K:1074:PRO:HD3	1.67	0.74
1:T:1154:PHE:HD2	1:T:1157:THR:HG21	1.52	0.74
1:E:1047:PHE:CZ	1:E:1077:VAL:HG21	2.21	0.74
1:R:1033:LYS:HB2	2:R:14:741:CL24	2.23	0.74
1:D:1058:ASN:C	1:D:1058:ASN:HD22	1.91	0.74
1:K:1156:MET:HG2	1:K:1174:LEU:HD21	1.69	0.74
1:S:1023:LYS:N	1:S:1023:LYS:HD2	2.03	0.74
1:D:1132:VAL:CG1	1:D:1134:ARG:HG3	2.18	0.74
1:J:1132:VAL:HG13	1:J:1134:ARG:HG3	1.70	0.74
1:C:996:ARG:HH12	1:C:1074:PRO:HD2	1.52	0.73
1:G:1127:ASN:OD1	1:G:1191:THR:HB	1.88	0.73
1:G:1112:MET:HE1	1:G:1206:ALA:HA	1.69	0.73
1:I:1254:LYS:CE	1:I:1254:LYS:N	2.48	0.73
1:I:1092:ARG:HD3	1:I:1095:ARG:NH1	2.02	0.73
1:R:1073:GLN:HB2	1:R:1074:PRO:HD3	1.70	0.73
1:T:1275:ARG:HA	1:T:1281:TYR:CD1	2.22	0.73
1:A:1058:ASN:C	1:A:1058:ASN:HD22	1.92	0.73
1:C:1109:LEU:HD22	1:C:1113:ILE:HG13	1.70	0.73
1:B:1044:ARG:NH1	1:B:1044:ARG:HG3	2.04	0.73
1:I:1254:LYS:NZ	1:I:1255:MET:HG2	2.03	0.73
1:L:1163:THR:HG22	1:L:1165:PTR:CD1	2.18	0.73
1:J:1088:LYS:HE3	1:J:1092:ARG:HH12	1.52	0.73
1:D:1112:MET:HE1	1:D:1206:ALA:HA	1.69	0.73
1:M:1139:ARG:NH2	1:M:1175:PRO:HG2	2.03	0.73
1:H:1092:ARG:HD2	1:H:1209:ALA:HB3	1.71	0.72
1:J:1139:ARG:HH22	1:J:1175:PRO:HG3	1.53	0.72
1:E:1258:SER:OG	1:E:1261:GLU:HG3	1.89	0.72
1:F:1235:ASP:O	1:F:1236:ASN:HB2	1.89	0.72
1:R:989:PRO:HG2	1:R:992:TRP:CD1	2.23	0.72
1:T:1058:ASN:ND2	1:T:1064:ARG:NH1	2.38	0.72
1:C:1127:ASN:OD1	1:C:1191:THR:HB	1.89	0.72
1:G:1047:PHE:CZ	1:G:1077:VAL:HG21	2.24	0.72
1:A:996:ARG:NH1	1:A:1074:PRO:HD2	2.04	0.72
1:D:1041:MET:O	1:D:1045:ILE:HG13	1.90	0.72
1:T:1184:LEU:HD22	1:T:1222:LEU:HD21	1.69	0.72
1:C:1133:HIS:HA	1:C:1157:THR:CG2	2.19	0.72
1:C:1186:ASP:HB2	1:C:1188:VAL:CG2	2.19	0.72
1:L:1003:ARG:HH11	1:L:1003:ARG:CG	2.02	0.72
1:E:1036:ASN:HD22	1:E:1038:ALA:HB3	1.55	0.72
1:M:998:LYS:HD2	1:M:1019:LYS:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1235:ASP:O	1:D:1236:ASN:HB2	1.89	0.71
1:E:1033:LYS:HE2	2:E:5:741:N27	2.05	0.71
1:K:1023:LYS:H	1:K:1023:LYS:HD2	1.56	0.71
1:E:1133:HIS:HA	1:E:1157:THR:HB	1.72	0.71
1:F:1047:PHE:CZ	1:F:1077:VAL:HG21	2.25	0.71
1:G:1186:ASP:HB2	1:G:1188:VAL:CG2	2.21	0.71
1:T:1161:PTR:HD1	1:T:1161:PTR:C	2.21	0.71
1:I:1109:LEU:HD22	1:I:1113:ILE:HG12	1.71	0.71
1:I:989:PRO:C	1:I:991:GLU:H	1.93	0.71
1:S:1267:LYS:HD2	1:S:1281:TYR:OH	1.91	0.71
1:I:1073:GLN:HB3	1:I:1074:PRO:CD	2.21	0.71
1:I:1243:GLU:O	1:I:1247:MET:HG3	1.90	0.71
1:T:1162:GLU:O	1:T:1163:THR:OG1	2.08	0.71
1:S:1058:ASN:CG	1:S:1064:ARG:HH12	1.93	0.71
1:B:1010:PHE:CD1	1:B:1047:PHE:CD1	2.78	0.70
1:D:1132:VAL:HG12	1:D:1134:ARG:HG3	1.73	0.70
1:H:1022:VAL:HG12	1:H:1025:GLU:HG3	1.71	0.70
1:I:1112:MET:CE	1:I:1205:ILE:HG22	2.22	0.70
1:M:1132:VAL:HG22	1:M:1160:ILE:HD13	1.74	0.70
1:B:1034:THR:HG22	1:B:1076:LEU:CD2	2.21	0.70
1:D:1112:MET:HE3	1:D:1206:ALA:HA	1.73	0.70
1:F:1082:MET:HB2	1:F:1142:MET:HE2	1.74	0.70
1:G:1235:ASP:O	1:G:1236:ASN:HB2	1.88	0.70
1:H:1004:GLU:HG2	1:H:1014:TYR:CE1	2.27	0.70
1:J:1161:PTR:O	1:J:1162:GLU:HB2	1.91	0.70
1:S:1258:SER:O	1:S:1262:ILE:HG13	1.90	0.70
1:A:1029:ARG:HB3	1:A:1081:LEU:HD12	1.73	0.70
1:D:1047:PHE:CZ	1:D:1077:VAL:HG21	2.27	0.70
1:E:1023:LYS:H	1:E:1023:LYS:CD	2.03	0.70
1:B:1112:MET:HE2	1:B:1206:ALA:HA	1.71	0.70
1:C:1162:GLU:O	1:C:1163:THR:CB	2.40	0.70
1:E:1223:ARG:HG3	1:E:1223:ARG:NH1	2.06	0.70
1:T:1121:ASP:HA	1:T:1263:ILE:HD11	1.72	0.70
1:A:1069:VAL:HG21	1:A:1076:LEU:HD12	1.72	0.69
1:S:996:ARG:HH21	1:S:1072:GLY:HA3	1.57	0.69
1:B:1186:ASP:HB2	1:B:1188:VAL:HG23	1.72	0.69
1:E:1015:GLU:OE2	1:E:1029:ARG:NH2	2.25	0.69
1:M:1156:MET:HG2	1:M:1174:LEU:HD21	1.73	0.69
1:M:984:ALA:O	1:M:988:VAL:HG22	1.93	0.69
1:R:1112:MET:CE	1:R:1206:ALA:HA	2.21	0.69
1:R:1058:ASN:C	1:R:1058:ASN:HD22	1.95	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1276:GLU:HG3	1:B:1277:VAL:HG13	1.75	0.69
1:E:1235:ASP:O	1:E:1236:ASN:HB2	1.92	0.69
1:F:996:ARG:NH1	1:F:1074:PRO:HD2	2.07	0.69
1:G:1044:ARG:HH11	1:G:1044:ARG:CB	2.06	0.69
1:H:1083:THR:O	2:H:8:741:H15	1.92	0.69
1:C:1186:ASP:HB2	1:C:1188:VAL:HG23	1.74	0.69
1:S:1023:LYS:O	1:S:1024:ASP:HB2	1.91	0.69
1:G:1114:GLN:O	1:G:1118:GLU:HG3	1.93	0.69
1:L:1275:ARG:HA	1:L:1281:TYR:CD1	2.28	0.69
1:F:1058:ASN:C	1:F:1058:ASN:HD22	1.96	0.69
1:R:1003:ARG:HD3	3:R:38:HOH:O	1.93	0.69
1:I:1092:ARG:HD3	1:I:1095:ARG:HH11	1.56	0.68
1:M:1036:ASN:HD22	1:M:1036:ASN:N	1.91	0.68
1:T:1275:ARG:HA	1:T:1281:TYR:HD1	1.57	0.68
1:E:1058:ASN:HD22	1:E:1058:ASN:C	1.96	0.68
1:S:1112:MET:HE1	1:S:1206:ALA:HA	1.75	0.68
1:S:1161:PTR:HD1	1:S:1161:PTR:C	2.23	0.68
1:D:996:ARG:HH12	1:D:1074:PRO:HD2	1.58	0.68
1:J:1036:ASN:HD21	1:J:1038:ALA:N	1.89	0.68
1:C:1036:ASN:O	1:C:1044:ARG:NH2	2.27	0.68
1:G:1247:MET:SD	1:H:986:VAL:HG11	2.34	0.68
1:A:1186:ASP:HB2	1:A:1188:VAL:HG23	1.74	0.68
1:H:1004:GLU:HG2	1:H:1014:TYR:HE1	1.58	0.68
1:D:1010:PHE:CD1	1:D:1047:PHE:CD1	2.82	0.68
1:E:1023:LYS:N	1:E:1023:LYS:HD2	2.09	0.68
1:G:1186:ASP:HB2	1:G:1188:VAL:HG23	1.76	0.68
1:C:1092:ARG:HD3	1:C:1095:ARG:HH11	1.58	0.68
1:G:1044:ARG:HB2	1:G:1044:ARG:NH1	2.09	0.68
1:H:1022:VAL:CG1	1:H:1025:GLU:HG3	2.24	0.68
1:H:1071:GLN:HE21	1:H:1071:GLN:N	1.92	0.68
1:E:1105:ALA:N	1:S:1007:GLN:NE2	2.39	0.68
1:T:1066:LEU:HB2	1:T:1078:ILE:HG22	1.75	0.68
1:M:1107:PRO:HD3	1:M:1208:LEU:HD21	1.75	0.67
1:D:1084:ARG:HD2	1:D:1144:ALA:O	1.93	0.67
1:E:1069:VAL:HB	1:E:1076:LEU:HB2	1.76	0.67
1:S:1161:PTR:HD1	1:S:1162:GLU:N	2.09	0.67
1:J:1139:ARG:NH2	1:J:1175:PRO:HG3	2.09	0.67
1:J:984:ALA:O	1:J:988:VAL:HG22	1.95	0.67
1:L:1235:ASP:O	1:L:1236:ASN:HB2	1.94	0.67
1:F:1092:ARG:NE	1:F:1095:ARG:HH11	1.92	0.67
1:I:1005:LEU:HD22	2:I:9:741:H13A	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1042:ARG:CG	1:R:1042:ARG:HH11	2.05	0.67
1:K:1275:ARG:HA	1:K:1281:TYR:CD1	2.30	0.67
1:R:1112:MET:HE2	1:R:1206:ALA:HA	1.76	0.67
1:S:1082:MET:HE2	1:S:1142:MET:HB2	1.76	0.67
1:C:1010:PHE:CD1	1:C:1047:PHE:CD1	2.82	0.67
1:C:1112:MET:HE3	1:C:1206:ALA:HA	1.75	0.67
1:G:1223:ARG:CG	1:G:1223:ARG:HH11	2.08	0.67
1:C:986:VAL:HG11	1:H:1247:MET:SD	2.34	0.67
1:H:1023:LYS:HD2	1:H:1023:LYS:N	2.01	0.67
1:H:996:ARG:HH12	1:H:1074:PRO:HD2	1.59	0.67
1:B:994:VAL:O	1:B:1069:VAL:HG22	1.96	0.66
1:C:1163:THR:HG23	1:C:1165:PTR:CE1	2.24	0.66
1:J:1178:TRP:CE2	3:J:8:HOH:O	2.47	0.66
1:S:1139:ARG:NH2	1:S:1175:PRO:HG3	2.09	0.66
1:A:1112:MET:HE3	1:A:1206:ALA:HA	1.78	0.66
1:F:1036:ASN:HD22	1:F:1038:ALA:HB3	1.60	0.66
1:S:984:ALA:O	1:S:988:VAL:HG22	1.95	0.66
1:A:1162:GLU:O	1:A:1163:THR:HB	1.95	0.66
1:H:1044:ARG:HH11	1:H:1044:ARG:HB2	1.60	0.66
1:I:1112:MET:HE2	1:I:1205:ILE:HG22	1.78	0.66
1:B:1069:VAL:HB	1:B:1076:LEU:HB2	1.78	0.66
1:C:1229:GLY:O	1:C:1230:LEU:HD23	1.95	0.66
1:F:1092:ARG:HE	1:F:1095:ARG:HH11	1.42	0.66
1:H:1275:ARG:HA	1:H:1281:TYR:CD1	2.31	0.66
1:R:1022:VAL:HG12	1:R:1023:LYS:HE2	1.77	0.66
1:A:1161:PTR:O	1:A:1162:GLU:HB2	1.95	0.66
1:E:1058:ASN:ND2	1:E:1064:ARG:HH21	1.94	0.66
1:M:1161:PTR:CD1	1:M:1162:GLU:HG3	2.26	0.66
1:I:984:ALA:O	1:I:988:VAL:HG22	1.95	0.66
1:A:1112:MET:HE1	1:A:1206:ALA:HA	1.75	0.66
1:E:996:ARG:NH1	1:E:1074:PRO:HD2	2.11	0.66
1:I:989:PRO:O	1:I:991:GLU:N	2.29	0.66
1:C:1235:ASP:O	1:C:1236:ASN:HB2	1.96	0.66
1:H:1234:PRO:HB2	1:H:1237:CYS:HB2	1.76	0.66
1:G:1034:THR:HG22	1:G:1076:LEU:CD2	2.25	0.66
1:G:1201:VAL:O	1:G:1205:ILE:HG13	1.96	0.66
1:R:1162:GLU:O	1:R:1163:THR:HB	1.96	0.66
1:T:1060:HIS:O	1:T:1150:LYS:HE3	1.95	0.66
1:A:1044:ARG:HB2	1:A:1044:ARG:HH11	1.61	0.65
2:A:1:741:O12	2:A:1:741:H16B	1.96	0.65
1:H:1097:GLU:HA	1:H:1097:GLU:OE2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:986:VAL:HG22	1:I:987:TYR:CD2	2.31	0.65
1:J:996:ARG:HB3	1:J:1069:VAL:HG11	1.77	0.65
1:R:1119:ILE:HG23	1:R:1151:ILE:HD11	1.78	0.65
1:T:1112:MET:HE1	1:T:1206:ALA:HA	1.78	0.65
1:A:984:ALA:O	1:A:988:VAL:HG22	1.97	0.65
1:G:1163:THR:CG2	1:G:1165:PTR:CE1	2.74	0.65
1:H:1073:GLN:HB3	1:H:1074:PRO:HD3	1.77	0.65
1:I:1254:LYS:HZ2	1:I:1255:MET:CG	2.10	0.65
1:K:1258:SER:O	1:K:1262:ILE:HG13	1.96	0.65
1:E:1275:ARG:HA	1:E:1281:TYR:CD1	2.30	0.65
1:D:1107:PRO:HD3	1:D:1208:LEU:HD21	1.78	0.65
1:M:1058:ASN:ND2	1:M:1064:ARG:CZ	2.58	0.65
1:G:1096:PRO:O	1:G:1097:GLU:HG3	1.97	0.65
1:J:1036:ASN:ND2	1:J:1038:ALA:N	2.38	0.65
1:C:1021:VAL:HG23	1:C:1022:VAL:HG23	1.78	0.65
1:C:1166:PTR:O2P	1:C:1166:PTR:HE1	1.97	0.65
1:D:1040:SER:OG	1:D:1043:GLU:HG2	1.96	0.65
1:L:1092:ARG:HG3	1:L:1209:ALA:HB3	1.77	0.65
1:M:1047:PHE:CZ	1:M:1077:VAL:HG21	2.31	0.65
1:H:1132:VAL:HG22	1:H:1160:ILE:HD13	1.77	0.65
1:C:1015:GLU:CD	1:C:1029:ARG:HH21	1.98	0.65
1:G:1036:ASN:ND2	1:G:1038:ALA:N	2.45	0.65
1:H:1161:PTR:O	1:H:1162:GLU:HB2	1.96	0.65
1:K:1081:LEU:HD13	1:K:1083:THR:HG22	1.79	0.65
1:T:1112:MET:CE	1:T:1206:ALA:HA	2.27	0.65
1:B:1121:ASP:HA	1:B:1263:ILE:HD11	1.79	0.65
1:E:993:GLU:OE2	1:E:1070:SER:OG	2.14	0.65
1:B:1168:LYS:HE2	3:B:147:HOH:O	1.95	0.64
1:B:1156:MET:HG2	1:B:1174:LEU:HD21	1.77	0.64
1:F:1166:PTR:O3P	1:F:1166:PTR:HE1	1.97	0.64
1:I:1252:ASN:HB3	1:I:1254:LYS:NZ	2.13	0.64
1:L:1051:ALA:O	1:L:1054:MET:HB2	1.97	0.64
1:F:1127:ASN:OD1	1:F:1191:THR:HB	1.96	0.64
1:B:1021:VAL:HG22	1:B:1022:VAL:HG23	1.79	0.64
1:E:1234:PRO:HB2	1:E:1237:CYS:HB2	1.78	0.64
1:G:1066:LEU:HB2	1:G:1078:ILE:HG22	1.79	0.64
1:S:1061:HIS:HD2	1:S:1118:GLU:HB3	1.61	0.64
1:D:1058:ASN:C	1:D:1058:ASN:ND2	2.50	0.64
1:I:1112:MET:HE1	1:I:1206:ALA:HA	1.79	0.64
1:A:1069:VAL:HB	1:A:1076:LEU:HB2	1.77	0.64
1:S:1127:ASN:OD1	1:S:1191:THR:HB	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1054:MET:HE1	3:D:120:HOH:O	1.98	0.64
1:G:984:ALA:O	1:G:988:VAL:HG22	1.98	0.64
1:L:1107:PRO:HD2	1:L:1112:MET:HE3	1.80	0.64
1:K:1112:MET:HE1	1:K:1206:ALA:HA	1.78	0.64
1:T:1010:PHE:CD1	1:T:1047:PHE:HD1	2.16	0.64
1:T:1127:ASN:OD1	1:T:1191:THR:HG22	1.98	0.64
1:A:1096:PRO:O	1:A:1097:GLU:HB2	1.96	0.64
1:G:1041:MET:O	1:G:1045:ILE:HG13	1.98	0.64
1:S:1092:ARG:HD3	1:S:1095:ARG:HD2	1.80	0.64
1:A:1247:MET:SD	1:B:986:VAL:HG11	2.38	0.63
1:E:1112:MET:HE2	1:E:1206:ALA:HA	1.78	0.63
1:D:1044:ARG:HD3	3:D:135:HOH:O	1.98	0.63
1:F:1112:MET:HE3	1:F:1206:ALA:HA	1.80	0.63
1:R:1109:LEU:O	1:R:1113:ILE:HG12	1.97	0.63
1:B:1023:LYS:H	1:B:1023:LYS:HD2	1.61	0.63
1:D:1047:PHE:HZ	1:D:1077:VAL:HG21	1.63	0.63
1:E:1042:ARG:CG	1:E:1042:ARG:HH11	2.02	0.63
1:E:1229:GLY:O	1:E:1230:LEU:HD23	1.97	0.63
1:E:1242:PHE:CE2	1:E:1246:ARG:HD2	2.33	0.63
1:G:1036:ASN:HD22	1:G:1038:ALA:N	1.96	0.63
1:M:1030:VAL:HG23	1:M:1032:ILE:HD11	1.81	0.63
1:R:1161:PTR:HD1	1:R:1162:GLU:HG3	1.79	0.63
1:S:1264:SER:HG	1:S:1280:TYR:HH	1.45	0.63
1:C:1162:GLU:O	1:C:1163:THR:HB	1.96	0.63
1:C:996:ARG:CZ	1:C:1074:PRO:HD2	2.27	0.63
1:I:1275:ARG:HA	1:I:1281:TYR:CD1	2.34	0.63
1:K:1132:VAL:HG23	1:K:1160:ILE:HD13	1.79	0.63
1:M:1166:PTR:OH	1:M:1168:LYS:CD	2.46	0.63
1:S:1259:PHE:O	1:S:1263:ILE:HG13	1.99	0.63
1:T:1184:LEU:HD13	1:T:1222:LEU:HD22	1.80	0.63
1:C:992:TRP:CH2	1:C:1055:LYS:HA	2.33	0.63
1:F:1201:VAL:O	1:F:1205:ILE:HG13	1.98	0.63
1:M:1044:ARG:O	1:M:1048:LEU:HB2	1.98	0.63
1:G:1267:LYS:HD2	1:G:1281:TYR:OH	1.99	0.63
1:T:984:ALA:O	1:T:988:VAL:HG22	1.99	0.63
1:E:1092:ARG:NH2	1:E:1095:ARG:NH1	2.47	0.63
1:I:989:PRO:HD3	1:I:1055:LYS:NZ	2.14	0.63
1:J:1092:ARG:HG3	1:J:1092:ARG:HH11	1.63	0.63
1:R:1243:GLU:OE2	1:R:1246:ARG:HD3	1.99	0.63
1:T:1161:PTR:HD1	1:T:1162:GLU:N	2.14	0.63
1:F:1012:MET:HG3	1:F:1014:TYR:CE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:985:ASP:OD1	1:I:1071:GLN:OE1	2.17	0.62
1:I:992:TRP:CZ2	1:I:1055:LYS:HB2	2.34	0.62
1:H:1275:ARG:HA	1:H:1281:TYR:HD1	1.64	0.62
1:L:1119:ILE:HG23	1:L:1151:ILE:HD11	1.81	0.62
1:S:1058:ASN:HD22	1:S:1058:ASN:C	2.02	0.62
1:E:1201:VAL:O	1:E:1205:ILE:HG13	2.00	0.62
1:K:1121:ASP:HA	1:K:1263:ILE:HD11	1.81	0.62
1:F:1047:PHE:C	1:F:1047:PHE:HD2	2.01	0.62
1:I:1023:LYS:CD	1:I:1023:LYS:N	2.58	0.62
1:J:1139:ARG:NH2	3:J:8:HOH:O	2.32	0.62
1:E:1242:PHE:O	1:E:1246:ARG:HG3	1.99	0.62
1:G:1103:VAL:O	1:G:1104:LEU:HD12	1.99	0.62
1:G:1023:LYS:H	1:G:1023:LYS:CD	2.13	0.62
1:J:1092:ARG:HG3	1:J:1092:ARG:NH1	2.13	0.62
1:D:1084:ARG:HG2	1:D:1084:ARG:NH1	2.08	0.62
1:E:996:ARG:HH12	1:E:1074:PRO:CG	2.13	0.62
1:G:1051:ALA:O	1:G:1054:MET:HB2	1.99	0.62
1:M:1112:MET:CE	1:M:1206:ALA:HA	2.30	0.62
1:M:1132:VAL:O	1:M:1157:THR:HB	2.00	0.62
1:B:1044:ARG:O	1:B:1048:LEU:HD22	1.99	0.62
1:C:1092:ARG:HD3	1:C:1095:ARG:HD2	1.81	0.62
1:G:1036:ASN:HD22	1:G:1038:ALA:H	1.46	0.62
1:D:1069:VAL:HG21	1:D:1076:LEU:HD12	1.80	0.62
1:K:1036:ASN:ND2	1:K:1038:ALA:H	1.98	0.62
1:B:1273:GLY:O	1:B:1276:GLU:HG2	2.00	0.61
1:F:1047:PHE:CD2	1:F:1047:PHE:C	2.74	0.61
1:H:1060:HIS:CD2	1:H:1277:VAL:HB	2.34	0.61
1:B:1084:ARG:NH2	1:B:1145:GLU:O	2.33	0.61
1:F:1109:LEU:HD22	1:F:1113:ILE:HG12	1.80	0.61
1:J:1207:THR:O	1:J:1210:GLU:HG3	2.00	0.61
1:J:1235:ASP:O	1:J:1236:ASN:HB2	1.98	0.61
1:D:1029:ARG:HB3	1:D:1081:LEU:HD12	1.82	0.61
1:F:1275:ARG:HA	1:F:1281:TYR:CD1	2.35	0.61
1:S:996:ARG:HB3	1:S:1069:VAL:HG11	1.82	0.61
1:S:1217:SER:OG	1:S:1220:GLN:HG3	2.00	0.61
1:C:1041:MET:O	1:C:1045:ILE:HG13	2.00	0.61
1:E:1010:PHE:CG	1:E:1047:PHE:HD1	2.17	0.61
1:F:1036:ASN:ND2	1:F:1038:ALA:HB3	2.16	0.61
1:H:1115:MET:HG2	1:H:1149:VAL:HG21	1.82	0.61
1:J:1060:HIS:O	1:J:1150:LYS:NZ	2.34	0.61
1:R:1047:PHE:HZ	1:R:1077:VAL:HG21	1.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:996:ARG:HH12	1:C:1074:PRO:CD	2.13	0.61
1:D:1084:ARG:HH11	1:D:1084:ARG:CG	2.09	0.61
1:D:1186:ASP:HB2	1:D:1188:VAL:HG23	1.80	0.61
1:E:1154:PHE:HD2	1:E:1157:THR:HG21	1.65	0.61
1:H:1022:VAL:HG21	1:H:1028:THR:HG21	1.82	0.61
1:J:994:VAL:HG22	1:J:1069:VAL:HG22	1.82	0.61
1:K:1042:ARG:HH11	1:K:1042:ARG:HG3	1.63	0.61
1:K:1134:ARG:NH1	1:K:1156:MET:O	2.32	0.61
1:B:1109:LEU:HD22	1:B:1113:ILE:HG12	1.82	0.61
1:K:1112:MET:CE	1:K:1206:ALA:HA	2.30	0.61
1:G:1035:VAL:HG21	1:G:1047:PHE:CE2	2.36	0.61
1:I:1035:VAL:HG21	1:I:1047:PHE:CE2	2.36	0.61
1:J:1154:PHE:HD2	1:J:1157:THR:HG21	1.65	0.61
1:B:998:LYS:HD3	1:B:1019:LYS:O	2.01	0.61
1:F:1161:PTR:O	1:F:1162:GLU:HB2	2.00	0.61
1:J:1063:VAL:HG23	1:J:1151:ILE:O	1.99	0.61
1:L:1161:PTR:HD1	1:L:1161:PTR:C	2.31	0.61
1:R:1163:THR:HG23	1:R:1165:PTR:CE1	2.30	0.61
1:A:1010:PHE:CD1	1:A:1047:PHE:HD1	2.19	0.61
1:E:989:PRO:HG2	1:E:992:TRP:CD1	2.36	0.61
1:G:1102:PRO:O	1:G:1103:VAL:HB	2.01	0.61
1:H:1112:MET:HE2	1:H:1206:ALA:CA	2.30	0.61
1:K:984:ALA:HA	1:K:1048:LEU:HD21	1.83	0.61
1:T:996:ARG:HE	1:T:1069:VAL:HG11	1.66	0.61
1:A:1229:GLY:O	1:A:1230:LEU:HD23	2.01	0.60
1:B:1058:ASN:C	1:B:1058:ASN:HD22	2.05	0.60
1:B:1034:THR:HG22	1:B:1076:LEU:HD23	1.83	0.60
1:F:1139:ARG:NH2	1:F:1175:PRO:HG2	2.16	0.60
1:K:1088:LYS:HE2	1:K:1092:ARG:NH2	2.16	0.60
1:A:1005:LEU:HD22	2:A:1:741:H13A	1.83	0.60
1:B:1143:VAL:HG22	1:B:1149:VAL:HG22	1.83	0.60
1:E:1073:GLN:HB2	1:E:1074:PRO:HD3	1.83	0.60
1:J:1217:SER:OG	1:J:1220:GLN:HG3	2.01	0.60
1:L:1092:ARG:O	1:L:1095:ARG:HG3	2.01	0.60
1:S:1162:GLU:O	1:S:1163:THR:CB	2.48	0.60
1:C:996:ARG:NH2	1:C:1074:PRO:O	2.32	0.60
1:H:1105:ALA:HB3	1:R:1007:GLN:HE21	1.65	0.60
1:T:992:TRP:CH2	1:T:1055:LYS:HA	2.37	0.60
1:D:1154:PHE:HD2	1:D:1157:THR:HG21	1.66	0.60
1:E:1042:ARG:NH2	1:E:1046:GLU:HG3	2.17	0.60
1:R:1022:VAL:CG1	1:R:1023:LYS:HE2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1025:GLU:HB3	1:F:1027:GLU:O	2.01	0.60
1:T:1023:LYS:O	1:T:1024:ASP:HB2	2.01	0.60
1:E:1157:THR:O	1:E:1158:ARG:HD3	2.01	0.60
1:H:1047:PHE:C	1:H:1047:PHE:CD2	2.75	0.60
1:M:1166:PTR:CE2	1:M:1168:LYS:HD3	2.30	0.60
1:M:988:VAL:O	1:M:988:VAL:HG23	2.00	0.60
1:T:989:PRO:O	1:T:992:TRP:HD1	1.83	0.60
1:B:1166:PTR:OH	1:B:1168:LYS:HD3	2.00	0.60
1:E:1158:ARG:HG3	1:E:1166:PTR:CD1	2.32	0.60
1:R:1162:GLU:O	1:R:1163:THR:CB	2.48	0.60
1:C:1058:ASN:ND2	1:C:1064:ARG:NH2	2.49	0.60
1:E:1010:PHE:CD1	1:E:1047:PHE:CD1	2.84	0.60
1:M:1037:GLU:C	1:M:1039:ALA:H	2.04	0.60
1:M:1078:ILE:HD12	1:M:1078:ILE:N	2.17	0.60
1:A:1092:ARG:O	1:A:1095:ARG:HG3	2.02	0.60
1:G:1047:PHE:HZ	1:G:1077:VAL:HG21	1.62	0.60
1:J:1092:ARG:NH1	1:J:1092:ARG:CG	2.61	0.60
1:L:1275:ARG:HA	1:L:1281:TYR:HD1	1.67	0.60
1:R:1184:LEU:HD13	1:R:1222:LEU:HD22	1.83	0.60
1:S:1092:ARG:HD3	1:S:1095:ARG:HH11	1.66	0.60
1:B:1186:ASP:HB2	1:B:1188:VAL:CG2	2.31	0.59
1:H:1032:ILE:CD1	1:H:1078:ILE:HD12	2.32	0.59
1:I:1040:SER:OG	1:I:1043:GLU:HG3	2.03	0.59
1:I:996:ARG:HH12	1:I:1074:PRO:HG2	1.66	0.59
1:R:984:ALA:O	1:R:988:VAL:HG22	2.01	0.59
1:S:1114:GLN:O	1:S:1118:GLU:HG3	2.02	0.59
1:A:1154:PHE:HD2	1:A:1157:THR:HG21	1.66	0.59
1:B:993:GLU:HG3	1:B:994:VAL:N	2.15	0.59
1:C:989:PRO:C	1:C:991:GLU:H	2.04	0.59
1:E:999:ILE:HG13	1:E:1078:ILE:HD11	1.84	0.59
1:K:1139:ARG:NH2	1:K:1175:PRO:HG2	2.17	0.59
1:C:1156:MET:HG2	1:C:1174:LEU:HD21	1.83	0.59
1:E:994:VAL:O	1:E:1069:VAL:HG22	2.03	0.59
1:F:1073:GLN:HB2	1:F:1074:PRO:HD3	1.84	0.59
1:J:984:ALA:HA	1:J:1048:LEU:HD21	1.84	0.59
1:K:1163:THR:HG22	1:K:1165:PTR:HE1	1.83	0.59
1:S:1134:ARG:HG2	1:S:1189:PHE:CD2	2.37	0.59
1:C:988:VAL:HG13	1:C:988:VAL:O	2.02	0.59
1:L:1023:LYS:O	1:L:1024:ASP:HB2	2.02	0.59
1:S:1015:GLU:HG3	1:S:1016:GLY:N	2.16	0.59
1:C:1069:VAL:HB	1:C:1076:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1211:GLN:HB3	1:K:1214:GLN:HG2	1.85	0.59
1:A:1162:GLU:O	1:A:1163:THR:CB	2.50	0.59
1:B:1023:LYS:H	1:B:1023:LYS:CD	2.14	0.59
1:C:1275:ARG:HA	1:C:1281:TYR:CD1	2.37	0.59
1:G:1234:PRO:HB2	1:G:1237:CYS:HB2	1.85	0.59
1:G:1271:GLU:OE2	1:G:1271:GLU:HA	2.01	0.59
1:A:1012:MET:HG2	1:A:1014:TYR:CZ	2.38	0.59
1:F:1022:VAL:HG13	1:F:1028:THR:OG1	2.03	0.59
1:F:1112:MET:HE1	1:F:1206:ALA:HA	1.81	0.59
1:H:1096:PRO:O	1:H:1097:GLU:HG2	2.03	0.59
1:S:1243:GLU:OE2	1:S:1246:ARG:NH1	2.36	0.59
1:F:1044:ARG:HH11	1:F:1044:ARG:CB	2.16	0.59
1:H:1000:THR:HG23	3:H:32:HOH:O	2.02	0.59
1:K:989:PRO:CG	1:K:992:TRP:HD1	1.99	0.59
1:L:1035:VAL:HG21	1:L:1047:PHE:CD2	2.38	0.59
1:S:1158:ARG:HG3	1:S:1166:PTR:CD1	2.33	0.59
1:C:1112:MET:CE	1:C:1206:ALA:HA	2.32	0.59
1:D:1065:LEU:HA	1:D:1079:MET:SD	2.42	0.59
1:H:1163:THR:O	1:H:1165:PTR:HD1	2.02	0.59
1:K:1222:LEU:HD12	1:K:1222:LEU:O	2.02	0.59
1:L:1035:VAL:HG21	1:L:1047:PHE:CE2	2.37	0.59
1:M:1042:ARG:NH1	1:M:1042:ARG:HG2	2.16	0.59
1:R:1092:ARG:HD3	1:R:1095:ARG:HH11	1.67	0.59
1:E:1065:LEU:HD23	1:E:1067:GLY:N	2.17	0.58
1:F:1049:ASN:O	1:F:1052:SER:HB3	2.03	0.58
1:M:1258:SER:O	1:M:1262:ILE:HG13	2.03	0.58
1:M:989:PRO:HB2	1:M:991:GLU:HG2	1.85	0.58
1:S:1161:PTR:HD1	1:S:1162:GLU:HG3	1.84	0.58
1:F:984:ALA:O	1:F:988:VAL:HG13	2.02	0.58
1:H:1029:ARG:HB3	1:H:1081:LEU:HD12	1.85	0.58
1:I:1095:ARG:NH2	1:I:1210:GLU:HG3	2.18	0.58
1:B:989:PRO:HB2	1:B:991:GLU:HG3	1.85	0.58
1:C:1132:VAL:CG2	1:C:1160:ILE:HD13	2.34	0.58
1:D:1023:LYS:H	1:D:1023:LYS:HD2	1.68	0.58
1:G:1023:LYS:H	1:G:1023:LYS:HD2	1.68	0.58
1:G:1064:ARG:O	1:G:1079:MET:HE3	2.03	0.58
1:S:1121:ASP:HA	1:S:1263:ILE:HD11	1.85	0.58
1:K:1036:ASN:C	1:K:1036:ASN:ND2	2.52	0.58
1:R:1005:LEU:HD22	2:R:14:741:H13A	1.84	0.58
1:C:1267:LYS:HD2	1:C:1281:TYR:OH	2.04	0.58
1:E:1030:VAL:HG23	1:E:1032:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1219:GLU:O	1:G:1223:ARG:HG2	2.03	0.58
1:H:1005:LEU:HD21	1:H:1015:GLU:HB2	1.84	0.58
1:T:1258:SER:OG	1:T:1261:GLU:HG3	2.04	0.58
1:B:1092:ARG:NH2	1:B:1095:ARG:CZ	2.66	0.58
1:F:1163:THR:HG22	1:F:1165:PTR:CD1	2.33	0.58
1:J:1036:ASN:O	1:J:1037:GLU:CB	2.51	0.58
1:C:1029:ARG:HB3	1:C:1081:LEU:HD12	1.85	0.58
1:H:1112:MET:HG2	1:H:1205:ILE:CG2	2.34	0.58
1:A:1223:ARG:O	1:A:1227:GLU:HG3	2.04	0.58
1:F:1092:ARG:CD	1:F:1209:ALA:HB3	2.29	0.58
1:I:1123:MET:HB3	1:I:1259:PHE:CE2	2.39	0.58
1:C:1010:PHE:H	1:C:1033:LYS:HZ1	1.51	0.58
1:D:1247:MET:SD	1:G:986:VAL:HG11	2.44	0.58
1:I:1252:ASN:HB3	1:I:1254:LYS:HZ3	1.68	0.58
1:K:1069:VAL:HB	1:K:1076:LEU:HB2	1.86	0.58
1:M:1235:ASP:O	1:M:1236:ASN:HB2	2.04	0.58
1:D:990:ASP:O	1:D:991:GLU:HG2	2.03	0.57
1:H:1235:ASP:O	1:H:1236:ASN:HB2	2.04	0.57
1:I:1036:ASN:ND2	1:I:1036:ASN:C	2.53	0.57
1:H:1036:ASN:HD21	1:H:1038:ALA:C	2.07	0.57
1:H:1109:LEU:HD22	1:H:1113:ILE:HG12	1.85	0.57
1:K:1023:LYS:N	1:K:1023:LYS:HD2	2.18	0.57
1:B:1010:PHE:HD1	1:B:1047:PHE:HD1	1.46	0.57
1:B:1105:ALA:HB3	1:J:1007:GLN:NE2	2.19	0.57
1:G:1061:HIS:HA	1:G:1150:LYS:HG2	1.85	0.57
1:K:1113:ILE:HD11	1:K:1240:MET:SD	2.44	0.57
2:L:13:741:C18	2:L:13:741:C32	2.82	0.57
1:M:1222:LEU:CD1	1:M:1226:MET:SD	2.92	0.57
1:S:1109:LEU:HD22	1:S:1113:ILE:HG12	1.87	0.57
1:T:1035:VAL:HG21	1:T:1047:PHE:CE2	2.39	0.57
1:C:993:GLU:HG3	1:C:1070:SER:OG	2.04	0.57
1:F:1023:LYS:O	1:F:1024:ASP:HB2	2.04	0.57
1:M:1092:ARG:HD3	1:M:1095:ARG:HH11	1.69	0.57
1:E:992:TRP:CZ2	1:E:1055:LYS:CB	2.88	0.57
1:G:996:ARG:HH12	1:G:1074:PRO:HG2	1.68	0.57
2:I:9:741:C18	2:I:9:741:C32	2.82	0.57
1:L:1073:GLN:HB3	1:L:1074:PRO:CD	2.35	0.57
1:L:1184:LEU:HD13	1:L:1222:LEU:HD23	1.85	0.57
1:S:1086:ASP:OD1	1:S:1089:SER:HB2	2.04	0.57
1:T:1054:MET:O	1:T:1055:LYS:C	2.42	0.57
1:F:1044:ARG:NH1	1:F:1044:ARG:HB2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1010:PHE:CD1	1:M:1047:PHE:HD1	2.23	0.57
1:B:1018:ALA:CB	1:B:1021:VAL:HG11	2.34	0.57
1:B:1201:VAL:O	1:B:1205:ILE:HG13	2.05	0.57
1:B:992:TRP:CH2	1:B:1055:LYS:HA	2.39	0.57
1:C:1065:LEU:HD23	1:C:1067:GLY:N	2.20	0.57
1:D:1184:LEU:HD22	1:D:1222:LEU:HD22	1.84	0.57
1:D:994:VAL:HG22	1:D:1069:VAL:HG22	1.87	0.57
1:F:1023:LYS:CD	1:F:1023:LYS:H	2.03	0.57
1:I:1154:PHE:HD2	1:I:1157:THR:HG21	1.69	0.57
1:I:1254:LYS:HZ2	1:I:1255:MET:N	2.03	0.57
1:M:1010:PHE:CD1	1:M:1047:PHE:CD1	2.92	0.57
1:R:1126:LEU:HD13	1:R:1131:PHE:HB2	1.87	0.57
1:R:995:ALA:HB1	1:R:997:GLU:OE2	2.05	0.57
1:M:1161:PTR:HD1	1:M:1162:GLU:HG3	1.87	0.57
1:C:1180:SER:CB	1:C:1182:GLU:OE2	2.53	0.56
1:I:1151:ILE:CD1	1:I:1151:ILE:N	2.68	0.56
1:I:1112:MET:CE	1:I:1206:ALA:HA	2.35	0.56
1:M:1163:THR:HG22	1:M:1165:PTR:HE1	1.86	0.56
1:F:1040:SER:O	1:F:1043:GLU:OE2	2.23	0.56
1:H:1071:GLN:CA	1:H:1071:GLN:HE21	2.18	0.56
1:H:1161:PTR:C	1:H:1161:PTR:HD1	2.35	0.56
1:I:1235:ASP:O	1:I:1236:ASN:HB2	2.04	0.56
1:J:1058:ASN:HD22	1:J:1058:ASN:C	2.07	0.56
1:S:1207:THR:HG22	1:S:1234:PRO:HB3	1.86	0.56
1:B:996:ARG:HH12	1:B:1074:PRO:HG2	1.70	0.56
1:C:1180:SER:OG	1:C:1182:GLU:OE2	2.23	0.56
1:F:1018:ALA:HB3	1:F:1021:VAL:HG11	1.87	0.56
1:H:1044:ARG:NH1	1:H:1044:ARG:HB2	2.20	0.56
1:R:1092:ARG:HD3	1:R:1095:ARG:NH1	2.19	0.56
1:R:1127:ASN:OD1	1:R:1191:THR:HB	2.05	0.56
1:T:1139:ARG:NH2	1:T:1175:PRO:HG2	2.19	0.56
1:A:1096:PRO:O	1:A:1097:GLU:CB	2.52	0.56
1:A:1158:ARG:HG3	1:A:1166:PTR:CD1	2.35	0.56
1:C:1047:PHE:CZ	1:C:1077:VAL:HG21	2.40	0.56
1:C:995:ALA:HB3	1:C:998:LYS:HG3	1.88	0.56
1:G:1018:ALA:HB1	1:G:1021:VAL:HG11	1.86	0.56
1:H:1019:LYS:CG	1:H:1027:GLU:HG2	2.34	0.56
1:L:1135:ASP:O	1:L:1140:ASN:ND2	2.38	0.56
1:L:989:PRO:C	1:L:991:GLU:H	2.07	0.56
1:M:1115:MET:HG2	1:M:1149:VAL:HG21	1.87	0.56
1:R:1121:ASP:HA	1:R:1263:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1069:VAL:HB	1:T:1076:LEU:HB2	1.87	0.56
1:A:1017:VAL:HG11	1:A:1027:GLU:OE1	2.05	0.56
1:B:1163:THR:HG22	1:B:1165:PTR:CD1	2.35	0.56
1:B:1127:ASN:OD1	1:B:1191:THR:HB	2.06	0.56
1:H:1108:SER:OG	1:H:1111:LYS:HG2	2.05	0.56
1:T:1127:ASN:CG	1:T:1191:THR:CG2	2.73	0.56
1:D:1044:ARG:NH1	1:D:1044:ARG:HB2	2.21	0.56
1:D:1069:VAL:HB	1:D:1076:LEU:HB2	1.87	0.56
1:F:1275:ARG:HA	1:F:1281:TYR:HD1	1.70	0.56
1:I:1163:THR:CG2	1:I:1165:PTR:CE1	2.84	0.56
1:L:1258:SER:O	1:L:1262:ILE:HG13	2.06	0.56
1:B:1235:ASP:O	1:B:1236:ASN:HB2	2.06	0.56
1:C:1092:ARG:CD	1:C:1095:ARG:HH11	2.17	0.56
1:D:1023:LYS:H	1:D:1023:LYS:CD	2.19	0.56
1:M:1161:PTR:HD1	1:M:1162:GLU:H	1.66	0.56
1:T:1022:VAL:HA	1:T:1023:LYS:HE2	1.87	0.56
1:A:1235:ASP:O	1:A:1236:ASN:CB	2.51	0.56
1:D:1112:MET:HG2	1:D:1205:ILE:CG2	2.36	0.56
1:H:1104:LEU:O	1:H:1105:ALA:O	2.24	0.56
1:K:996:ARG:NH2	1:K:1074:PRO:HD2	2.21	0.56
1:L:1163:THR:CG2	1:L:1165:PTR:CE1	2.79	0.56
2:T:16:741:O12	2:T:16:741:H16B	2.06	0.56
1:R:1023:LYS:O	1:R:1023:LYS:HD2	2.06	0.56
1:T:1179:MET:HE2	1:T:1184:LEU:HD23	1.88	0.56
1:B:1177:ARG:CZ	1:B:1211:GLN:NE2	2.70	0.55
1:C:984:ALA:HA	1:C:1048:LEU:HD21	1.88	0.55
1:A:1051:ALA:O	1:A:1054:MET:HB2	2.05	0.55
1:C:1034:THR:HG22	1:C:1076:LEU:CD2	2.36	0.55
1:C:998:LYS:O	1:C:1019:LYS:HG3	2.06	0.55
1:F:1015:GLU:HG2	1:F:1016:GLY:N	2.21	0.55
1:H:1044:ARG:HH11	1:H:1044:ARG:CB	2.19	0.55
1:K:1047:PHE:CZ	1:K:1077:VAL:HG21	2.42	0.55
1:T:1023:LYS:N	1:T:1023:LYS:HE2	2.22	0.55
1:T:1161:PTR:O	1:T:1162:GLU:HB2	2.05	0.55
1:B:996:ARG:NH1	1:B:1074:PRO:HD2	2.21	0.55
1:D:1121:ASP:HA	1:D:1263:ILE:HD11	1.87	0.55
1:G:1036:ASN:HD21	1:G:1038:ALA:HB3	1.71	0.55
1:I:989:PRO:C	1:I:991:GLU:N	2.60	0.55
1:R:1036:ASN:N	1:R:1036:ASN:HD22	2.00	0.55
1:T:1023:LYS:H	1:T:1023:LYS:CE	2.19	0.55
1:E:1121:ASP:HA	1:E:1263:ILE:HD11	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1107:PRO:HD3	1:H:1208:LEU:HD21	1.89	0.55
1:B:1041:MET:O	1:B:1045:ILE:HG13	2.06	0.55
1:F:1222:LEU:C	1:F:1222:LEU:HD12	2.27	0.55
1:I:1253:PRO:C	1:I:1254:LYS:HE3	2.24	0.55
1:J:1069:VAL:HB	1:J:1076:LEU:HB2	1.89	0.55
1:K:1146:ASP:O	1:K:1147:PHE:HB2	2.07	0.55
1:T:1179:MET:CE	1:T:1184:LEU:HD23	2.36	0.55
1:G:984:ALA:HA	1:G:1048:LEU:HD21	1.89	0.55
1:I:1243:GLU:OE2	1:I:1246:ARG:HD3	2.07	0.55
1:K:1036:ASN:ND2	1:K:1038:ALA:N	2.54	0.55
1:R:1058:ASN:C	1:R:1058:ASN:ND2	2.60	0.55
1:B:993:GLU:HA	1:B:1068:VAL:O	2.07	0.55
1:C:996:ARG:HH12	1:C:1074:PRO:HG2	1.70	0.55
1:I:989:PRO:CD	1:I:1055:LYS:NZ	2.69	0.55
1:T:1154:PHE:CD2	1:T:1157:THR:HG21	2.38	0.55
1:B:1054:MET:O	1:B:1057:PHE:N	2.39	0.55
1:B:1135:ASP:O	1:B:1140:ASN:ND2	2.39	0.55
1:B:1167:ARG:NH1	1:B:1188:VAL:HG22	2.21	0.55
1:I:1254:LYS:H	1:I:1254:LYS:CE	2.17	0.55
1:A:1092:ARG:NH1	1:A:1095:ARG:NH1	2.55	0.55
1:I:1167:ARG:NH1	1:I:1167:ARG:HG3	2.22	0.55
1:J:1229:GLY:O	1:J:1230:LEU:HD23	2.06	0.55
1:M:993:GLU:OE1	1:M:1071:GLN:HG2	2.07	0.55
1:C:1025:GLU:HB3	1:C:1027:GLU:O	2.07	0.55
1:C:1036:ASN:HD21	1:C:1038:ALA:CB	2.20	0.55
1:F:984:ALA:HA	1:F:1048:LEU:HD21	1.89	0.55
1:I:1041:MET:O	1:I:1045:ILE:HG13	2.06	0.55
1:I:1254:LYS:NZ	1:I:1255:MET:H	2.05	0.55
1:M:998:LYS:HG3	1:M:998:LYS:O	2.05	0.55
1:S:1127:ASN:H	1:S:1127:ASN:HD22	1.52	0.55
1:D:1234:PRO:HB2	1:D:1237:CYS:HB2	1.89	0.54
1:F:1044:ARG:HH11	1:F:1044:ARG:HB2	1.72	0.54
1:I:1167:ARG:CG	1:I:1167:ARG:HH11	2.19	0.54
1:A:1113:ILE:HG23	1:A:1266:ILE:HD12	1.88	0.54
1:B:1065:LEU:HA	1:B:1079:MET:SD	2.48	0.54
1:C:1286:LYS:OXT	1:C:1286:LYS:HD3	2.08	0.54
1:G:1010:PHE:CD1	1:G:1047:PHE:CD1	2.95	0.54
1:H:988:VAL:HG23	1:H:988:VAL:O	2.08	0.54
1:L:1003:ARG:HH11	1:L:1003:ARG:HG2	1.73	0.54
1:E:1018:ALA:HB1	1:E:1021:VAL:HG11	1.89	0.54
1:J:1088:LYS:CE	1:J:1092:ARG:HH12	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1243:GLU:O	1:K:1247:MET:HG3	2.08	0.54
1:L:1161:PTR:O	1:L:1162:GLU:HB2	2.06	0.54
1:R:1166:PTR:O2P	1:R:1166:PTR:HE1	2.06	0.54
1:E:996:ARG:HH12	1:E:1074:PRO:HD2	1.73	0.54
1:I:1029:ARG:HB3	1:I:1081:LEU:HD12	1.89	0.54
1:I:1162:GLU:O	1:I:1163:THR:OG1	2.20	0.54
1:I:1234:PRO:HB2	1:I:1237:CYS:HB2	1.88	0.54
1:C:1058:ASN:ND2	1:C:1058:ASN:C	2.57	0.54
1:C:1177:ARG:HG3	3:C:37:HOH:O	2.08	0.54
1:D:1271:GLU:HB3	1:D:1272:PRO:HD2	1.90	0.54
1:M:994:VAL:CG2	1:M:1069:VAL:HG22	2.34	0.54
1:S:1162:GLU:O	1:S:1163:THR:HB	2.07	0.54
1:B:1054:MET:O	1:B:1055:LYS:C	2.46	0.54
1:C:1154:PHE:HB3	1:C:1157:THR:OG1	2.07	0.54
1:E:1065:LEU:HD23	1:E:1067:GLY:H	1.73	0.54
1:M:1177:ARG:HG2	1:M:1213:TYR:HD2	1.72	0.54
1:T:1010:PHE:CD1	1:T:1047:PHE:CD1	2.95	0.54
1:D:1139:ARG:HH22	1:D:1175:PRO:HG3	1.72	0.54
1:E:996:ARG:NH2	1:E:1074:PRO:O	2.39	0.54
1:F:1047:PHE:HZ	1:F:1077:VAL:HG21	1.67	0.54
1:I:1216:LEU:HD23	1:I:1216:LEU:N	2.23	0.54
1:S:1112:MET:CE	1:S:1206:ALA:HA	2.37	0.54
1:S:1139:ARG:HH22	1:S:1175:PRO:CG	2.18	0.54
1:C:1036:ASN:ND2	1:C:1038:ALA:H	2.06	0.54
1:M:998:LYS:CD	1:M:1019:LYS:O	2.55	0.54
1:M:1094:LEU:HD13	1:M:1106:PRO:HB2	1.90	0.54
1:A:1058:ASN:ND2	1:A:1064:ARG:NH2	2.55	0.54
1:A:1139:ARG:NH2	1:A:1175:PRO:HG2	2.23	0.54
1:C:1119:ILE:HG23	1:C:1151:ILE:HD11	1.90	0.54
1:H:1036:ASN:ND2	1:H:1036:ASN:C	2.60	0.54
1:J:1234:PRO:HB2	1:J:1237:CYS:HB2	1.90	0.54
1:R:1047:PHE:CE2	1:R:1077:VAL:HG21	2.42	0.54
1:R:1161:PTR:CD1	1:R:1162:GLU:HG3	2.38	0.54
1:C:1081:LEU:HD13	1:C:1083:THR:HG22	1.90	0.54
1:E:984:ALA:O	1:E:988:VAL:CG2	2.56	0.54
1:H:1285:ASN:O	1:H:1286:LYS:HB2	2.08	0.54
1:K:986:VAL:HG22	1:K:987:TYR:CD2	2.43	0.54
1:M:1112:MET:HG2	1:M:1205:ILE:HG22	1.90	0.54
1:R:1042:ARG:HG2	1:R:1042:ARG:NH1	2.11	0.54
1:B:1007:GLN:HA	1:B:1007:GLN:OE1	2.08	0.53
1:F:1163:THR:HG22	1:F:1165:PTR:CE1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1036:ASN:ND2	1:G:1038:ALA:HB3	2.23	0.53
1:H:1007:GLN:OE1	1:H:1007:GLN:HA	2.08	0.53
1:J:1092:ARG:HD2	1:J:1095:ARG:HD2	1.90	0.53
1:K:1208:LEU:O	1:K:1209:ALA:HB3	2.08	0.53
1:R:1058:ASN:ND2	1:R:1064:ARG:NH2	2.56	0.53
1:S:1047:PHE:CZ	1:S:1077:VAL:HG21	2.43	0.53
1:S:1066:LEU:HB2	1:S:1078:ILE:HG22	1.90	0.53
1:T:1065:LEU:HD23	1:T:1067:GLY:N	2.23	0.53
1:A:1010:PHE:CD1	1:A:1047:PHE:CD1	2.96	0.53
1:F:1018:ALA:O	1:F:1021:VAL:HG12	2.08	0.53
1:I:1121:ASP:HA	1:I:1263:ILE:HD11	1.88	0.53
1:I:1132:VAL:CG2	1:I:1160:ILE:HD13	2.38	0.53
1:I:993:GLU:OE2	1:I:1071:GLN:NE2	2.35	0.53
1:J:1066:LEU:HB2	1:J:1078:ILE:HG22	1.90	0.53
1:J:1132:VAL:CG1	1:J:1134:ARG:HG3	2.37	0.53
1:K:987:TYR:OH	1:R:1257:PRO:HD3	2.09	0.53
1:D:1023:LYS:O	1:D:1024:ASP:HB2	2.08	0.53
1:D:1112:MET:CE	1:D:1205:ILE:HG22	2.38	0.53
1:D:1229:GLY:O	1:D:1230:LEU:HD23	2.09	0.53
1:M:1166:PTR:OH	1:M:1168:LYS:HD3	2.08	0.53
1:R:1132:VAL:CG2	1:R:1160:ILE:HD13	2.38	0.53
1:T:1047:PHE:CZ	1:T:1077:VAL:HG21	2.44	0.53
1:T:1135:ASP:O	1:T:1140:ASN:ND2	2.42	0.53
1:B:1248:CYS:O	1:B:1256:ARG:HD3	2.07	0.53
1:D:1021:VAL:HG21	1:D:1066:LEU:HB3	1.90	0.53
1:E:998:LYS:HD3	1:E:1019:LYS:O	2.08	0.53
1:J:1177:ARG:HB2	1:J:1178:TRP:CZ3	2.44	0.53
1:M:1121:ASP:HA	1:M:1263:ILE:HD11	1.90	0.53
1:C:1181:PRO:HG3	1:C:1225:VAL:HG12	1.91	0.53
1:C:1275:ARG:HA	1:C:1281:TYR:HD1	1.73	0.53
1:J:1088:LYS:HE3	1:J:1092:ARG:NH1	2.21	0.53
1:J:1133:HIS:HA	1:J:1157:THR:HB	1.91	0.53
1:M:1130:LYS:NZ	1:M:1164:ASP:OD1	2.42	0.53
1:T:1161:PTR:O	1:T:1162:GLU:CB	2.55	0.53
1:I:1114:GLN:O	1:I:1118:GLU:HG3	2.08	0.53
1:S:1127:ASN:ND2	1:S:1127:ASN:N	2.56	0.53
1:H:1054:MET:HE1	1:H:1154:PHE:HD1	1.73	0.53
1:J:1243:GLU:OE2	1:J:1246:ARG:NH1	2.38	0.53
2:S:15:741:C18	2:S:15:741:C32	2.86	0.53
1:F:1030:VAL:CA	1:F:1081:LEU:HB2	2.39	0.53
1:G:1154:PHE:HB3	1:G:1157:THR:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1022:VAL:HG21	1:I:1028:THR:HG21	1.90	0.53
1:J:1010:PHE:H	1:J:1033:LYS:HZ1	1.57	0.53
1:L:1132:VAL:HG12	1:L:1134:ARG:HG3	1.91	0.53
1:M:1243:GLU:O	1:M:1247:MET:HG3	2.09	0.53
1:A:1015:GLU:HG2	1:A:1016:GLY:N	2.24	0.53
1:A:1023:LYS:O	1:A:1024:ASP:HB2	2.08	0.53
1:B:1023:LYS:N	1:B:1023:LYS:HD2	2.23	0.53
1:K:990:ASP:O	1:K:991:GLU:HB2	2.07	0.53
1:L:1082:MET:O	2:L:13:741:H3	2.09	0.53
1:M:1119:ILE:HG23	1:M:1151:ILE:HD11	1.91	0.53
1:R:1235:ASP:O	1:R:1236:ASN:HB2	2.08	0.53
1:S:1061:HIS:CD2	1:S:1118:GLU:HB3	2.44	0.53
1:J:1257:PRO:HD3	1:S:987:TYR:OH	2.08	0.53
1:A:1203:TRP:O	1:A:1207:THR:HG23	2.08	0.52
1:B:1229:GLY:O	1:B:1230:LEU:HD23	2.07	0.52
1:D:1084:ARG:NH1	1:D:1084:ARG:CG	2.68	0.52
1:H:1069:VAL:HB	1:H:1076:LEU:HB2	1.91	0.52
1:M:1023:LYS:O	1:M:1025:GLU:HB2	2.09	0.52
1:S:1081:LEU:HD22	1:S:1082:MET:N	2.24	0.52
1:T:1010:PHE:HD1	1:T:1047:PHE:HD1	1.56	0.52
1:I:992:TRP:CD1	1:I:1055:LYS:HE2	2.44	0.52
1:J:1134:ARG:HG2	1:J:1189:PHE:CD2	2.44	0.52
1:M:1058:ASN:ND2	1:M:1064:ARG:NH2	2.42	0.52
1:T:1087:LEU:HB3	1:T:1138:ALA:O	2.09	0.52
1:A:1058:ASN:ND2	1:A:1064:ARG:HH22	2.06	0.52
1:F:1065:LEU:HD23	1:F:1067:GLY:N	2.24	0.52
1:H:1047:PHE:HD2	1:H:1047:PHE:O	1.92	0.52
1:I:1051:ALA:O	1:I:1054:MET:HB2	2.09	0.52
1:I:989:PRO:CD	1:I:1055:LYS:HZ1	2.23	0.52
1:K:1166:PTR:O2P	1:K:1166:PTR:HE1	2.09	0.52
1:M:1036:ASN:ND2	1:M:1036:ASN:H	2.02	0.52
1:F:1162:GLU:O	1:F:1163:THR:OG1	2.25	0.52
1:M:1113:ILE:HD11	1:M:1240:MET:SD	2.49	0.52
1:R:988:VAL:O	1:R:988:VAL:HG23	2.08	0.52
1:A:1092:ARG:CZ	1:A:1095:ARG:HH11	2.21	0.52
1:A:1114:GLN:O	1:A:1118:GLU:HG3	2.09	0.52
1:J:1207:THR:HB	1:J:1210:GLU:HG3	1.91	0.52
1:A:1026:PRO:HD2	1:A:1027:GLU:H	1.74	0.52
1:G:1095:ARG:NH1	1:G:1208:LEU:O	2.42	0.52
1:I:1112:MET:HE3	1:I:1205:ILE:HG22	1.90	0.52
1:L:1003:ARG:HG3	1:L:1003:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:VAL:HG23	1:A:1151:ILE:O	2.09	0.52
1:C:1010:PHE:CG	1:C:1047:PHE:CD1	2.93	0.52
1:D:1054:MET:O	1:D:1057:PHE:N	2.41	0.52
1:T:1023:LYS:HE2	1:T:1023:LYS:H	1.74	0.52
1:B:1058:ASN:C	1:B:1058:ASN:ND2	2.63	0.52
1:E:1223:ARG:HH11	1:E:1223:ARG:CG	2.20	0.52
1:F:1073:GLN:NE2	1:F:1073:GLN:HA	2.20	0.52
1:I:1047:PHE:CZ	1:I:1077:VAL:HG21	2.45	0.52
1:R:1161:PTR:HD1	1:R:1161:PTR:C	2.40	0.52
1:T:1092:ARG:O	1:T:1095:ARG:HG3	2.10	0.52
1:A:1007:GLN:OE1	1:A:1012:MET:HE3	2.10	0.52
1:A:1207:THR:OG1	1:A:1210:GLU:HB2	2.09	0.52
1:F:1135:ASP:O	1:F:1140:ASN:ND2	2.40	0.52
1:S:1082:MET:CE	1:S:1142:MET:HB2	2.39	0.52
1:D:1036:ASN:HD22	1:D:1036:ASN:C	2.13	0.52
1:I:999:ILE:CG2	1:I:1032:ILE:HD12	2.40	0.52
1:J:1065:LEU:HD23	1:J:1067:GLY:H	1.75	0.52
1:J:1139:ARG:HH22	1:J:1175:PRO:CG	2.23	0.52
1:M:1132:VAL:CG2	1:M:1160:ILE:HD13	2.40	0.52
1:T:1127:ASN:ND2	1:T:1191:THR:HG22	2.25	0.52
1:B:1112:MET:HE1	1:B:1206:ALA:HA	1.88	0.51
1:D:1233:LYS:NZ	1:D:1239:ASP:OD2	2.43	0.51
1:E:1109:LEU:HD22	1:E:1113:ILE:HG12	1.92	0.51
1:I:1184:LEU:HD22	1:I:1222:LEU:HD22	1.91	0.51
1:R:1069:VAL:HB	1:R:1076:LEU:HB2	1.91	0.51
1:S:1015:GLU:HG3	1:S:1016:GLY:H	1.76	0.51
1:B:1198:PHE:O	1:B:1201:VAL:HG13	2.09	0.51
1:D:1030:VAL:HG23	1:D:1032:ILE:HD11	1.93	0.51
1:G:1097:GLU:OE1	1:G:1097:GLU:C	2.49	0.51
1:I:1161:PTR:HD1	1:I:1162:GLU:H	1.70	0.51
1:J:1092:ARG:HG2	1:J:1092:ARG:HH11	1.75	0.51
1:L:1276:GLU:HG3	1:L:1277:VAL:HG13	1.92	0.51
1:M:1203:TRP:O	1:M:1207:THR:HG23	2.10	0.51
1:S:988:VAL:O	1:S:988:VAL:HG23	2.10	0.51
1:B:1084:ARG:CZ	1:B:1147:PHE:CZ	2.93	0.51
1:C:1040:SER:OG	1:C:1043:GLU:HG3	2.10	0.51
1:G:1109:LEU:HD22	1:G:1109:LEU:O	2.10	0.51
1:H:1010:PHE:H	1:H:1033:LYS:HZ1	1.58	0.51
1:M:1029:ARG:HB3	1:M:1081:LEU:HD12	1.92	0.51
1:T:982:SER:O	1:T:985:ASP:OD2	2.28	0.51
1:A:996:ARG:CZ	1:A:1074:PRO:HD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1047:PHE:CZ	1:B:1077:VAL:HG21	2.45	0.51
1:C:996:ARG:NH2	1:C:1074:PRO:HD2	2.26	0.51
1:I:1252:ASN:C	1:I:1254:LYS:CE	2.79	0.51
1:T:1065:LEU:HD23	1:T:1067:GLY:H	1.75	0.51
1:F:984:ALA:HA	1:F:1048:LEU:CD2	2.40	0.51
1:F:1066:LEU:HB2	1:F:1078:ILE:HG22	1.93	0.51
1:I:1215:GLY:C	1:I:1216:LEU:HD23	2.31	0.51
1:C:1224:PHE:CE1	1:C:1229:GLY:HA3	2.45	0.51
1:K:1060:HIS:O	1:K:1150:LYS:HE2	2.10	0.51
1:D:1109:LEU:HD22	1:D:1113:ILE:HG12	1.91	0.51
1:D:1215:GLY:O	1:D:1216:LEU:HD23	2.11	0.51
1:E:1166:PTR:HE1	1:E:1166:PTR:O2P	2.11	0.51
1:F:1092:ARG:HD3	1:F:1209:ALA:CB	2.34	0.51
1:F:1235:ASP:O	1:F:1236:ASN:CB	2.57	0.51
1:H:1035:VAL:CG2	1:H:1047:PHE:HE1	2.23	0.51
1:H:1073:GLN:CB	1:H:1074:PRO:HD3	2.40	0.51
1:B:1264:SER:HB2	1:B:1280:TYR:OH	2.11	0.51
1:D:1001:MET:HE3	1:D:1014:TYR:CG	2.46	0.51
1:D:1186:ASP:CB	1:D:1188:VAL:HG23	2.41	0.51
1:A:1276:GLU:OE1	1:R:1283:GLU:CG	2.57	0.51
1:B:1021:VAL:HG21	1:B:1066:LEU:HD13	1.93	0.51
1:C:1054:MET:O	1:C:1057:PHE:N	2.41	0.51
1:G:987:TYR:CE2	1:G:1045:ILE:HD13	2.45	0.51
1:J:1036:ASN:ND2	1:J:1037:GLU:N	2.59	0.51
1:R:1079:MET:HG3	2:R:14:741:N33	2.25	0.51
1:S:1054:MET:O	1:S:1055:LYS:C	2.49	0.51
1:C:1180:SER:HB2	1:C:1182:GLU:OE2	2.11	0.51
1:H:1139:ARG:NH2	1:H:1175:PRO:HG2	2.26	0.51
1:L:989:PRO:O	1:L:991:GLU:N	2.43	0.51
1:D:1084:ARG:HB2	1:D:1143:VAL:HB	1.92	0.50
1:E:1010:PHE:CG	1:E:1047:PHE:CD1	2.99	0.50
1:E:989:PRO:HG2	1:E:992:TRP:HD1	1.77	0.50
1:K:1275:ARG:HA	1:K:1281:TYR:HD1	1.75	0.50
1:R:1092:ARG:HG2	1:R:1209:ALA:HB3	1.93	0.50
1:S:1177:ARG:HG2	1:S:1213:TYR:HD2	1.75	0.50
1:S:1207:THR:CG2	1:S:1234:PRO:HB3	2.41	0.50
1:G:1027:GLU:OE2	1:S:1019:LYS:NZ	2.44	0.50
1:I:989:PRO:HD3	1:I:1055:LYS:HZ1	1.75	0.50
1:T:1058:ASN:C	1:T:1058:ASN:ND2	2.64	0.50
1:C:1241:LEU:O	1:C:1245:MET:HG3	2.11	0.50
1:D:1092:ARG:O	1:D:1095:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:741:C18	2:E:5:741:C32	2.89	0.50
1:K:1054:MET:O	1:K:1055:LYS:C	2.50	0.50
1:L:1134:ARG:HD3	1:L:1156:MET:O	2.11	0.50
1:S:1036:ASN:HD22	1:S:1036:ASN:N	2.09	0.50
1:T:1036:ASN:N	1:T:1036:ASN:HD22	2.09	0.50
1:T:995:ALA:HB1	1:T:997:GLU:OE1	2.12	0.50
1:C:1054:MET:O	1:C:1055:LYS:C	2.49	0.50
1:D:1037:GLU:C	1:D:1039:ALA:H	2.15	0.50
1:D:1060:HIS:O	1:D:1150:LYS:HE2	2.11	0.50
1:D:1112:MET:HG2	1:D:1205:ILE:HG21	1.92	0.50
1:F:1010:PHE:H	1:F:1033:LYS:HZ1	1.59	0.50
1:H:1079:MET:HG2	2:H:8:741:CL24	2.49	0.50
1:H:1095:ARG:HB3	1:H:1096:PRO:HD2	1.92	0.50
1:T:1235:ASP:O	1:T:1236:ASN:HB2	2.10	0.50
1:B:1107:PRO:HD2	1:B:1112:MET:HE3	1.92	0.50
1:E:1012:MET:CG	1:E:1014:TYR:CE2	2.93	0.50
1:E:989:PRO:C	1:E:991:GLU:H	2.15	0.50
1:F:1023:LYS:N	1:F:1023:LYS:HD3	2.18	0.50
1:G:1071:GLN:OE1	1:G:1071:GLN:HA	2.11	0.50
1:H:1112:MET:HG2	1:H:1205:ILE:HG22	1.92	0.50
1:C:1184:LEU:HD22	1:C:1222:LEU:HD22	1.91	0.50
1:E:989:PRO:O	1:E:991:GLU:N	2.45	0.50
1:T:1216:LEU:HD22	1:T:1220:GLN:HB3	1.94	0.50
1:A:1022:VAL:HG21	1:A:1028:THR:HG21	1.93	0.50
1:I:1062:VAL:HG13	1:I:1154:PHE:HZ	1.76	0.50
1:K:1042:ARG:HG2	1:K:1042:ARG:NH1	2.23	0.50
1:K:1035:VAL:HG21	1:K:1047:PHE:CE2	2.47	0.50
1:K:1154:PHE:HD2	1:K:1157:THR:HG21	1.77	0.50
1:R:1018:ALA:HB1	1:R:1021:VAL:HG11	1.92	0.50
1:R:1154:PHE:HD2	1:R:1157:THR:HG21	1.76	0.50
1:B:996:ARG:NH2	1:B:1072:GLY:HA3	2.26	0.50
1:B:1134:ARG:HD3	1:B:1156:MET:O	2.12	0.50
1:E:1012:MET:HG2	1:E:1014:TYR:CE2	2.47	0.50
1:F:1112:MET:HG2	1:F:1205:ILE:CG2	2.42	0.50
1:J:1080:GLU:OE1	1:J:1150:LYS:HE3	2.12	0.50
1:R:1184:LEU:HD22	1:R:1222:LEU:CD2	2.42	0.50
1:R:1275:ARG:HA	1:R:1281:TYR:CD1	2.45	0.50
1:T:1060:HIS:O	1:T:1150:LYS:CE	2.60	0.50
1:G:1161:PTR:O	1:G:1162:GLU:HB2	2.12	0.50
1:G:995:ALA:HB1	1:G:997:GLU:HG2	1.94	0.50
1:I:1139:ARG:NH2	1:I:1175:PRO:HG2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:989:PRO:CG	1:K:992:TRP:CD1	2.84	0.50
1:R:1092:ARG:O	1:R:1095:ARG:HG3	2.12	0.50
1:S:1132:VAL:HG23	1:S:1160:ILE:HD13	1.94	0.50
1:C:986:VAL:CG1	1:H:1247:MET:SD	3.00	0.49
1:K:1247:MET:SD	1:M:986:VAL:HG11	2.52	0.49
1:D:1036:ASN:HD22	1:D:1038:ALA:N	2.10	0.49
1:D:1168:LYS:HE2	1:D:1171:LYS:O	2.12	0.49
1:J:1109:LEU:HD22	1:J:1113:ILE:HG12	1.93	0.49
1:K:1161:PTR:O	1:K:1162:GLU:HB2	2.12	0.49
1:L:996:ARG:HH21	1:L:1072:GLY:HA3	1.76	0.49
1:M:1133:HIS:O	1:M:1134:ARG:HB2	2.12	0.49
1:S:1161:PTR:CD1	1:S:1162:GLU:HG3	2.42	0.49
1:B:1015:GLU:HG2	1:B:1016:GLY:N	2.27	0.49
1:C:1127:ASN:HB3	3:C:123:HOH:O	2.13	0.49
1:C:1247:MET:SD	1:D:986:VAL:HG11	2.51	0.49
1:E:996:ARG:HH12	1:E:1074:PRO:CD	2.25	0.49
1:F:1065:LEU:HD23	1:F:1067:GLY:H	1.77	0.49
1:G:1035:VAL:CG2	1:G:1047:PHE:CE2	2.95	0.49
1:H:996:ARG:NH2	1:H:1074:PRO:O	2.41	0.49
1:H:1161:PTR:HD1	1:H:1162:GLU:N	2.27	0.49
1:H:1127:ASN:OD1	1:H:1191:THR:HB	2.12	0.49
1:I:1161:PTR:O	1:I:1162:GLU:HB2	2.11	0.49
1:J:1259:PHE:O	1:J:1263:ILE:HG13	2.13	0.49
1:L:1161:PTR:CD1	1:L:1161:PTR:C	2.91	0.49
1:M:1022:VAL:CG1	1:M:1028:THR:OG1	2.60	0.49
1:M:1030:VAL:HG23	1:M:1032:ILE:CD1	2.43	0.49
1:M:984:ALA:HA	1:M:1048:LEU:HD21	1.94	0.49
1:R:987:TYR:CZ	1:R:1045:ILE:HD13	2.47	0.49
1:S:1058:ASN:ND2	1:S:1064:ARG:NH2	2.55	0.49
1:S:1244:LEU:HD21	1:S:1262:ILE:HG23	1.94	0.49
1:A:1234:PRO:HB2	1:A:1237:CYS:HB2	1.94	0.49
1:A:992:TRP:CZ2	1:A:1055:LYS:CB	2.94	0.49
1:E:989:PRO:C	1:E:991:GLU:N	2.66	0.49
1:G:1054:MET:CE	1:G:1154:PHE:HD1	2.25	0.49
1:G:1163:THR:O	1:G:1165:PTR:HD1	2.12	0.49
1:J:1029:ARG:HB3	1:J:1081:LEU:HD12	1.94	0.49
1:J:1146:ASP:O	1:J:1147:PHE:HB2	2.13	0.49
1:M:1112:MET:HG2	1:M:1205:ILE:CG2	2.42	0.49
1:R:1022:VAL:HG23	1:R:1028:THR:OG1	2.12	0.49
1:S:1058:ASN:HD22	1:S:1064:ARG:HH22	1.55	0.49
1:T:1165:PTR:CD2	1:T:1165:PTR:C	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1095:ARG:NH2	1:K:1210:GLU:HG3	2.28	0.49
1:S:1235:ASP:O	1:S:1236:ASN:HB2	2.12	0.49
1:G:1030:VAL:HG23	1:G:1032:ILE:HD11	1.94	0.49
1:I:1167:ARG:HH11	1:I:1167:ARG:HG3	1.77	0.49
1:I:1254:LYS:NZ	1:I:1255:MET:N	2.59	0.49
1:I:1275:ARG:HA	1:I:1281:TYR:HD1	1.77	0.49
1:J:1023:LYS:O	1:J:1024:ASP:HB2	2.13	0.49
1:L:1156:MET:HG2	1:L:1174:LEU:HD21	1.93	0.49
1:S:1216:LEU:HD22	1:S:1220:GLN:HB3	1.93	0.49
1:A:1007:GLN:HA	1:A:1012:MET:HE2	1.94	0.49
1:A:1044:ARG:O	1:A:1048:LEU:HD22	2.13	0.49
1:C:996:ARG:HH12	1:C:1074:PRO:CG	2.25	0.49
1:D:1092:ARG:NH2	1:D:1095:ARG:NH1	2.61	0.49
1:F:1112:MET:HG2	1:F:1205:ILE:HG22	1.94	0.49
1:G:1084:ARG:HB2	1:G:1143:VAL:HB	1.94	0.49
1:G:1275:ARG:HA	1:G:1281:TYR:CD1	2.48	0.49
1:H:1106:PRO:HB2	1:H:1112:MET:HE1	1.94	0.49
1:H:1236:ASN:HA	1:R:1038:ALA:HB3	1.94	0.49
1:I:1142:MET:HE1	2:I:9:741:C4	2.43	0.49
1:K:1163:THR:O	1:K:1164:ASP:HB2	2.13	0.49
1:M:1054:MET:O	1:M:1055:LYS:C	2.51	0.49
1:H:1268:GLU:OE2	1:H:1268:GLU:HA	2.13	0.49
1:S:999:ILE:CG2	1:S:1032:ILE:HD13	2.43	0.49
1:F:1139:ARG:HH22	1:F:1175:PRO:HG2	1.78	0.49
1:H:994:VAL:O	1:H:1069:VAL:HG13	2.13	0.49
1:I:1010:PHE:CD2	1:I:1047:PHE:HB2	2.47	0.49
1:K:1252:ASN:C	1:K:1252:ASN:OD1	2.51	0.49
1:M:1166:PTR:OH	1:M:1168:LYS:NZ	2.42	0.49
1:A:1134:ARG:HD3	1:A:1156:MET:O	2.12	0.49
1:E:1073:GLN:HA	1:E:1073:GLN:HE21	1.77	0.49
1:H:1115:MET:HG2	1:H:1149:VAL:CG2	2.42	0.49
1:J:1036:ASN:C	1:J:1036:ASN:HD22	2.15	0.49
1:L:1095:ARG:HH22	1:L:1210:GLU:HG2	1.77	0.49
1:L:1161:PTR:HE1	1:L:1162:GLU:OE1	2.12	0.49
1:S:1015:GLU:CG	1:S:1016:GLY:N	2.76	0.49
1:I:987:TYR:OH	1:T:1257:PRO:HD3	2.13	0.49
1:M:1036:ASN:ND2	1:M:1036:ASN:N	2.60	0.48
1:R:1042:ARG:CG	1:R:1042:ARG:NH1	2.68	0.48
1:R:1064:ARG:HG2	3:R:81:HOH:O	2.12	0.48
1:S:1002:SER:OG	1:S:1003:ARG:N	2.45	0.48
1:S:986:VAL:HG22	1:S:987:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1034:THR:HG22	1:D:1076:LEU:CD2	2.42	0.48
1:F:1021:VAL:HG22	1:F:1022:VAL:HG12	1.95	0.48
1:F:1043:GLU:OE1	1:F:1043:GLU:N	2.42	0.48
1:F:1195:VAL:O	1:F:1198:PHE:HB3	2.13	0.48
1:G:1082:MET:CE	1:G:1150:LYS:HD2	2.43	0.48
1:I:1258:SER:O	1:I:1262:ILE:HG13	2.13	0.48
1:K:1119:ILE:HG23	1:K:1151:ILE:HD11	1.95	0.48
1:K:1114:GLN:OE1	1:K:1271:GLU:HG2	2.13	0.48
1:R:1115:MET:HG2	1:R:1149:VAL:HG21	1.94	0.48
1:R:1139:ARG:NH2	1:R:1175:PRO:HG2	2.28	0.48
1:S:1163:THR:HG23	1:S:1165:PTR:CE1	2.43	0.48
1:A:996:ARG:NH2	1:A:1074:PRO:O	2.37	0.48
1:B:1037:GLU:C	1:B:1039:ALA:H	2.15	0.48
1:D:1092:ARG:HG2	1:D:1209:ALA:HB3	1.95	0.48
1:L:1030:VAL:HG12	1:L:1066:LEU:HD12	1.96	0.48
1:L:991:GLU:HG2	1:L:991:GLU:H	1.48	0.48
1:A:1044:ARG:O	1:A:1048:LEU:CD2	2.61	0.48
1:E:1185:LYS:HG3	1:E:1226:MET:CE	2.43	0.48
1:L:1133:HIS:O	1:L:1134:ARG:HB2	2.13	0.48
1:S:1184:LEU:HD13	1:S:1222:LEU:HD22	1.94	0.48
1:S:1257:PRO:HA	1:S:1261:GLU:OE1	2.13	0.48
1:D:989:PRO:O	1:D:991:GLU:N	2.44	0.48
1:E:1036:ASN:ND2	1:E:1038:ALA:HB3	2.25	0.48
1:G:1037:GLU:C	1:G:1039:ALA:H	2.16	0.48
1:L:984:ALA:O	1:L:988:VAL:HG22	2.13	0.48
1:S:1195:VAL:O	1:S:1198:PHE:HB3	2.13	0.48
1:B:1018:ALA:HB1	1:B:1021:VAL:CG1	2.40	0.48
1:B:1161:PTR:O	1:B:1162:GLU:HB2	2.12	0.48
1:D:1112:MET:HE1	1:D:1206:ALA:CA	2.42	0.48
1:D:1250:GLN:HE21	1:D:1250:GLN:CA	2.13	0.48
1:G:1134:ARG:HD3	1:G:1156:MET:O	2.13	0.48
1:J:1036:ASN:HD22	1:J:1037:GLU:N	2.12	0.48
1:K:1151:ILE:HG22	1:K:1154:PHE:CZ	2.49	0.48
1:S:1222:LEU:O	1:S:1226:MET:HB2	2.13	0.48
1:A:1112:MET:CE	1:A:1206:ALA:CA	2.87	0.48
1:A:1270:MET:HE2	1:A:1274:PHE:CD1	2.48	0.48
1:B:1273:GLY:O	1:B:1276:GLU:CG	2.62	0.48
1:F:1022:VAL:HA	3:F:114:HOH:O	2.13	0.48
1:M:996:ARG:HH22	1:M:1074:PRO:C	2.17	0.48
1:T:994:VAL:O	1:T:1069:VAL:HG22	2.14	0.48
1:D:1153:ASP:OD1	1:D:1153:ASP:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1012:MET:HG2	1:E:1014:TYR:HE2	1.78	0.48
1:H:1047:PHE:CD2	1:H:1047:PHE:O	2.66	0.48
1:J:1109:LEU:O	1:J:1113:ILE:HG12	2.13	0.48
2:K:11:741:C18	2:K:11:741:C32	2.92	0.48
1:L:1084:ARG:HB2	1:L:1143:VAL:HB	1.96	0.48
1:L:1154:PHE:HD2	1:L:1157:THR:HG21	1.79	0.48
1:S:1004:GLU:HG3	1:S:1014:TYR:CE1	2.48	0.48
1:T:1082:MET:CE	1:T:1142:MET:HB2	2.44	0.48
1:A:1151:ILE:N	1:A:1151:ILE:CD1	2.77	0.48
1:D:1139:ARG:NH2	1:D:1175:PRO:HG3	2.28	0.48
1:D:1199:GLY:O	1:D:1202:LEU:HB2	2.13	0.48
1:H:1032:ILE:HD13	1:H:1078:ILE:HD12	1.95	0.48
1:I:1203:TRP:O	1:I:1207:THR:HG23	2.13	0.48
1:K:1204:GLU:O	1:K:1209:ALA:N	2.47	0.48
1:K:1217:SER:O	1:K:1220:GLN:N	2.47	0.48
1:H:1104:LEU:O	1:R:1007:GLN:NE2	2.47	0.48
1:S:1154:PHE:HD2	1:S:1157:THR:HG21	1.79	0.48
1:A:1026:PRO:CD	1:A:1027:GLU:H	2.27	0.48
1:F:1032:ILE:CD1	1:F:1078:ILE:HG13	2.43	0.48
1:I:1248:CYS:O	1:I:1256:ARG:HD3	2.14	0.48
1:J:1047:PHE:CZ	1:J:1077:VAL:HG21	2.49	0.48
1:J:1113:ILE:HD11	1:J:1240:MET:SD	2.54	0.48
1:J:1177:ARG:HB2	1:J:1178:TRP:CE3	2.49	0.48
1:J:1196:TRP:CE3	1:J:1249:TRP:HA	2.49	0.48
1:L:1003:ARG:NH1	1:L:1003:ARG:CG	2.70	0.48
1:I:987:TYR:CZ	1:I:1045:ILE:HD13	2.49	0.47
2:J:10:741:C32	2:J:10:741:C18	2.92	0.47
1:J:1157:THR:HG22	3:J:13:HOH:O	2.12	0.47
1:K:1113:ILE:HG21	1:K:1269:GLU:HB3	1.96	0.47
1:F:1207:THR:OG1	1:F:1210:GLU:HB2	2.14	0.47
1:R:1022:VAL:HG21	1:R:1028:THR:HG21	1.95	0.47
1:S:1252:ASN:HB3	1:S:1255:MET:HG3	1.94	0.47
1:B:1080:GLU:O	2:B:2:741:H8	2.13	0.47
1:C:1250:GLN:HA	1:C:1250:GLN:NE2	2.29	0.47
1:D:1112:MET:CE	1:D:1206:ALA:CA	2.84	0.47
2:I:9:741:O38	2:I:9:741:C36	2.59	0.47
1:J:1092:ARG:CD	1:J:1095:ARG:HH11	2.27	0.47
1:E:1125:TYR:HD1	1:E:1279:PHE:CD1	2.31	0.47
1:T:992:TRP:CE3	1:T:1065:LEU:HD22	2.49	0.47
1:A:1058:ASN:ND2	1:A:1058:ASN:C	2.65	0.47
1:C:987:TYR:CE2	1:C:1045:ILE:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1044:ARG:HH11	1:D:1044:ARG:CB	2.27	0.47
1:F:1009:SER:OG	2:F:6:741:H28	2.15	0.47
1:K:1207:THR:O	1:K:1208:LEU:HB2	2.13	0.47
1:R:1023:LYS:H	1:R:1023:LYS:CE	2.27	0.47
1:R:995:ALA:HB1	1:R:997:GLU:HG2	1.97	0.47
1:S:1081:LEU:HD22	1:S:1082:MET:H	1.78	0.47
1:T:1154:PHE:HA	1:T:1157:THR:HG23	1.96	0.47
1:A:1065:LEU:HD23	1:A:1067:GLY:N	2.29	0.47
1:B:1084:ARG:NH2	1:B:1147:PHE:CE2	2.83	0.47
1:C:1123:MET:HB3	1:C:1259:PHE:CE2	2.50	0.47
1:E:1065:LEU:HA	1:E:1079:MET:SD	2.55	0.47
1:E:1154:PHE:O	1:E:1157:THR:HG23	2.14	0.47
1:F:1030:VAL:HA	1:F:1081:LEU:HB2	1.95	0.47
1:G:1177:ARG:NH1	1:G:1221:VAL:HG21	2.29	0.47
1:G:1185:LYS:HG3	1:G:1226:MET:CE	2.45	0.47
2:G:7:741:O12	2:G:7:741:H16B	2.14	0.47
2:R:14:741:H36	2:R:14:741:H37	1.62	0.47
1:A:1078:ILE:N	1:A:1078:ILE:HD12	2.30	0.47
1:D:1207:THR:HG22	1:D:1234:PRO:HB3	1.97	0.47
1:G:1252:ASN:ND2	1:G:1255:MET:HG2	2.29	0.47
1:H:1097:GLU:OE2	1:H:1097:GLU:CA	2.62	0.47
1:I:1035:VAL:HG21	1:I:1047:PHE:CD2	2.50	0.47
1:I:1108:SER:O	1:I:1112:MET:HG3	2.14	0.47
1:J:1217:SER:O	1:J:1218:ASN:C	2.51	0.47
1:L:992:TRP:CZ2	1:L:1055:LYS:CB	2.97	0.47
1:L:1107:PRO:HD3	1:L:1208:LEU:HD21	1.97	0.47
1:L:1243:GLU:O	1:L:1247:MET:HG3	2.14	0.47
1:B:1021:VAL:HG22	1:B:1022:VAL:N	2.30	0.47
1:B:1242:PHE:CE2	1:B:1246:ARG:HD2	2.49	0.47
1:C:1047:PHE:CE2	1:C:1077:VAL:HG21	2.49	0.47
1:E:1082:MET:O	2:E:5:741:H3	2.14	0.47
1:F:1216:LEU:HA	1:F:1220:GLN:OE1	2.14	0.47
1:I:1003:ARG:HD2	1:I:1003:ARG:H	1.80	0.47
1:M:1041:MET:O	1:M:1045:ILE:HG13	2.15	0.47
1:S:996:ARG:NH2	1:S:1072:GLY:HA3	2.28	0.47
1:S:993:GLU:HG3	1:S:1070:SER:OG	2.15	0.47
1:A:1112:MET:HG2	1:A:1205:ILE:CG2	2.45	0.47
1:D:1258:SER:O	1:D:1262:ILE:HG13	2.15	0.47
1:E:1012:MET:HE2	1:E:1012:MET:HB2	1.79	0.47
1:I:1167:ARG:CG	1:I:1167:ARG:NH1	2.78	0.47
1:B:999:ILE:HG12	1:B:1078:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1104:LEU:CD1	1:F:1208:LEU:HD12	2.45	0.47
1:J:1207:THR:HG22	1:J:1234:PRO:HB3	1.95	0.47
1:K:1133:HIS:O	1:K:1134:ARG:HB2	2.14	0.47
1:T:1009:SER:OG	1:T:1033:LYS:NZ	2.47	0.47
1:L:1061:HIS:HA	1:L:1150:LYS:HG2	1.97	0.47
1:S:1034:THR:HG22	1:S:1076:LEU:CD2	2.46	0.47
1:B:1166:PTR:OH	1:B:1168:LYS:CD	2.63	0.46
1:C:1084:ARG:CZ	1:C:1147:PHE:CZ	2.98	0.46
1:E:1195:VAL:O	1:E:1198:PHE:HB3	2.16	0.46
1:F:1121:ASP:HA	1:F:1263:ILE:HD11	1.96	0.46
1:F:1167:ARG:HA	1:F:1187:GLY:O	2.14	0.46
1:H:1044:ARG:HG2	1:H:1048:LEU:CD2	2.45	0.46
1:S:1092:ARG:HG2	1:S:1209:ALA:HB3	1.97	0.46
1:C:1087:LEU:HB3	1:C:1138:ALA:O	2.14	0.46
1:F:1096:PRO:O	1:F:1097:GLU:C	2.54	0.46
1:H:1121:ASP:HA	1:H:1263:ILE:HD11	1.96	0.46
1:I:1159:ASP:OD1	1:I:1160:ILE:N	2.48	0.46
1:S:1161:PTR:C	1:S:1161:PTR:CD1	2.93	0.46
1:T:989:PRO:O	1:T:990:ASP:C	2.52	0.46
1:A:1130:LYS:HA	1:A:1130:LYS:HD2	1.67	0.46
1:A:1285:ASN:O	1:A:1286:LYS:HB2	2.15	0.46
1:E:1215:GLY:C	1:E:1216:LEU:HD23	2.36	0.46
1:G:1034:THR:HG22	1:G:1076:LEU:HD22	1.97	0.46
1:G:1121:ASP:HA	1:G:1263:ILE:HD11	1.97	0.46
1:J:1051:ALA:O	1:J:1054:MET:HB2	2.16	0.46
1:K:1132:VAL:CG2	1:K:1160:ILE:HD13	2.43	0.46
1:K:1222:LEU:C	1:K:1222:LEU:HD12	2.36	0.46
1:R:1157:THR:HG23	3:R:29:HOH:O	2.15	0.46
1:R:1107:PRO:HG3	1:R:1208:LEU:HD21	1.96	0.46
1:B:1105:ALA:HB3	1:J:1007:GLN:HE21	1.79	0.46
2:C:3:741:C18	2:C:3:741:C32	2.94	0.46
1:D:1001:MET:CE	1:D:1014:TYR:CG	2.99	0.46
1:E:1012:MET:HG3	1:E:1014:TYR:CE2	2.50	0.46
1:E:1060:HIS:CD2	1:E:1277:VAL:HB	2.50	0.46
1:G:1133:HIS:HA	1:G:1157:THR:HB	1.97	0.46
1:I:1095:ARG:HB3	1:I:1096:PRO:HD2	1.97	0.46
1:I:1154:PHE:O	1:I:1157:THR:HG23	2.14	0.46
1:L:1146:ASP:O	1:L:1147:PHE:HB2	2.16	0.46
1:S:1023:LYS:H	1:S:1023:LYS:HD3	1.76	0.46
1:T:1036:ASN:H	1:T:1036:ASN:HD22	1.63	0.46
1:T:1132:VAL:HG23	1:T:1160:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1285:ASN:O	1:T:1286:LYS:HG3	2.15	0.46
1:A:1044:ARG:HB2	1:A:1044:ARG:NH1	2.28	0.46
1:A:1166:PTR:O2P	1:A:1166:PTR:HE1	2.16	0.46
1:C:1079:MET:HE2	1:C:1079:MET:HB3	1.71	0.46
1:C:1134:ARG:HD3	1:C:1156:MET:O	2.14	0.46
1:D:1285:ASN:O	1:D:1286:LYS:HG3	2.16	0.46
1:E:1012:MET:CG	1:E:1014:TYR:HE2	2.27	0.46
1:E:1058:ASN:C	1:E:1058:ASN:ND2	2.66	0.46
1:F:1023:LYS:N	1:F:1023:LYS:CD	2.77	0.46
2:H:8:741:H36	2:H:8:741:H37A	1.59	0.46
1:L:1207:THR:HG22	1:L:1234:PRO:HB3	1.98	0.46
1:M:1106:PRO:HA	1:M:1107:PRO:HA	1.55	0.46
1:M:1207:THR:HG22	1:M:1234:PRO:HB3	1.97	0.46
1:R:992:TRP:CZ2	1:R:1055:LYS:CB	2.98	0.46
2:D:4:741:H37	2:D:4:741:H36	1.47	0.46
1:E:1005:LEU:HD11	1:E:1015:GLU:HB2	1.98	0.46
1:J:1137:ALA:CB	3:J:8:HOH:O	2.63	0.46
1:M:1275:ARG:HA	1:M:1281:TYR:CD1	2.51	0.46
1:S:1161:PTR:HE1	1:S:1162:GLU:HG3	1.98	0.46
1:A:1109:LEU:HD22	1:A:1109:LEU:O	2.16	0.46
1:D:1061:HIS:HA	1:D:1150:LYS:HG2	1.97	0.46
1:E:1042:ARG:HH22	1:E:1046:GLU:HG3	1.81	0.46
1:G:1202:LEU:HD11	1:G:1244:LEU:HD13	1.96	0.46
1:H:1032:ILE:HD12	1:H:1078:ILE:HD12	1.98	0.46
1:H:1276:GLU:HG3	1:H:1277:VAL:HG13	1.98	0.46
1:I:1083:THR:O	2:I:9:741:H15A	2.15	0.46
1:J:1133:HIS:O	1:J:1134:ARG:HB2	2.14	0.46
1:R:1223:ARG:O	1:R:1227:GLU:HG3	2.15	0.46
1:T:1082:MET:HE2	1:T:1142:MET:HB2	1.98	0.46
1:A:989:PRO:C	1:A:991:GLU:H	2.18	0.46
1:D:1275:ARG:HA	1:D:1281:TYR:CD1	2.51	0.46
1:F:1095:ARG:HH21	1:F:1104:LEU:HD21	1.79	0.46
1:G:1132:VAL:HG23	1:G:1160:ILE:HD13	1.97	0.46
1:K:1024:ASP:N	1:K:1024:ASP:OD2	2.49	0.46
1:M:1082:MET:HE2	1:M:1142:MET:HB2	1.98	0.46
1:S:1069:VAL:HB	1:S:1076:LEU:HB2	1.96	0.46
2:B:2:741:C32	2:B:2:741:C18	2.94	0.46
1:I:1127:ASN:OD1	1:I:1191:THR:HB	2.16	0.46
1:I:1254:LYS:NZ	1:I:1255:MET:CG	2.74	0.46
1:J:1207:THR:CG2	1:J:1234:PRO:HB3	2.45	0.46
1:K:1042:ARG:NH1	1:K:1042:ARG:CG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1222:LEU:HD12	1:M:1226:MET:SD	2.56	0.46
1:T:1283:GLU:OE2	1:T:1283:GLU:HA	2.16	0.46
1:B:989:PRO:C	1:B:991:GLU:H	2.19	0.46
1:F:1022:VAL:CG1	1:F:1028:THR:OG1	2.64	0.46
1:H:1114:GLN:O	1:H:1118:GLU:HG3	2.16	0.46
1:I:989:PRO:CG	1:I:1055:LYS:HZ3	2.29	0.46
1:L:1002:SER:OG	1:L:1003:ARG:N	2.48	0.46
1:R:1033:LYS:CB	2:R:14:741:CL24	2.99	0.46
1:A:1092:ARG:CZ	1:A:1095:ARG:NH1	2.79	0.45
1:A:1132:VAL:CG2	1:A:1160:ILE:HG21	2.46	0.45
1:A:1133:HIS:O	1:A:1134:ARG:HB2	2.16	0.45
1:C:1207:THR:HB	1:C:1210:GLU:HG3	1.99	0.45
1:G:1119:ILE:HG23	1:G:1151:ILE:HD11	1.98	0.45
1:I:1162:GLU:O	1:I:1163:THR:CB	2.64	0.45
1:I:1207:THR:HG22	1:I:1234:PRO:HB3	1.97	0.45
1:J:1134:ARG:NH1	1:J:1156:MET:HG3	2.31	0.45
1:R:1201:VAL:O	1:R:1205:ILE:HG13	2.16	0.45
1:S:1201:VAL:O	1:S:1205:ILE:HG13	2.16	0.45
1:T:988:VAL:CG1	1:T:1048:LEU:HD12	2.46	0.45
1:C:1010:PHE:HB2	1:C:1047:PHE:CD1	2.52	0.45
1:C:1242:PHE:O	1:C:1246:ARG:HG3	2.16	0.45
1:E:996:ARG:HH22	1:E:1074:PRO:C	2.20	0.45
1:G:1161:PTR:O	1:G:1162:GLU:CB	2.63	0.45
1:G:1162:GLU:O	1:G:1163:THR:CB	2.64	0.45
1:B:1236:ASN:HA	1:J:1038:ALA:CB	2.46	0.45
1:M:1044:ARG:NH1	1:M:1044:ARG:HB2	2.30	0.45
1:R:1049:ASN:HA	1:R:1049:ASN:HD22	1.63	0.45
1:S:1060:HIS:O	1:S:1150:LYS:HE2	2.16	0.45
1:B:1021:VAL:CG2	1:B:1022:VAL:N	2.77	0.45
1:B:1018:ALA:HB2	1:B:1030:VAL:HG21	1.98	0.45
1:C:1132:VAL:CG2	1:C:1160:ILE:HG21	2.47	0.45
1:C:1168:LYS:HE2	1:C:1171:LYS:O	2.16	0.45
1:H:1156:MET:HG2	1:H:1174:LEU:HD21	1.98	0.45
1:I:1275:ARG:HB2	1:I:1275:ARG:HE	1.50	0.45
1:K:1234:PRO:HB2	1:K:1237:CYS:HB2	1.96	0.45
1:M:1154:PHE:HD2	1:M:1157:THR:HG21	1.82	0.45
1:R:1112:MET:HE1	1:R:1206:ALA:HA	1.96	0.45
1:R:999:ILE:HG23	1:R:1032:ILE:CD1	2.47	0.45
2:S:15:741:H14A	2:S:15:741:H36B	1.51	0.45
1:G:1032:ILE:HD12	1:G:1078:ILE:HG13	1.99	0.45
1:L:1229:GLY:O	1:L:1230:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1236:ASN:HD22	1:S:1236:ASN:N	2.12	0.45
1:A:1151:ILE:HG22	1:A:1154:PHE:CZ	2.51	0.45
1:C:1064:ARG:O	1:C:1079:MET:HE3	2.16	0.45
1:C:999:ILE:HG12	1:C:1078:ILE:CD1	2.43	0.45
1:K:996:ARG:HE	1:K:1072:GLY:HA3	1.82	0.45
1:L:1162:GLU:O	1:L:1163:THR:OG1	2.30	0.45
1:M:1035:VAL:HG21	1:M:1047:PHE:CE2	2.51	0.45
1:M:1082:MET:HB2	1:M:1142:MET:CE	2.47	0.45
1:M:1112:MET:HE2	1:M:1206:ALA:HA	1.98	0.45
1:M:1254:LYS:HB2	1:M:1254:LYS:HE3	1.47	0.45
1:R:994:VAL:O	1:R:1069:VAL:HG22	2.16	0.45
1:C:1059:CYS:HB2	1:C:1125:TYR:CD2	2.51	0.45
1:D:1201:VAL:O	1:D:1205:ILE:HG13	2.17	0.45
1:E:1087:LEU:HB3	1:E:1138:ALA:O	2.17	0.45
1:E:1259:PHE:O	1:E:1263:ILE:HG13	2.17	0.45
1:G:994:VAL:HG22	1:G:1069:VAL:HG22	1.98	0.45
1:I:1252:ASN:CG	1:I:1254:LYS:CE	2.80	0.45
1:K:1114:GLN:CD	1:K:1271:GLU:HG2	2.37	0.45
1:K:996:ARG:CZ	1:K:1074:PRO:HD2	2.47	0.45
1:R:1058:ASN:HD21	1:R:1064:ARG:NH2	2.14	0.45
1:T:1022:VAL:CA	1:T:1023:LYS:HE2	2.47	0.45
1:C:1256:ARG:HB3	1:C:1257:PRO:HD2	1.99	0.45
1:I:1064:ARG:HG3	1:I:1065:LEU:N	2.30	0.45
1:L:1082:MET:HE2	1:L:1142:MET:HB2	1.97	0.45
2:M:12:741:C18	2:M:12:741:C32	2.94	0.45
1:R:1037:GLU:C	1:R:1039:ALA:H	2.19	0.45
1:S:1048:LEU:HA	1:S:1048:LEU:HD12	1.86	0.45
1:S:1275:ARG:HA	1:S:1281:TYR:CD1	2.52	0.45
1:G:992:TRP:CH2	1:G:1055:LYS:HB2	2.50	0.45
1:G:1096:PRO:O	1:G:1097:GLU:CB	2.65	0.45
1:I:996:ARG:HH21	1:I:1072:GLY:HA3	1.81	0.45
1:J:1121:ASP:HA	1:J:1263:ILE:HD11	1.98	0.45
1:M:992:TRP:CZ2	1:M:1055:LYS:CB	3.00	0.45
1:R:1022:VAL:CG2	1:R:1028:THR:HG21	2.47	0.45
1:E:1123:MET:HB3	1:E:1259:PHE:CE2	2.51	0.45
1:F:1009:SER:N	1:F:1033:LYS:NZ	2.64	0.45
1:L:1241:LEU:HD12	1:L:1241:LEU:HA	1.84	0.45
1:S:1047:PHE:CZ	1:S:1077:VAL:CG2	3.00	0.45
1:T:1057:PHE:HB3	1:T:1125:TYR:HE2	1.81	0.45
1:D:1154:PHE:HA	1:D:1157:THR:HG23	1.98	0.45
1:E:1039:ALA:O	1:E:1044:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:741:C32	2:E:5:741:C23	2.95	0.45
1:G:1247:MET:SD	1:H:986:VAL:CG1	3.04	0.45
1:I:992:TRP:NE1	1:I:1055:LYS:HE2	2.31	0.45
1:I:1254:LYS:HZ2	1:I:1255:MET:CB	2.29	0.45
1:L:989:PRO:C	1:L:991:GLU:N	2.71	0.45
1:T:1107:PRO:HB2	1:T:1112:MET:CG	2.47	0.45
1:D:1132:VAL:HG23	1:D:1160:ILE:HD13	1.99	0.44
1:E:1158:ARG:HG3	1:E:1166:PTR:CE1	2.47	0.44
1:F:1234:PRO:HB2	1:F:1237:CYS:HB2	1.98	0.44
1:F:1114:GLN:CD	1:F:1271:GLU:HG2	2.38	0.44
1:G:1146:ASP:O	1:G:1147:PHE:HB2	2.17	0.44
1:H:1201:VAL:HA	1:H:1204:GLU:HB2	1.99	0.44
1:R:1023:LYS:O	1:R:1025:GLU:HG3	2.17	0.44
1:B:996:ARG:HH21	1:B:1072:GLY:HA3	1.82	0.44
2:F:6:741:C32	2:F:6:741:C18	2.95	0.44
1:G:1250:GLN:HB2	1:G:1256:ARG:HG2	1.99	0.44
1:I:1135:ASP:O	1:I:1140:ASN:ND2	2.49	0.44
1:I:987:TYR:CE1	1:I:1045:ILE:HG23	2.53	0.44
1:J:1179:MET:HE2	1:J:1184:LEU:HD23	1.99	0.44
1:J:989:PRO:HG2	1:J:992:TRP:CD1	2.52	0.44
1:K:1012:MET:HG3	1:K:1013:VAL:N	2.32	0.44
1:L:1153:ASP:C	1:L:1153:ASP:OD1	2.55	0.44
1:T:1073:GLN:HB2	1:T:1074:PRO:HD3	1.99	0.44
1:T:1132:VAL:CG2	1:T:1160:ILE:HD13	2.47	0.44
1:T:1184:LEU:HD22	1:T:1222:LEU:CD2	2.42	0.44
1:A:1025:GLU:HA	1:A:1026:PRO:HD3	1.87	0.44
1:B:1112:MET:HE2	1:B:1206:ALA:CA	2.42	0.44
1:E:1215:GLY:O	1:E:1216:LEU:HD23	2.17	0.44
1:F:996:ARG:CZ	1:F:1074:PRO:HD2	2.46	0.44
1:J:1132:VAL:O	1:J:1157:THR:HB	2.17	0.44
1:R:1035:VAL:HG21	1:R:1047:PHE:CE2	2.53	0.44
1:R:1062:VAL:HG13	1:R:1154:PHE:HZ	1.81	0.44
1:C:1065:LEU:HD23	1:C:1067:GLY:H	1.81	0.44
1:C:1115:MET:O	1:C:1119:ILE:HG13	2.18	0.44
1:D:1264:SER:HA	1:D:1267:LYS:HD3	1.99	0.44
1:F:1023:LYS:HE3	1:F:1023:LYS:HB2	1.81	0.44
1:G:1030:VAL:CG2	1:G:1032:ILE:HD11	2.46	0.44
1:G:987:TYR:CZ	1:G:1045:ILE:HD13	2.53	0.44
1:R:1037:GLU:O	1:R:1039:ALA:N	2.50	0.44
1:R:1165:PTR:HE2	1:R:1165:PTR:O1P	2.17	0.44
1:S:1040:SER:OG	1:S:1043:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:GLN:OE1	1:A:1012:MET:CE	2.65	0.44
1:A:1186:ASP:CB	1:A:1188:VAL:HG23	2.43	0.44
1:D:1005:LEU:HD11	1:D:1015:GLU:HB2	1.99	0.44
1:E:1030:VAL:CG2	1:E:1032:ILE:HD11	2.47	0.44
1:E:1184:LEU:HD13	1:E:1222:LEU:HD13	2.00	0.44
1:F:1078:ILE:HD12	1:F:1078:ILE:N	2.32	0.44
1:G:1162:GLU:O	1:G:1163:THR:OG1	2.34	0.44
1:K:1154:PHE:HA	1:K:1157:THR:HG23	2.00	0.44
1:T:1109:LEU:HD22	1:T:1113:ILE:HG12	1.98	0.44
1:B:1018:ALA:O	1:B:1021:VAL:HG13	2.18	0.44
1:C:1060:HIS:CD2	1:C:1277:VAL:CG2	3.00	0.44
1:C:1201:VAL:O	1:C:1205:ILE:HG13	2.17	0.44
1:C:988:VAL:CG1	1:C:988:VAL:O	2.64	0.44
1:F:1039:ALA:O	1:F:1040:SER:O	2.36	0.44
1:G:1109:LEU:HD22	1:G:1113:ILE:HG12	1.98	0.44
1:I:1058:ASN:ND2	1:I:1058:ASN:C	2.71	0.44
1:R:1216:LEU:HD22	1:R:1220:GLN:HB3	1.99	0.44
1:S:1146:ASP:C	1:S:1146:ASP:OD1	2.55	0.44
1:C:1139:ARG:NH2	1:C:1175:PRO:HG2	2.33	0.44
1:C:1060:HIS:CD2	1:C:1277:VAL:HG21	2.53	0.44
1:C:989:PRO:O	1:C:991:GLU:N	2.51	0.44
1:D:1133:HIS:HA	1:D:1157:THR:HG22	2.00	0.44
1:E:1009:SER:N	1:E:1033:LYS:NZ	2.65	0.44
1:E:1015:GLU:HG2	1:E:1016:GLY:N	2.33	0.44
1:I:1087:LEU:O	1:I:1091:LEU:HG	2.18	0.44
1:J:1054:MET:O	1:J:1055:LYS:C	2.56	0.44
1:K:1029:ARG:HB3	1:K:1081:LEU:HD12	2.00	0.44
1:L:989:PRO:HG2	1:L:992:TRP:CD1	2.52	0.44
1:M:1233:LYS:HA	1:M:1234:PRO:HD3	1.87	0.44
1:A:1219:GLU:OE1	1:A:1223:ARG:NH2	2.49	0.44
1:F:1007:GLN:OE1	1:F:1012:MET:HE2	2.17	0.44
1:F:1112:MET:CE	1:F:1206:ALA:CA	2.90	0.44
1:I:1109:LEU:HD22	1:I:1109:LEU:O	2.18	0.44
1:J:1065:LEU:HD23	1:J:1067:GLY:N	2.32	0.44
1:K:1163:THR:HG22	1:K:1165:PTR:CE1	2.47	0.44
1:R:1207:THR:HG22	1:R:1234:PRO:HB3	1.98	0.44
1:S:1132:VAL:CG2	1:S:1160:ILE:HD13	2.47	0.44
1:S:1161:PTR:CE1	1:S:1162:GLU:HG3	2.48	0.44
1:T:1112:MET:HE1	1:T:1206:ALA:CA	2.45	0.44
1:B:1084:ARG:HG3	1:B:1144:ALA:O	2.18	0.44
1:B:1197:SER:O	1:B:1201:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:987:TYR:CZ	1:C:1045:ILE:HD13	2.53	0.44
1:C:1061:HIS:HA	1:C:1150:LYS:HG2	1.98	0.44
1:E:1058:ASN:ND2	1:E:1064:ARG:NH2	2.64	0.44
1:F:1030:VAL:CG1	1:F:1066:LEU:HD12	2.48	0.44
1:G:1069:VAL:HB	1:G:1076:LEU:HB2	1.99	0.44
1:H:1113:ILE:HD13	1:H:1113:ILE:HA	1.74	0.44
1:H:989:PRO:HB2	1:H:992:TRP:HD1	1.82	0.44
1:I:1252:ASN:CB	1:I:1254:LYS:HE2	2.48	0.44
1:K:1002:SER:OG	1:K:1003:ARG:N	2.49	0.44
1:M:1154:PHE:HA	1:M:1157:THR:HG23	2.00	0.44
1:S:1065:LEU:HD23	1:S:1067:GLY:N	2.33	0.44
1:T:1201:VAL:O	1:T:1205:ILE:HG13	2.17	0.44
1:T:1112:MET:HE3	1:T:1206:ALA:HA	1.99	0.44
1:T:1207:THR:OG1	1:T:1207:THR:O	2.36	0.44
1:T:1252:ASN:HA	1:T:1253:PRO:HD3	1.88	0.44
1:C:1092:ARG:O	1:C:1095:ARG:HG3	2.18	0.43
1:D:1060:HIS:CD2	1:D:1277:VAL:CB	2.95	0.43
1:E:1022:VAL:HG21	1:E:1028:THR:HG21	1.99	0.43
1:E:1213:TYR:CE1	1:E:1231:LEU:HG	2.52	0.43
1:H:1133:HIS:O	1:H:1134:ARG:HB2	2.18	0.43
1:H:1162:GLU:O	1:H:1163:THR:HG23	2.18	0.43
1:H:1260:LEU:HA	1:H:1260:LEU:HD23	1.87	0.43
2:T:16:741:C18	2:T:16:741:C32	2.96	0.43
1:D:1001:MET:CE	1:D:1014:TYR:CD2	3.01	0.43
1:D:1060:HIS:HD2	1:D:1277:VAL:HB	1.73	0.43
1:E:1081:LEU:HD13	1:E:1083:THR:HG22	1.99	0.43
1:I:1224:PHE:CZ	1:I:1229:GLY:HA3	2.53	0.43
1:J:1137:ALA:HB1	3:J:8:HOH:O	2.18	0.43
1:K:1118:GLU:OE2	1:K:1148:THR:HG23	2.19	0.43
1:M:1233:LYS:HA	1:M:1242:PHE:CD1	2.53	0.43
1:R:1126:LEU:HD13	1:R:1131:PHE:CB	2.47	0.43
1:T:1271:GLU:HB3	1:T:1272:PRO:HD2	1.99	0.43
1:B:1133:HIS:C	1:B:1135:ASP:H	2.21	0.43
1:C:1079:MET:HE3	1:C:1079:MET:HA	2.00	0.43
1:E:1166:PTR:CD2	1:E:1166:PTR:C	2.96	0.43
1:E:1260:LEU:HD23	1:E:1260:LEU:HA	1.65	0.43
1:I:1133:HIS:HA	1:I:1157:THR:HB	2.00	0.43
1:J:1095:ARG:HH22	1:J:1210:GLU:HG2	1.83	0.43
1:L:1037:GLU:HG3	1:L:1038:ALA:N	2.33	0.43
1:T:1106:PRO:HA	1:T:1107:PRO:HD3	1.81	0.43
1:C:1114:GLN:O	1:C:1118:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1207:THR:HG22	1:C:1234:PRO:HB3	2.00	0.43
1:D:1126:LEU:HA	1:D:1126:LEU:HD23	1.82	0.43
1:H:1105:ALA:HB3	1:R:1007:GLN:NE2	2.33	0.43
1:I:1095:ARG:HH22	1:I:1210:GLU:HG3	1.81	0.43
1:I:1213:TYR:CE1	1:I:1231:LEU:HG	2.52	0.43
1:K:1066:LEU:HB2	1:K:1078:ILE:HG22	2.01	0.43
1:R:1040:SER:OG	1:R:1043:GLU:CG	2.62	0.43
1:T:1057:PHE:N	1:T:1057:PHE:CD1	2.85	0.43
1:A:1109:LEU:HD22	1:A:1113:ILE:HG12	2.00	0.43
1:E:1030:VAL:HG23	1:E:1032:ILE:CD1	2.48	0.43
1:F:994:VAL:HG22	1:F:1069:VAL:CG2	2.49	0.43
1:I:1142:MET:HE1	2:I:9:741:C5	2.48	0.43
1:J:1247:MET:SD	1:S:986:VAL:HG11	2.59	0.43
1:K:1271:GLU:HG2	1:K:1271:GLU:H	1.67	0.43
1:K:996:ARG:O	1:K:999:ILE:N	2.44	0.43
1:S:1123:MET:HB3	1:S:1259:PHE:CE2	2.53	0.43
1:A:1092:ARG:NH1	1:A:1095:ARG:HH12	2.17	0.43
1:B:1012:MET:HB2	1:B:1012:MET:HE2	1.90	0.43
1:F:1113:ILE:HD11	1:F:1240:MET:SD	2.59	0.43
1:H:1119:ILE:HG23	1:H:1151:ILE:HD11	2.00	0.43
1:A:1044:ARG:HG2	1:A:1048:LEU:HD21	2.00	0.43
1:A:1065:LEU:HD23	1:A:1067:GLY:H	1.83	0.43
2:B:2:741:C32	2:B:2:741:C23	2.97	0.43
1:C:1047:PHE:C	1:C:1047:PHE:CD2	2.92	0.43
1:F:1031:ALA:HB1	2:F:6:741:H23	2.01	0.43
1:F:1058:ASN:C	1:F:1058:ASN:ND2	2.68	0.43
1:G:1235:ASP:O	1:G:1236:ASN:CB	2.60	0.43
1:H:1092:ARG:O	1:H:1095:ARG:HG3	2.19	0.43
1:J:1042:ARG:HD2	3:J:133:HOH:O	2.19	0.43
1:L:1113:ILE:HD11	1:L:1240:MET:CE	2.49	0.43
1:S:1021:VAL:HG23	1:S:1022:VAL:N	2.34	0.43
1:S:1036:ASN:H	1:S:1036:ASN:HD22	1.67	0.43
1:C:1058:ASN:ND2	1:C:1058:ASN:O	2.48	0.43
1:F:1073:GLN:CB	1:F:1074:PRO:HD3	2.49	0.43
1:G:992:TRP:CZ2	1:G:1055:LYS:CB	2.90	0.43
1:H:1012:MET:HG2	1:H:1014:TYR:CZ	2.53	0.43
1:I:1233:LYS:HD2	1:I:1242:PHE:CD2	2.53	0.43
1:I:988:VAL:HG23	1:I:988:VAL:O	2.19	0.43
1:J:1244:LEU:HA	1:J:1244:LEU:HD23	1.83	0.43
1:K:1222:LEU:CD1	1:K:1226:MET:SD	3.06	0.43
1:A:1087:LEU:O	1:A:1091:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1058:ASN:ND2	1:C:1064:ARG:HH22	2.16	0.43
1:C:1079:MET:HG3	2:C:3:741:CL24	2.56	0.43
1:D:1054:MET:CE	3:D:120:HOH:O	2.61	0.43
1:G:1102:PRO:HB2	1:G:1103:VAL:H	1.58	0.43
1:H:1112:MET:CE	1:H:1205:ILE:HG22	2.48	0.43
1:I:1129:ASN:O	1:I:1130:LYS:HB2	2.19	0.43
1:M:1040:SER:OG	1:M:1043:GLU:HB2	2.18	0.43
2:A:1:741:O38	2:A:1:741:H36	2.16	0.43
1:C:1163:THR:O	1:C:1165:PTR:HD1	2.19	0.43
1:C:994:VAL:HG22	1:C:1069:VAL:HG22	2.00	0.43
1:F:1063:VAL:HG21	1:F:1142:MET:HG3	2.01	0.43
1:H:1087:LEU:O	1:H:1091:LEU:HG	2.19	0.43
1:K:989:PRO:O	1:K:991:GLU:N	2.52	0.43
1:L:1047:PHE:CZ	1:L:1077:VAL:HG21	2.54	0.43
1:M:989:PRO:HG2	1:M:992:TRP:CD1	2.54	0.43
1:R:1081:LEU:HD13	1:R:1083:THR:HG22	2.01	0.43
1:T:1134:ARG:HD3	1:T:1156:MET:O	2.18	0.43
1:T:1161:PTR:CD1	1:T:1161:PTR:C	2.91	0.43
1:B:1159:ASP:OD1	1:B:1160:ILE:N	2.52	0.42
1:C:1132:VAL:HG22	1:C:1160:ILE:HD13	2.00	0.42
1:D:1044:ARG:HH11	1:D:1044:ARG:HB2	1.84	0.42
1:G:1126:LEU:HA	1:G:1126:LEU:HD22	1.89	0.42
1:G:1154:PHE:HD2	1:G:1157:THR:HG21	1.84	0.42
1:H:1051:ALA:O	1:H:1054:MET:HB2	2.18	0.42
1:J:1156:MET:HG2	1:J:1174:LEU:HD21	2.01	0.42
1:K:1010:PHE:CD1	1:K:1047:PHE:CD1	3.07	0.42
1:M:1054:MET:O	1:M:1057:PHE:N	2.51	0.42
1:A:1126:LEU:HD22	1:A:1126:LEU:HA	1.83	0.42
1:C:1042:ARG:HB3	1:C:1042:ARG:HE	1.71	0.42
1:C:1132:VAL:HG23	1:C:1160:ILE:HG21	2.00	0.42
1:L:1095:ARG:NH2	1:L:1210:GLU:HG2	2.34	0.42
1:L:1217:SER:O	1:L:1218:ASN:C	2.57	0.42
1:M:1030:VAL:CG1	1:M:1066:LEU:HD12	2.49	0.42
1:T:988:VAL:HG12	1:T:1048:LEU:HD12	2.01	0.42
1:C:1030:VAL:CG2	1:C:1032:ILE:HD11	2.49	0.42
1:F:1081:LEU:CD1	1:F:1083:THR:HG23	2.49	0.42
1:G:1154:PHE:HB3	1:G:1157:THR:HG21	2.00	0.42
1:G:1223:ARG:H	1:G:1223:ARG:HG2	1.49	0.42
1:I:1058:ASN:ND2	1:I:1064:ARG:NH2	2.67	0.42
1:K:1083:THR:O	2:K:11:741:H15A	2.18	0.42
1:L:1066:LEU:HB2	1:L:1078:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1245:MET:HB3	1:S:1249:TRP:CZ3	2.54	0.42
1:T:1240:MET:HG2	1:T:1241:LEU:N	2.32	0.42
1:B:1174:LEU:HD23	1:B:1174:LEU:HA	1.71	0.42
1:C:1036:ASN:ND2	1:C:1038:ALA:N	2.67	0.42
1:C:992:TRP:CZ2	1:C:1055:LYS:CB	3.02	0.42
1:C:1235:ASP:O	1:C:1236:ASN:CB	2.67	0.42
1:D:1165:PTR:CD2	1:D:1165:PTR:C	2.97	0.42
1:E:1092:ARG:CZ	1:E:1095:ARG:NH1	2.82	0.42
1:G:1064:ARG:HE	1:G:1064:ARG:HB2	1.37	0.42
1:G:1107:PRO:HD3	1:G:1208:LEU:HD21	2.02	0.42
1:I:1130:LYS:HD3	1:I:1130:LYS:HA	1.88	0.42
1:I:1151:ILE:N	1:I:1151:ILE:HD13	2.34	0.42
1:R:1023:LYS:C	1:R:1023:LYS:HD2	2.40	0.42
1:R:1168:LYS:HA	1:R:1168:LYS:HD2	1.79	0.42
1:R:1095:ARG:HH22	1:R:1210:GLU:CG	2.32	0.42
1:S:1137:ALA:HA	1:S:1201:VAL:HG12	2.01	0.42
2:A:1:741:C16	2:A:1:741:O12	2.66	0.42
1:B:1044:ARG:NH1	1:B:1044:ARG:CG	2.75	0.42
1:B:1106:PRO:HB2	1:B:1112:MET:HE1	2.01	0.42
1:F:1033:LYS:HD3	2:F:6:741:S25	2.59	0.42
1:G:1010:PHE:CD2	1:G:1047:PHE:HB2	2.55	0.42
1:G:1073:GLN:HB2	1:G:1074:PRO:CD	2.49	0.42
1:G:991:GLU:HG2	1:G:991:GLU:H	1.50	0.42
1:H:1154:PHE:HD2	1:H:1157:THR:HG21	1.84	0.42
1:K:1217:SER:O	1:K:1218:ASN:C	2.57	0.42
1:M:1044:ARG:HH11	1:M:1044:ARG:HB2	1.85	0.42
1:R:1023:LYS:C	1:R:1024:ASP:OD2	2.56	0.42
1:R:1184:LEU:HD22	1:R:1222:LEU:HD21	2.00	0.42
1:E:1236:ASN:HA	1:S:1038:ALA:CB	2.49	0.42
1:S:1154:PHE:HA	1:S:1157:THR:HG23	2.00	0.42
1:T:1107:PRO:HD3	1:T:1208:LEU:HD21	2.01	0.42
1:A:1018:ALA:HB3	1:A:1021:VAL:HG21	2.00	0.42
1:A:1060:HIS:CD2	1:A:1277:VAL:HB	2.55	0.42
1:C:1159:ASP:OD1	1:C:1160:ILE:N	2.53	0.42
1:C:996:ARG:NH1	1:C:1074:PRO:CD	2.72	0.42
1:E:1018:ALA:HB1	1:E:1021:VAL:CG1	2.50	0.42
1:F:994:VAL:O	1:F:1069:VAL:HG22	2.20	0.42
1:I:1113:ILE:HD13	1:I:1113:ILE:HA	1.79	0.42
1:J:1145:GLU:CA	1:J:1145:GLU:OE1	2.67	0.42
1:K:988:VAL:HG23	1:K:988:VAL:O	2.19	0.42
1:M:1042:ARG:CG	1:M:1042:ARG:NH1	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1095:ARG:HH22	1:R:1210:GLU:HG2	1.85	0.42
1:R:1161:PTR:HD1	1:R:1162:GLU:CG	2.47	0.42
1:S:1092:ARG:HD3	1:S:1095:ARG:NH1	2.32	0.42
2:S:15:741:H37A	2:S:15:741:H36	1.61	0.42
1:T:1058:ASN:HD22	1:T:1058:ASN:C	2.22	0.42
1:T:1059:CYS:HB2	1:T:1125:TYR:CD2	2.54	0.42
1:A:995:ALA:HB1	1:A:997:GLU:HG2	2.01	0.42
1:B:1054:MET:O	1:B:1056:GLU:N	2.53	0.42
1:E:1013:VAL:HG21	3:E:151:HOH:O	2.19	0.42
1:I:1106:PRO:N	1:I:1107:PRO:CD	2.82	0.42
1:L:1081:LEU:HD13	1:L:1083:THR:HG22	2.02	0.42
1:M:1030:VAL:CG2	1:M:1032:ILE:HD11	2.49	0.42
1:S:1035:VAL:HG12	1:S:1035:VAL:O	2.19	0.42
1:S:1081:LEU:HD13	1:S:1083:THR:HG22	2.02	0.42
1:A:1168:LYS:HD2	1:A:1168:LYS:HA	1.63	0.42
1:A:1201:VAL:O	1:A:1205:ILE:HG13	2.19	0.42
1:C:1007:GLN:HA	1:C:1007:GLN:OE1	2.19	0.42
1:D:1037:GLU:O	1:D:1039:ALA:N	2.39	0.42
1:H:1207:THR:HG22	1:H:1234:PRO:HB3	2.01	0.42
1:I:1069:VAL:HB	1:I:1076:LEU:HB2	2.01	0.42
1:J:1060:HIS:CD2	1:J:1277:VAL:HB	2.54	0.42
1:K:1174:LEU:HA	1:K:1175:PRO:HD3	1.94	0.42
1:L:1081:LEU:HD23	1:L:1081:LEU:HA	1.92	0.42
1:L:1268:GLU:OE2	1:L:1268:GLU:HA	2.19	0.42
1:M:1037:GLU:O	1:M:1039:ALA:N	2.49	0.42
1:S:1005:LEU:HD12	1:S:1014:TYR:C	2.40	0.42
1:S:1113:ILE:HD11	1:S:1240:MET:SD	2.60	0.42
1:T:1058:ASN:O	1:T:1058:ASN:ND2	2.53	0.42
1:T:1159:ASP:OD1	1:T:1160:ILE:N	2.52	0.42
1:T:1222:LEU:HA	1:T:1222:LEU:HD22	1.60	0.42
1:A:1153:ASP:OD1	1:A:1153:ASP:C	2.59	0.42
1:B:1163:THR:CG2	1:B:1165:PTR:CE1	2.91	0.42
1:D:1275:ARG:O	1:D:1275:ARG:HG3	2.19	0.42
1:I:1112:MET:HE1	1:I:1206:ALA:CA	2.48	0.42
1:R:990:ASP:N	1:R:990:ASP:OD1	2.52	0.42
1:T:1047:PHE:CZ	1:T:1077:VAL:CG2	3.03	0.42
1:T:998:LYS:O	1:T:999:ILE:HD13	2.20	0.42
1:E:1082:MET:H	2:E:5:741:C8	2.33	0.42
1:F:1063:VAL:HG23	1:F:1151:ILE:O	2.20	0.42
1:M:996:ARG:CZ	1:M:1074:PRO:HD2	2.42	0.42
1:R:1243:GLU:O	1:R:1247:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1271:GLU:HB3	1:R:1272:PRO:HD2	2.02	0.42
1:A:1104:LEU:HD23	1:A:1104:LEU:O	2.20	0.41
1:D:1112:MET:HG2	1:D:1205:ILE:HG22	2.02	0.41
1:E:996:ARG:CZ	1:E:1074:PRO:HD2	2.50	0.41
1:H:1044:ARG:O	1:H:1048:LEU:HD23	2.19	0.41
1:J:989:PRO:C	1:J:991:GLU:H	2.22	0.41
1:M:1005:LEU:HD11	1:M:1015:GLU:HB2	2.02	0.41
1:M:1037:GLU:C	1:M:1039:ALA:N	2.72	0.41
1:M:1130:LYS:HA	1:M:1130:LYS:HD2	1.58	0.41
1:T:1040:SER:HB2	1:T:1043:GLU:H	1.85	0.41
1:A:1216:LEU:N	1:A:1216:LEU:HD23	2.35	0.41
1:B:996:ARG:NH1	1:B:1074:PRO:HG2	2.33	0.41
1:E:1008:GLY:C	1:E:1033:LYS:HZ2	2.24	0.41
1:E:1082:MET:HE2	1:E:1150:LYS:HB2	2.02	0.41
1:E:1134:ARG:HD3	1:E:1156:MET:O	2.20	0.41
1:M:1022:VAL:CG1	1:M:1025:GLU:HB3	2.40	0.41
1:M:988:VAL:O	1:M:988:VAL:CG2	2.67	0.41
1:R:1049:ASN:HA	1:R:1052:SER:HB2	2.02	0.41
1:B:1025:GLU:HA	1:B:1026:PRO:HD3	1.80	0.41
1:B:1151:ILE:HG22	1:B:1154:PHE:CZ	2.55	0.41
1:B:1165:PTR:C	1:B:1165:PTR:CD2	2.99	0.41
1:C:1047:PHE:HZ	1:C:1077:VAL:HG21	1.85	0.41
1:C:1082:MET:HB2	1:C:1142:MET:CE	2.50	0.41
1:C:989:PRO:C	1:C:991:GLU:N	2.70	0.41
1:F:1081:LEU:HD13	1:F:1083:THR:HG23	2.02	0.41
1:F:1162:GLU:O	1:F:1163:THR:CB	2.68	0.41
1:G:1096:PRO:O	1:G:1097:GLU:CG	2.66	0.41
1:G:1054:MET:HE3	2:G:7:741:H31	2.02	0.41
1:I:1078:ILE:HD13	1:I:1078:ILE:N	2.35	0.41
1:K:1047:PHE:CZ	1:K:1077:VAL:CG2	3.03	0.41
1:K:1062:VAL:HG13	1:K:1154:PHE:HZ	1.84	0.41
1:K:1132:VAL:HG12	1:K:1134:ARG:HG3	2.02	0.41
1:K:1213:TYR:O	1:K:1214:GLN:C	2.57	0.41
1:L:1004:GLU:HG2	1:L:1004:GLU:H	1.50	0.41
1:L:1109:LEU:HD22	1:L:1113:ILE:HG12	2.01	0.41
1:L:1132:VAL:CG2	1:L:1160:ILE:HD13	2.36	0.41
1:L:1165:PTR:CD2	1:L:1165:PTR:C	2.98	0.41
1:S:1084:ARG:HB2	1:S:1143:VAL:HB	2.02	0.41
1:C:1166:PTR:O2P	1:C:1166:PTR:CE1	2.66	0.41
1:D:1081:LEU:HD23	1:D:1081:LEU:HA	1.90	0.41
1:G:1036:ASN:ND2	1:G:1038:ALA:CA	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1275:ARG:HG3	1:G:1275:ARG:O	2.19	0.41
1:H:1030:VAL:HA	1:H:1081:LEU:HB2	2.03	0.41
1:B:1236:ASN:HA	1:J:1038:ALA:HB3	2.01	0.41
1:J:1083:THR:O	2:J:10:741:H15	2.19	0.41
1:L:1048:LEU:HA	1:L:1048:LEU:HD12	1.81	0.41
1:L:997:GLU:OE2	1:L:997:GLU:N	2.54	0.41
1:M:1109:LEU:HD22	1:M:1109:LEU:O	2.20	0.41
1:M:1114:GLN:O	1:M:1118:GLU:HG3	2.20	0.41
1:M:989:PRO:HB2	1:M:992:TRP:HD1	1.84	0.41
1:A:1095:ARG:HA	1:A:1096:PRO:HD3	1.85	0.41
1:B:1259:PHE:O	1:B:1263:ILE:HG13	2.21	0.41
1:D:1058:ASN:ND2	1:D:1064:ARG:HH22	2.18	0.41
1:D:996:ARG:NH2	1:D:1072:GLY:HA3	2.36	0.41
1:D:1084:ARG:CB	1:D:1143:VAL:HB	2.51	0.41
1:E:1008:GLY:N	1:E:1011:GLY:O	2.53	0.41
1:G:1032:ILE:CD1	1:G:1078:ILE:HG13	2.51	0.41
1:H:1088:LYS:O	1:H:1092:ARG:HG2	2.20	0.41
2:I:9:741:H36A	2:I:9:741:H14A	1.76	0.41
1:B:1105:ALA:N	1:J:1007:GLN:NE2	2.69	0.41
1:K:1095:ARG:HG2	1:K:1208:LEU:HD12	2.01	0.41
1:L:1030:VAL:CG1	1:L:1066:LEU:HD12	2.50	0.41
1:L:1069:VAL:HB	1:L:1076:LEU:HB2	2.03	0.41
1:S:1058:ASN:ND2	1:S:1058:ASN:C	2.72	0.41
1:D:1244:LEU:HD23	1:D:1244:LEU:HA	1.72	0.41
1:D:999:ILE:HG21	1:D:1076:LEU:HD13	2.02	0.41
1:G:1132:VAL:CG2	1:G:1160:ILE:HD13	2.51	0.41
1:H:1213:TYR:CE1	1:H:1231:LEU:HG	2.56	0.41
1:I:1168:LYS:HD2	1:I:1168:LYS:HA	1.40	0.41
1:R:989:PRO:C	1:R:991:GLU:H	2.24	0.41
1:S:1161:PTR:O	1:S:1162:GLU:O	2.38	0.41
1:T:1030:VAL:HG23	1:T:1032:ILE:HD11	2.03	0.41
1:T:992:TRP:N	1:T:992:TRP:CD1	2.88	0.41
1:B:1049:ASN:HA	1:B:1049:ASN:HD22	1.65	0.41
1:C:1023:LYS:O	1:C:1024:ASP:HB2	2.20	0.41
1:H:1079:MET:CG	2:H:8:741:CL24	3.05	0.41
1:H:1244:LEU:HA	1:H:1244:LEU:HD23	1.83	0.41
1:J:1049:ASN:HA	1:J:1049:ASN:HD22	1.63	0.41
1:L:1151:ILE:N	1:L:1151:ILE:CD1	2.83	0.41
1:M:1048:LEU:HA	1:M:1048:LEU:HD12	1.71	0.41
1:M:1126:LEU:HD23	1:M:1126:LEU:HA	1.93	0.41
1:A:1047:PHE:CZ	1:A:1077:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:996:ARG:NH2	1:F:1072:GLY:HA3	2.35	0.41
1:G:1079:MET:HE3	1:G:1079:MET:HA	2.03	0.41
1:H:989:PRO:O	1:H:991:GLU:N	2.42	0.41
1:J:1057:PHE:N	1:J:1057:PHE:CD1	2.88	0.41
1:J:1163:THR:O	1:J:1164:ASP:HB2	2.21	0.41
1:L:1133:HIS:HA	1:L:1157:THR:HG22	2.03	0.41
1:M:1166:PTR:OH	1:M:1168:LYS:HD2	2.18	0.41
1:S:1033:LYS:HB2	2:S:15:741:CL24	2.58	0.41
1:T:1275:ARG:HG3	1:T:1281:TYR:CD1	2.56	0.41
1:A:1041:MET:O	1:A:1045:ILE:HG13	2.21	0.41
1:F:984:ALA:O	1:F:988:VAL:CG1	2.69	0.41
1:I:1092:ARG:CD	1:I:1095:ARG:NH1	2.78	0.41
1:J:1048:LEU:HD12	1:J:1048:LEU:HA	1.78	0.41
1:K:1126:LEU:HA	1:K:1126:LEU:HD22	1.71	0.41
1:K:1095:ARG:HH22	1:K:1210:GLU:HG3	1.85	0.41
1:L:1049:ASN:HA	1:L:1049:ASN:HD22	1.68	0.41
1:R:1222:LEU:HD22	1:R:1222:LEU:HA	1.86	0.41
1:T:1030:VAL:CG2	1:T:1032:ILE:HD11	2.51	0.41
1:D:1250:GLN:OE1	1:G:1045:ILE:HD12	2.20	0.41
1:E:1174:LEU:HA	1:E:1175:PRO:HD3	1.97	0.41
1:F:1133:HIS:O	1:F:1134:ARG:HB2	2.21	0.41
2:F:6:741:H36	2:F:6:741:H37	1.75	0.41
1:F:994:VAL:HG22	1:F:1069:VAL:HG22	2.01	0.41
1:G:1036:ASN:HD21	1:G:1038:ALA:CA	2.33	0.41
1:H:992:TRP:CZ2	1:H:1055:LYS:CB	3.04	0.41
1:I:1241:LEU:HA	1:I:1241:LEU:HD12	1.83	0.41
1:L:1201:VAL:O	1:L:1205:ILE:HG13	2.20	0.41
1:L:1245:MET:HB3	1:L:1249:TRP:CZ3	2.56	0.41
1:M:1241:LEU:HA	1:M:1241:LEU:HD12	1.69	0.41
1:M:989:PRO:O	1:M:991:GLU:N	2.48	0.41
1:S:1132:VAL:HG12	1:S:1134:ARG:HG3	2.01	0.41
1:A:989:PRO:C	1:A:991:GLU:N	2.74	0.41
1:B:1257:PRO:HB2	1:B:1262:ILE:HG13	2.02	0.41
1:D:996:ARG:HH12	1:D:1074:PRO:CD	2.32	0.41
1:E:1223:ARG:HG2	1:E:1223:ARG:H	1.73	0.41
1:F:1021:VAL:HG13	1:F:1022:VAL:CG1	2.51	0.41
1:J:1042:ARG:NH1	3:J:133:HOH:O	2.52	0.41
1:J:989:PRO:HB2	1:J:991:GLU:HG2	2.03	0.41
1:K:1177:ARG:HB3	1:K:1212:PRO:HB2	2.03	0.41
1:L:1079:MET:HE2	2:L:13:741:N33	2.35	0.41
1:M:1092:ARG:HG2	1:M:1209:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:LEU:HD13	2:A:1:741:C2	2.52	0.40
1:A:1121:ASP:HA	1:A:1263:ILE:HD11	2.02	0.40
1:A:1154:PHE:CD2	1:A:1157:THR:HG21	2.52	0.40
1:B:1215:GLY:O	1:B:1216:LEU:HD23	2.21	0.40
1:C:1286:LYS:HD3	1:C:1286:LYS:C	2.42	0.40
1:E:1082:MET:HG3	1:E:1142:MET:CB	2.51	0.40
1:F:1022:VAL:HG11	1:F:1028:THR:HG21	2.04	0.40
1:F:996:ARG:NH2	1:F:1074:PRO:O	2.43	0.40
1:I:1092:ARG:CD	1:I:1095:ARG:HH11	2.30	0.40
1:J:1174:LEU:HA	1:J:1175:PRO:HD2	1.93	0.40
1:K:1112:MET:CE	1:K:1205:ILE:HG22	2.51	0.40
1:L:1121:ASP:HA	1:L:1263:ILE:HD11	2.02	0.40
1:M:1217:SER:O	1:M:1218:ASN:C	2.59	0.40
1:M:992:TRP:CH2	1:M:1055:LYS:HA	2.56	0.40
1:S:1063:VAL:HG23	1:S:1151:ILE:O	2.21	0.40
1:T:1057:PHE:HE1	1:T:1131:PHE:CE2	2.39	0.40
1:T:1270:MET:HE3	1:T:1270:MET:HB3	1.87	0.40
1:T:996:ARG:O	1:T:999:ILE:N	2.47	0.40
1:A:1196:TRP:CD1	1:A:1196:TRP:C	2.95	0.40
1:A:994:VAL:O	1:A:1069:VAL:HG22	2.21	0.40
1:B:1112:MET:HG2	1:B:1205:ILE:CG2	2.51	0.40
1:B:1139:ARG:NH2	1:B:1175:PRO:HG2	2.36	0.40
1:C:1163:THR:CG2	1:C:1165:PTR:CD1	3.00	0.40
1:D:1036:ASN:C	1:D:1036:ASN:ND2	2.74	0.40
1:G:1052:SER:O	1:G:1055:LYS:CG	2.61	0.40
2:I:9:741:C23	2:I:9:741:C32	2.99	0.40
1:J:1084:ARG:HD2	1:J:1143:VAL:HG12	2.02	0.40
1:J:1184:LEU:HD22	1:J:1222:LEU:CD2	2.51	0.40
1:K:1095:ARG:O	1:K:1096:PRO:C	2.59	0.40
1:K:1244:LEU:HA	1:K:1244:LEU:HD23	1.82	0.40
1:K:1242:PHE:O	1:K:1246:ARG:HG3	2.21	0.40
1:M:1069:VAL:HG21	1:M:1076:LEU:HD12	2.02	0.40
1:M:1082:MET:CE	1:M:1142:MET:HB2	2.51	0.40
1:R:1133:HIS:O	1:R:1134:ARG:HB2	2.21	0.40
1:S:1044:ARG:O	1:S:1048:LEU:HD22	2.21	0.40
1:A:1077:VAL:C	1:A:1078:ILE:HD12	2.41	0.40
1:B:1177:ARG:NE	1:B:1211:GLN:HE21	2.18	0.40
1:D:1112:MET:HE3	1:D:1205:ILE:HG22	2.02	0.40
1:E:1162:GLU:O	1:E:1163:THR:OG1	2.35	0.40
1:I:1217:SER:O	1:I:1218:ASN:C	2.59	0.40
1:K:1063:VAL:HG23	1:K:1151:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1208:LEU:O	1:K:1209:ALA:CB	2.69	0.40
1:M:1186:ASP:HB2	1:M:1188:VAL:HG23	2.04	0.40
1:M:995:ALA:HB1	1:M:997:GLU:OE1	2.21	0.40
1:R:1249:TRP:O	1:R:1250:GLN:C	2.58	0.40
1:T:1254:LYS:HE3	1:T:1254:LYS:HB2	1.64	0.40
1:C:1092:ARG:CG	1:C:1092:ARG:NH1	2.51	0.40
1:C:1201:VAL:O	1:C:1204:GLU:HB2	2.21	0.40
1:D:1058:ASN:ND2	1:D:1064:ARG:NH2	2.69	0.40
1:G:1121:ASP:HA	1:G:1263:ILE:CD1	2.51	0.40
1:G:1161:PTR:C	1:G:1162:GLU:O	2.70	0.40
1:H:1087:LEU:HB3	1:H:1138:ALA:O	2.22	0.40
1:J:1035:VAL:HG21	1:J:1047:PHE:CE2	2.57	0.40
1:J:1036:ASN:C	1:J:1036:ASN:ND2	2.74	0.40
1:J:1153:ASP:C	1:J:1153:ASP:OD1	2.59	0.40
1:M:1030:VAL:HG12	1:M:1066:LEU:HD12	2.02	0.40
1:M:1182:GLU:HG2	1:M:1183:SER:N	2.36	0.40
1:R:1079:MET:CB	2:R:14:741:N33	2.85	0.40
1:T:1078:ILE:HD12	1:T:1078:ILE:N	2.36	0.40
1:C:1023:LYS:CD	1:C:1023:LYS:H	2.34	0.40
1:F:1104:LEU:HD13	1:F:1104:LEU:HA	1.54	0.40
1:F:1142:MET:HB3	1:F:1142:MET:HE3	1.98	0.40
1:G:1005:LEU:HA	1:G:1005:LEU:HD23	1.85	0.40
1:I:1059:CYS:HB2	1:I:1125:TYR:CD2	2.56	0.40
1:K:1243:GLU:OE2	1:K:1246:ARG:NH1	2.54	0.40
1:R:1023:LYS:CD	1:R:1023:LYS:N	2.84	0.40
1:R:1023:LYS:HD2	1:R:1023:LYS:N	2.35	0.40
1:T:1054:MET:HE3	2:T:16:741:C31	2.51	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	295/308 (96%)	267 (90%)	22 (8%)	6 (2%)	7	27
1	B	294/308 (96%)	273 (93%)	17 (6%)	4 (1%)	11	36
1	C	297/308 (96%)	271 (91%)	20 (7%)	6 (2%)	7	27
1	D	293/308 (95%)	271 (92%)	18 (6%)	4 (1%)	11	36
1	E	295/308 (96%)	271 (92%)	20 (7%)	4 (1%)	11	36
1	F	295/308 (96%)	268 (91%)	21 (7%)	6 (2%)	7	27
1	G	295/308 (96%)	275 (93%)	16 (5%)	4 (1%)	11	36
1	H	295/308 (96%)	265 (90%)	22 (8%)	8 (3%)	5	19
1	I	290/308 (94%)	272 (94%)	15 (5%)	3 (1%)	15	45
1	J	289/308 (94%)	266 (92%)	20 (7%)	3 (1%)	15	45
1	K	289/308 (94%)	266 (92%)	17 (6%)	6 (2%)	7	26
1	L	289/308 (94%)	270 (93%)	16 (6%)	3 (1%)	15	45
1	M	291/308 (94%)	268 (92%)	14 (5%)	9 (3%)	4	16
1	R	290/308 (94%)	268 (92%)	19 (7%)	3 (1%)	15	45
1	S	291/308 (94%)	264 (91%)	24 (8%)	3 (1%)	15	45
1	T	291/308 (94%)	265 (91%)	21 (7%)	5 (2%)	9	31
All	All	4679/4928 (95%)	4300 (92%)	302 (6%)	77 (2%)	9	32

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1097	GLU
1	C	1055	LYS
1	C	1163	THR
1	D	1038	ALA
1	D	1163	THR
1	F	1040	SER
1	H	1097	GLU
1	H	1105	ALA
1	I	990	ASP
1	K	991	GLU
1	K	1163	THR
1	M	991	GLU
1	M	1163	THR
1	R	1163	THR
1	S	1163	THR
1	A	1163	THR

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Mol	Chain	Res	Type
1	A	1236	ASN
1	B	1055	LYS
1	C	1038	ALA
1	D	990	ASP
1	E	1163	THR
1	F	1163	THR
1	G	1038	ALA
1	H	990	ASP
1	H	1040	SER
1	H	1096	PRO
1	H	1163	THR
1	I	1162	GLU
1	I	1163	THR
1	J	1037	GLU
1	J	1163	THR
1	K	1209	ALA
1	M	990	ASP
1	M	997	GLU
1	M	1020	GLY
1	L	990	ASP
1	R	1162	GLU
1	S	1162	GLU
1	T	991	GLU
1	B	1040	SER
1	B	1162	GLU
1	C	990	ASP
1	C	1162	GLU
1	E	990	ASP
1	F	1162	GLU
1	G	1096	PRO
1	G	1163	THR
1	H	1038	ALA
1	K	990	ASP
1	M	1055	LYS
1	M	1162	GLU
1	L	1162	GLU
1	A	1162	GLU
1	B	1038	ALA
1	E	1162	GLU
1	F	990	ASP
1	F	1074	PRO
1	G	1162	GLU

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Mol	Chain	Res	Type
1	K	1162	GLU
1	M	1038	ALA
1	L	1163	THR
1	A	1074	PRO
1	F	1038	ALA
1	J	990	ASP
1	R	1038	ALA
1	S	1055	LYS
1	T	990	ASP
1	T	1162	GLU
1	A	1038	ALA
1	D	991	GLU
1	K	1055	LYS
1	C	1074	PRO
1	E	1074	PRO
1	T	989	PRO
1	T	1107	PRO
1	H	1106	PRO
1	M	1074	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/265 (98%)	228 (88%)	31 (12%)	5	15
1	B	258/265 (97%)	217 (84%)	41 (16%)	2	7
1	C	257/265 (97%)	222 (86%)	35 (14%)	3	11
1	D	257/265 (97%)	231 (90%)	26 (10%)	7	23
1	E	256/265 (97%)	219 (86%)	37 (14%)	3	9
1	F	259/265 (98%)	223 (86%)	36 (14%)	3	10
1	G	260/265 (98%)	223 (86%)	37 (14%)	3	10
1	H	259/265 (98%)	226 (87%)	33 (13%)	4	13
1	I	256/265 (97%)	212 (83%)	44 (17%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	254/265 (96%)	230 (91%)	24 (9%)	8	26
1	K	254/265 (96%)	224 (88%)	30 (12%)	5	16
1	L	254/265 (96%)	226 (89%)	28 (11%)	6	19
1	M	255/265 (96%)	220 (86%)	35 (14%)	3	11
1	R	255/265 (96%)	223 (88%)	32 (12%)	4	14
1	S	256/265 (97%)	223 (87%)	33 (13%)	4	13
1	T	256/265 (97%)	220 (86%)	36 (14%)	3	10
All	All	4105/4240 (97%)	3567 (87%)	538 (13%)	4	12

All (538) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	986	VAL
1	A	991	GLU
1	A	997	GLU
1	A	1000	THR
1	A	1012	MET
1	A	1017	VAL
1	A	1021	VAL
1	A	1023	LYS
1	A	1035	VAL
1	A	1036	ASN
1	A	1042	ARG
1	A	1046	GLU
1	A	1056	GLU
1	A	1058	ASN
1	A	1064	ARG
1	A	1071	GLN
1	A	1081	LEU
1	A	1109	LEU
1	A	1126	LEU
1	A	1130	LYS
1	A	1139	ARG
1	A	1145	GLU
1	A	1151	ILE
1	A	1157	THR
1	A	1179	MET
1	A	1222	LEU
1	A	1239	ASP
1	A	1240	MET

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Mol	Chain	Res	Type
1	A	1244	LEU
1	A	1264	SER
1	A	1271	GLU
1	B	986	VAL
1	B	988	VAL
1	B	991	GLU
1	B	994	VAL
1	B	997	GLU
1	B	1000	THR
1	B	1002	SER
1	B	1023	LYS
1	B	1024	ASP
1	B	1032	ILE
1	B	1036	ASN
1	B	1040	SER
1	B	1042	ARG
1	B	1044	ARG
1	B	1046	GLU
1	B	1048	LEU
1	B	1056	GLU
1	B	1058	ASN
1	B	1064	ARG
1	B	1068	VAL
1	B	1071	GLN
1	B	1080	GLU
1	B	1081	LEU
1	B	1092	ARG
1	B	1109	LEU
1	B	1126	LEU
1	B	1132	VAL
1	B	1142	MET
1	B	1162	GLU
1	B	1163	THR
1	B	1171	LYS
1	B	1188	VAL
1	B	1201	VAL
1	B	1219	GLU
1	B	1222	LEU
1	B	1239	ASP
1	B	1244	LEU
1	B	1250	GLN
1	B	1269	GLU

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Mol	Chain	Res	Type
1	B	1275	ARG
1	B	1284	GLU
1	C	986	VAL
1	C	994	VAL
1	C	997	GLU
1	C	999	ILE
1	C	1000	THR
1	C	1001	MET
1	C	1007	GLN
1	C	1032	ILE
1	C	1036	ASN
1	C	1042	ARG
1	C	1048	LEU
1	C	1054	MET
1	C	1056	GLU
1	C	1058	ASN
1	C	1064	ARG
1	C	1068	VAL
1	C	1079	MET
1	C	1081	LEU
1	C	1092	ARG
1	C	1109	LEU
1	C	1126	LEU
1	C	1139	ARG
1	C	1157	THR
1	C	1182	GLU
1	C	1188	VAL
1	C	1193	SER
1	C	1222	LEU
1	C	1239	ASP
1	C	1240	MET
1	C	1243	GLU
1	C	1244	LEU
1	C	1250	GLN
1	C	1264	SER
1	C	1268	GLU
1	C	1269	GLU
1	D	986	VAL
1	D	988	VAL
1	D	997	GLU
1	D	1000	THR
1	D	1021	VAL

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Mol	Chain	Res	Type
1	D	1023	LYS
1	D	1032	ILE
1	D	1035	VAL
1	D	1036	ASN
1	D	1046	GLU
1	D	1058	ASN
1	D	1068	VAL
1	D	1073	GLN
1	D	1081	LEU
1	D	1109	LEU
1	D	1110	SER
1	D	1126	LEU
1	D	1132	VAL
1	D	1145	GLU
1	D	1162	GLU
1	D	1171	LYS
1	D	1201	VAL
1	D	1222	LEU
1	D	1244	LEU
1	D	1268	GLU
1	D	1275	ARG
1	E	986	VAL
1	E	988	VAL
1	E	991	GLU
1	E	993	GLU
1	E	994	VAL
1	E	997	GLU
1	E	1000	THR
1	E	1002	SER
1	E	1023	LYS
1	E	1025	GLU
1	E	1032	ILE
1	E	1042	ARG
1	E	1043	GLU
1	E	1046	GLU
1	E	1048	LEU
1	E	1056	GLU
1	E	1058	ASN
1	E	1064	ARG
1	E	1068	VAL
1	E	1071	GLN
1	E	1073	GLN

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Mol	Chain	Res	Type
1	E	1081	LEU
1	E	1095	ARG
1	E	1109	LEU
1	E	1126	LEU
1	E	1139	ARG
1	E	1157	THR
1	E	1167	ARG
1	E	1191	THR
1	E	1201	VAL
1	E	1222	LEU
1	E	1223	ARG
1	E	1240	MET
1	E	1250	GLN
1	E	1268	GLU
1	E	1275	ARG
1	E	1276	GLU
1	F	985	ASP
1	F	986	VAL
1	F	988	VAL
1	F	999	ILE
1	F	1000	THR
1	F	1003	ARG
1	F	1021	VAL
1	F	1022	VAL
1	F	1023	LYS
1	F	1035	VAL
1	F	1042	ARG
1	F	1046	GLU
1	F	1047	PHE
1	F	1049	ASN
1	F	1056	GLU
1	F	1058	ASN
1	F	1068	VAL
1	F	1073	GLN
1	F	1081	LEU
1	F	1095	ARG
1	F	1097	GLU
1	F	1103	VAL
1	F	1104	LEU
1	F	1109	LEU
1	F	1132	VAL
1	F	1163	THR

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Mol	Chain	Res	Type
1	F	1171	LYS
1	F	1176	VAL
1	F	1201	VAL
1	F	1222	LEU
1	F	1240	MET
1	F	1243	GLU
1	F	1244	LEU
1	F	1264	SER
1	F	1269	GLU
1	F	1276	GLU
1	G	986	VAL
1	G	991	GLU
1	G	993	GLU
1	G	994	VAL
1	G	997	GLU
1	G	1000	THR
1	G	1023	LYS
1	G	1037	GLU
1	G	1042	ARG
1	G	1044	ARG
1	G	1046	GLU
1	G	1048	LEU
1	G	1055	LYS
1	G	1064	ARG
1	G	1068	VAL
1	G	1081	LEU
1	G	1088	LYS
1	G	1097	GLU
1	G	1104	LEU
1	G	1109	LEU
1	G	1126	LEU
1	G	1130	LYS
1	G	1139	ARG
1	G	1157	THR
1	G	1162	GLU
1	G	1163	THR
1	G	1188	VAL
1	G	1201	VAL
1	G	1219	GLU
1	G	1222	LEU
1	G	1223	ARG
1	G	1239	ASP

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Mol	Chain	Res	Type
1	G	1243	GLU
1	G	1244	LEU
1	G	1269	GLU
1	G	1271	GLU
1	G	1275	ARG
1	H	986	VAL
1	H	991	GLU
1	H	994	VAL
1	H	997	GLU
1	H	1021	VAL
1	H	1023	LYS
1	H	1028	THR
1	H	1036	ASN
1	H	1042	ARG
1	H	1046	GLU
1	H	1047	PHE
1	H	1048	LEU
1	H	1058	ASN
1	H	1064	ARG
1	H	1068	VAL
1	H	1071	GLN
1	H	1073	GLN
1	H	1081	LEU
1	H	1097	GLU
1	H	1109	LEU
1	H	1132	VAL
1	H	1139	ARG
1	H	1171	LYS
1	H	1176	VAL
1	H	1191	THR
1	H	1201	VAL
1	H	1214	GLN
1	H	1222	LEU
1	H	1226	MET
1	H	1239	ASP
1	H	1240	MET
1	H	1244	LEU
1	H	1264	SER
1	I	994	VAL
1	I	997	GLU
1	I	998	LYS
1	I	1000	THR

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Mol	Chain	Res	Type
1	I	1001	MET
1	I	1003	ARG
1	I	1023	LYS
1	I	1032	ILE
1	I	1036	ASN
1	I	1040	SER
1	I	1042	ARG
1	I	1046	GLU
1	I	1048	LEU
1	I	1052	SER
1	I	1053	VAL
1	I	1058	ASN
1	I	1064	ARG
1	I	1068	VAL
1	I	1073	GLN
1	I	1080	GLU
1	I	1081	LEU
1	I	1109	LEU
1	I	1110	SER
1	I	1126	LEU
1	I	1151	ILE
1	I	1157	THR
1	I	1163	THR
1	I	1167	ARG
1	I	1168	LYS
1	I	1171	LYS
1	I	1177	ARG
1	I	1186	ASP
1	I	1191	THR
1	I	1201	VAL
1	I	1222	LEU
1	I	1235	ASP
1	I	1240	MET
1	I	1243	GLU
1	I	1244	LEU
1	I	1250	GLN
1	I	1254	LYS
1	I	1268	GLU
1	I	1269	GLU
1	I	1275	ARG
1	J	986	VAL
1	J	991	GLU

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Mol	Chain	Res	Type
1	J	1000	THR
1	J	1003	ARG
1	J	1036	ASN
1	J	1048	LEU
1	J	1058	ASN
1	J	1068	VAL
1	J	1081	LEU
1	J	1092	ARG
1	J	1109	LEU
1	J	1126	LEU
1	J	1130	LYS
1	J	1132	VAL
1	J	1145	GLU
1	J	1151	ILE
1	J	1157	THR
1	J	1214	GLN
1	J	1219	GLU
1	J	1222	LEU
1	J	1240	MET
1	J	1243	GLU
1	J	1244	LEU
1	J	1268	GLU
1	K	982	SER
1	K	986	VAL
1	K	994	VAL
1	K	997	GLU
1	K	1001	MET
1	K	1009	SER
1	K	1023	LYS
1	K	1024	ASP
1	K	1036	ASN
1	K	1042	ARG
1	K	1043	GLU
1	K	1046	GLU
1	K	1048	LEU
1	K	1052	SER
1	K	1064	ARG
1	K	1068	VAL
1	K	1081	LEU
1	K	1109	LEU
1	K	1110	SER
1	K	1113	ILE

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Mol	Chain	Res	Type
1	K	1126	LEU
1	K	1157	THR
1	K	1163	THR
1	K	1177	ARG
1	K	1222	LEU
1	K	1235	ASP
1	K	1240	MET
1	K	1244	LEU
1	K	1269	GLU
1	K	1271	GLU
1	M	980	SER
1	M	986	VAL
1	M	994	VAL
1	M	996	ARG
1	M	1000	THR
1	M	1001	MET
1	M	1003	ARG
1	M	1022	VAL
1	M	1025	GLU
1	M	1032	ILE
1	M	1033	LYS
1	M	1036	ASN
1	M	1037	GLU
1	M	1040	SER
1	M	1042	ARG
1	M	1043	GLU
1	M	1052	SER
1	M	1056	GLU
1	M	1068	VAL
1	M	1070	SER
1	M	1073	GLN
1	M	1080	GLU
1	M	1081	LEU
1	M	1095	ARG
1	M	1109	LEU
1	M	1130	LYS
1	M	1156	MET
1	M	1157	THR
1	M	1163	THR
1	M	1201	VAL
1	M	1208	LEU
1	M	1219	GLU

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Mol	Chain	Res	Type
1	M	1222	LEU
1	M	1240	MET
1	M	1244	LEU
1	L	986	VAL
1	L	991	GLU
1	L	994	VAL
1	L	997	GLU
1	L	1003	ARG
1	L	1004	GLU
1	L	1017	VAL
1	L	1019	LYS
1	L	1023	LYS
1	L	1032	ILE
1	L	1036	ASN
1	L	1037	GLU
1	L	1042	ARG
1	L	1048	LEU
1	L	1080	GLU
1	L	1081	LEU
1	L	1109	LEU
1	L	1126	LEU
1	L	1151	ILE
1	L	1163	THR
1	L	1177	ARG
1	L	1201	VAL
1	L	1211	GLN
1	L	1222	LEU
1	L	1240	MET
1	L	1243	GLU
1	L	1244	LEU
1	L	1268	GLU
1	R	986	VAL
1	R	994	VAL
1	R	997	GLU
1	R	1000	THR
1	R	1003	ARG
1	R	1004	GLU
1	R	1009	SER
1	R	1021	VAL
1	R	1023	LYS
1	R	1024	ASP
1	R	1032	ILE

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Mol	Chain	Res	Type
1	R	1036	ASN
1	R	1046	GLU
1	R	1048	LEU
1	R	1052	SER
1	R	1058	ASN
1	R	1064	ARG
1	R	1068	VAL
1	R	1080	GLU
1	R	1081	LEU
1	R	1109	LEU
1	R	1110	SER
1	R	1126	LEU
1	R	1177	ARG
1	R	1214	GLN
1	R	1219	GLU
1	R	1222	LEU
1	R	1240	MET
1	R	1244	LEU
1	R	1264	SER
1	R	1269	GLU
1	R	1275	ARG
1	S	986	VAL
1	S	994	VAL
1	S	997	GLU
1	S	1000	THR
1	S	1001	MET
1	S	1003	ARG
1	S	1023	LYS
1	S	1035	VAL
1	S	1036	ASN
1	S	1042	ARG
1	S	1048	LEU
1	S	1053	VAL
1	S	1058	ASN
1	S	1068	VAL
1	S	1071	GLN
1	S	1081	LEU
1	S	1088	LYS
1	S	1109	LEU
1	S	1126	LEU
1	S	1127	ASN
1	S	1157	THR

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Mol	Chain	Res	Type
1	S	1168	LYS
1	S	1177	ARG
1	S	1191	THR
1	S	1211	GLN
1	S	1214	GLN
1	S	1222	LEU
1	S	1223	ARG
1	S	1239	ASP
1	S	1240	MET
1	S	1244	LEU
1	S	1254	LYS
1	S	1269	GLU
1	T	985	ASP
1	T	991	GLU
1	T	994	VAL
1	T	1000	THR
1	T	1003	ARG
1	T	1004	GLU
1	T	1009	SER
1	T	1019	LYS
1	T	1023	LYS
1	T	1025	GLU
1	T	1032	ILE
1	T	1036	ASN
1	T	1040	SER
1	T	1042	ARG
1	T	1046	GLU
1	T	1052	SER
1	T	1056	GLU
1	T	1057	PHE
1	T	1058	ASN
1	T	1064	ARG
1	T	1068	VAL
1	T	1081	LEU
1	T	1109	LEU
1	T	1110	SER
1	T	1126	LEU
1	T	1163	THR
1	T	1191	THR
1	T	1207	THR
1	T	1214	GLN
1	T	1222	LEU

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Mol	Chain	Res	Type
1	T	1240	MET
1	T	1244	LEU
1	T	1264	SER
1	T	1268	GLU
1	T	1269	GLU
1	T	1275	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1036	ASN
1	A	1049	ASN
1	A	1058	ASN
1	A	1060	HIS
1	A	1214	GLN
1	A	1236	ASN
1	B	1036	ASN
1	B	1049	ASN
1	B	1058	ASN
1	B	1211	GLN
1	B	1236	ASN
1	C	1036	ASN
1	C	1058	ASN
1	C	1060	HIS
1	C	1236	ASN
1	D	1036	ASN
1	D	1049	ASN
1	D	1058	ASN
1	D	1060	HIS
1	D	1073	GLN
1	D	1236	ASN
1	E	1058	ASN
1	E	1060	HIS
1	E	1073	GLN
1	E	1214	GLN
1	E	1236	ASN
1	F	1049	ASN
1	F	1058	ASN
1	F	1073	GLN
1	F	1236	ASN
1	G	1036	ASN
1	G	1049	ASN

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Mol	Chain	Res	Type
1	G	1060	HIS
1	G	1236	ASN
1	H	1036	ASN
1	H	1060	HIS
1	H	1071	GLN
1	H	1236	ASN
1	H	1250	GLN
1	I	1036	ASN
1	I	1058	ASN
1	I	1073	GLN
1	I	1214	GLN
1	J	1007	GLN
1	J	1036	ASN
1	J	1049	ASN
1	J	1058	ASN
1	J	1060	HIS
1	J	1214	GLN
1	K	1036	ASN
1	K	1058	ASN
1	K	1060	HIS
1	K	1236	ASN
1	M	1036	ASN
1	M	1049	ASN
1	M	1058	ASN
1	M	1060	HIS
1	M	1214	GLN
1	L	1036	ASN
1	L	1058	ASN
1	L	1073	GLN
1	L	1236	ASN
1	R	1007	GLN
1	R	1036	ASN
1	R	1058	ASN
1	R	1236	ASN
1	S	1007	GLN
1	S	1036	ASN
1	S	1058	ASN
1	S	1061	HIS
1	S	1127	ASN
1	S	1236	ASN
1	T	1036	ASN
1	T	1049	ASN

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Mol	Chain	Res	Type
1	T	1058	ASN
1	T	1073	GLN
1	T	1127	ASN
1	T	1236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PTR	R	1165	1	15,16,17	1.97	2 (13%)	19,22,24	0.63	0
1	PTR	D	1166	1	15,16,17	2.00	2 (13%)	19,22,24	0.80	1 (5%)
1	PTR	J	1166	1	15,16,17	1.95	2 (13%)	19,22,24	0.97	1 (5%)
1	PTR	S	1165	1	15,16,17	1.94	1 (6%)	19,22,24	0.73	1 (5%)
1	PTR	J	1165	1	15,16,17	2.00	2 (13%)	19,22,24	0.75	1 (5%)
1	PTR	S	1161	1	11,12,17	0.55	0	12,15,24	0.24	0
1	PTR	R	1166	1	15,16,17	1.90	2 (13%)	19,22,24	0.66	0
1	PTR	E	1166	1	15,16,17	1.97	2 (13%)	19,22,24	0.60	0
1	PTR	M	1165	1	15,16,17	1.95	1 (6%)	19,22,24	0.64	1 (5%)
1	PTR	B	1165	1	15,16,17	1.98	1 (6%)	19,22,24	0.65	1 (5%)
1	PTR	E	1161	1	11,12,17	0.72	0	12,15,24	0.52	0
1	PTR	B	1161	1	11,12,17	0.70	0	12,15,24	0.22	0
1	PTR	H	1166	1	15,16,17	1.92	2 (13%)	19,22,24	0.70	0
1	PTR	E	1165	1	15,16,17	2.03	1 (6%)	19,22,24	0.91	2 (10%)
1	PTR	C	1161	1	11,12,17	0.76	0	12,15,24	0.30	0
1	PTR	B	1166	1	15,16,17	2.16	2 (13%)	19,22,24	1.11	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PTR	S	1166	1	15,16,17	1.96	2 (13%)	19,22,24	0.76	1 (5%)
1	PTR	M	1166	1	15,16,17	2.13	3 (20%)	19,22,24	1.72	6 (31%)
1	PTR	T	1165	1	15,16,17	1.99	1 (6%)	19,22,24	0.65	0
1	PTR	H	1165	1	15,16,17	1.93	2 (13%)	19,22,24	0.69	0
1	PTR	F	1161	1	11,12,17	0.77	0	12,15,24	0.29	0
1	PTR	G	1166	1	15,16,17	2.03	2 (13%)	19,22,24	0.71	1 (5%)
1	PTR	F	1165	1	15,16,17	1.93	1 (6%)	19,22,24	0.81	1 (5%)
1	PTR	K	1161	1	11,12,17	0.66	0	12,15,24	0.27	0
1	PTR	G	1165	1	15,16,17	1.95	2 (13%)	19,22,24	0.81	1 (5%)
1	PTR	I	1166	1	15,16,17	1.99	2 (13%)	19,22,24	1.01	2 (10%)
1	PTR	R	1161	1	11,12,17	0.63	0	12,15,24	0.29	0
1	PTR	I	1165	1	15,16,17	2.02	1 (6%)	19,22,24	0.54	0
1	PTR	L	1161	1	11,12,17	0.75	0	12,15,24	0.34	0
1	PTR	H	1161	1	11,12,17	0.68	0	12,15,24	0.41	0
1	PTR	C	1165	1	15,16,17	2.01	2 (13%)	19,22,24	0.60	0
1	PTR	J	1161	1	11,12,17	0.70	0	12,15,24	0.19	0
1	PTR	F	1166	1	15,16,17	1.97	2 (13%)	19,22,24	0.86	1 (5%)
1	PTR	K	1166	1	15,16,17	1.91	2 (13%)	19,22,24	0.88	0
1	PTR	A	1166	1	15,16,17	2.01	2 (13%)	19,22,24	0.78	1 (5%)
1	PTR	M	1161	1	11,12,17	0.77	0	12,15,24	0.31	0
1	PTR	K	1165	1	15,16,17	1.97	1 (6%)	19,22,24	0.48	0
1	PTR	C	1166	1	15,16,17	2.07	1 (6%)	19,22,24	0.69	1 (5%)
1	PTR	I	1161	1	11,12,17	0.61	0	12,15,24	0.29	0
1	PTR	T	1166	1	15,16,17	1.91	2 (13%)	19,22,24	0.81	1 (5%)
1	PTR	L	1165	1	15,16,17	1.96	1 (6%)	19,22,24	0.49	0
1	PTR	A	1165	1	15,16,17	1.93	1 (6%)	19,22,24	0.52	0
1	PTR	T	1161	1	11,12,17	0.61	0	12,15,24	0.51	0
1	PTR	G	1161	1	11,12,17	0.57	0	12,15,24	0.29	0
1	PTR	D	1161	1	11,12,17	0.68	0	12,15,24	0.46	0
1	PTR	A	1161	1	15,16,17	1.98	2 (13%)	19,22,24	0.86	1 (5%)
1	PTR	L	1166	1	15,16,17	2.01	2 (13%)	19,22,24	0.94	2 (10%)
1	PTR	D	1165	1	15,16,17	1.96	1 (6%)	19,22,24	0.65	1 (5%)

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
1	PTR	R	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	D	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	J	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	S	1165	1	-	1/10/11/13	0/1/1/1
1	PTR	J	1165	1	-	1/10/11/13	0/1/1/1
1	PTR	S	1161	1	-	2/5/6/13	0/1/1/1
1	PTR	R	1166	1	-	2/10/11/13	0/1/1/1
1	PTR	E	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	M	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	E	1161	1	-	2/5/6/13	0/1/1/1
1	PTR	B	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	H	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	E	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	C	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	B	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	S	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	M	1166	1	-	2/10/11/13	0/1/1/1
1	PTR	T	1165	1	-	2/10/11/13	0/1/1/1
1	PTR	H	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	F	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	G	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	F	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	K	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	G	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	I	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	R	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	I	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	L	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	H	1161	1	-	1/5/6/13	0/1/1/1
1	PTR	C	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	J	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	F	1166	1	-	1/10/11/13	0/1/1/1
1	PTR	K	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	M	1161	1	-	2/5/6/13	0/1/1/1
1	PTR	K	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	C	1166	1	-	2/10/11/13	0/1/1/1
1	PTR	I	1161	1	-	2/5/6/13	0/1/1/1
1	PTR	T	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	L	1165	1	-	0/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	T	1161	1	-	2/5/6/13	0/1/1/1
1	PTR	G	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	D	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	A	1161	1	-	0/10/11/13	0/1/1/1
1	PTR	L	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	D	1165	1	-	1/10/11/13	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1166	PTR	OH-CZ	-7.68	1.23	1.40
1	E	1165	PTR	OH-CZ	-7.59	1.23	1.40
1	G	1166	PTR	OH-CZ	-7.47	1.23	1.40
1	I	1165	PTR	OH-CZ	-7.46	1.23	1.40
1	T	1165	PTR	OH-CZ	-7.36	1.23	1.40
1	L	1165	PTR	OH-CZ	-7.35	1.24	1.40
1	K	1165	PTR	OH-CZ	-7.33	1.24	1.40
1	C	1165	PTR	OH-CZ	-7.33	1.24	1.40
1	A	1166	PTR	OH-CZ	-7.31	1.24	1.40
1	B	1165	PTR	OH-CZ	-7.28	1.24	1.40
1	D	1166	PTR	OH-CZ	-7.27	1.24	1.40
1	J	1165	PTR	OH-CZ	-7.26	1.24	1.40
1	D	1165	PTR	OH-CZ	-7.25	1.24	1.40
1	R	1165	PTR	OH-CZ	-7.21	1.24	1.40
1	L	1166	PTR	OH-CZ	-7.19	1.24	1.40
1	F	1166	PTR	OH-CZ	-7.19	1.24	1.40
1	M	1165	PTR	OH-CZ	-7.14	1.24	1.40
1	S	1165	PTR	OH-CZ	-7.13	1.24	1.40
1	A	1161	PTR	OH-CZ	-7.13	1.24	1.40
1	A	1165	PTR	OH-CZ	-7.12	1.24	1.40
1	E	1166	PTR	OH-CZ	-7.10	1.24	1.40
1	I	1166	PTR	OH-CZ	-7.10	1.24	1.40
1	F	1165	PTR	OH-CZ	-7.09	1.24	1.40
1	J	1166	PTR	OH-CZ	-7.04	1.24	1.40
1	S	1166	PTR	OH-CZ	-7.01	1.24	1.40
1	H	1165	PTR	OH-CZ	-6.97	1.24	1.40
1	G	1165	PTR	OH-CZ	-6.93	1.24	1.40
1	T	1166	PTR	OH-CZ	-6.93	1.24	1.40
1	R	1166	PTR	OH-CZ	-6.88	1.25	1.40
1	B	1166	PTR	OH-CZ	-6.86	1.25	1.40
1	H	1166	PTR	OH-CZ	-6.77	1.25	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	1166	PTR	OH-CZ	-6.77	1.25	1.40
1	M	1166	PTR	OH-CZ	-6.53	1.25	1.40
1	B	1166	PTR	P-OH	3.61	1.64	1.59
1	M	1166	PTR	P-OH	3.45	1.64	1.59
1	I	1166	PTR	P-OH	2.67	1.63	1.59
1	H	1166	PTR	P-OH	2.64	1.63	1.59
1	L	1166	PTR	P-OH	2.57	1.63	1.59
1	K	1166	PTR	P-OH	2.54	1.63	1.59
1	S	1166	PTR	P-OH	2.52	1.63	1.59
1	M	1166	PTR	CE1-CD1	2.46	1.43	1.38
1	G	1165	PTR	P-OH	2.42	1.63	1.59
1	E	1166	PTR	P-OH	2.29	1.62	1.59
1	J	1165	PTR	P-OH	2.27	1.62	1.59
1	J	1166	PTR	P-OH	2.25	1.62	1.59
1	C	1165	PTR	P-OH	2.24	1.62	1.59
1	T	1166	PTR	P-OH	2.24	1.62	1.59
1	F	1166	PTR	P-OH	2.23	1.62	1.59
1	D	1166	PTR	P-OH	2.21	1.62	1.59
1	R	1166	PTR	P-OH	2.20	1.62	1.59
1	A	1161	PTR	P-OH	2.19	1.62	1.59
1	H	1165	PTR	P-OH	2.15	1.62	1.59
1	A	1166	PTR	P-OH	2.12	1.62	1.59
1	R	1165	PTR	P-OH	2.07	1.62	1.59
1	G	1166	PTR	P-OH	2.00	1.62	1.59

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1166	PTR	OH-CZ-CE1	3.60	129.95	119.23
1	I	1166	PTR	O3P-P-OH	3.26	115.43	105.24
1	M	1166	PTR	O3P-P-OH	2.97	114.52	105.24
1	J	1166	PTR	O2P-P-OH	2.82	114.06	105.24
1	A	1161	PTR	CB-CA-C	-2.65	106.50	111.47
1	M	1166	PTR	O2P-P-OH	2.65	113.51	105.24
1	B	1166	PTR	O2P-P-OH	2.60	113.37	105.24
1	F	1166	PTR	O3P-P-OH	2.52	113.12	105.24
1	L	1166	PTR	CB-CA-C	-2.48	106.81	111.47
1	E	1165	PTR	O2P-P-OH	2.48	113.00	105.24
1	M	1166	PTR	OH-CZ-CE2	-2.48	111.86	119.23
1	B	1165	PTR	O2P-P-OH	2.46	112.93	105.24
1	S	1166	PTR	O3P-P-OH	2.43	112.84	105.24
1	G	1166	PTR	O3P-P-OH	2.42	112.80	105.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1166	PTR	O2P-P-OH	2.41	112.79	105.24
1	T	1166	PTR	O2P-P-OH	2.41	112.78	105.24
1	A	1166	PTR	O2P-P-OH	2.39	112.73	105.24
1	D	1166	PTR	O2P-P-OH	2.39	112.71	105.24
1	M	1166	PTR	CB-CA-C	-2.38	107.00	111.47
1	S	1165	PTR	O3P-P-OH	2.34	112.57	105.24
1	J	1165	PTR	O2P-P-OH	2.33	112.53	105.24
1	B	1166	PTR	O3P-P-OH	2.32	112.50	105.24
1	L	1166	PTR	O2P-P-OH	2.30	112.45	105.24
1	M	1165	PTR	O2P-P-OH	2.27	112.33	105.24
1	G	1165	PTR	O2P-P-OH	2.22	112.17	105.24
1	M	1166	PTR	O2P-P-O1P	-2.21	102.02	110.68
1	D	1165	PTR	O2P-P-OH	2.21	112.15	105.24
1	F	1165	PTR	O2P-P-OH	2.14	111.92	105.24
1	I	1166	PTR	P-OH-CZ	2.12	130.53	123.75
1	E	1165	PTR	CB-CA-C	-2.06	107.61	111.47

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	1166	PTR	CZ-OH-P-O1P
1	C	1166	PTR	CZ-OH-P-O1P
1	S	1165	PTR	N-CA-CB-CG
1	D	1165	PTR	N-CA-CB-CG
1	M	1161	PTR	CA-CB-CG-CD1
1	R	1166	PTR	CZ-OH-P-O3P
1	M	1161	PTR	CA-CB-CG-CD2
1	I	1161	PTR	CA-CB-CG-CD2
1	E	1161	PTR	CA-CB-CG-CD1
1	I	1161	PTR	CA-CB-CG-CD1
1	E	1161	PTR	CA-CB-CG-CD2
1	J	1165	PTR	N-CA-CB-CG
1	T	1165	PTR	CA-CB-CG-CD1
1	T	1165	PTR	CA-CB-CG-CD2
1	T	1161	PTR	CA-CB-CG-CD1
1	T	1161	PTR	CA-CB-CG-CD2
1	S	1161	PTR	CA-CB-CG-CD2
1	S	1161	PTR	CA-CB-CG-CD1
1	M	1166	PTR	CE2-CZ-OH-P
1	M	1166	PTR	CE1-CZ-OH-P
1	C	1166	PTR	CZ-OH-P-O3P

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Mol	Chain	Res	Type	Atoms
1	H	1161	PTR	CA-CB-CG-CD2
1	R	1166	PTR	CE1-CZ-OH-P

There are no ring outliers.

37 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	1165	PTR	2	0
1	S	1165	PTR	1	0
1	S	1161	PTR	8	0
1	R	1166	PTR	1	0
1	E	1166	PTR	4	0
1	M	1165	PTR	2	0
1	B	1165	PTR	4	0
1	B	1161	PTR	1	0
1	B	1166	PTR	2	0
1	S	1166	PTR	1	0
1	M	1166	PTR	6	0
1	T	1165	PTR	2	0
1	H	1165	PTR	1	0
1	F	1161	PTR	1	0
1	G	1166	PTR	1	0
1	F	1165	PTR	2	0
1	K	1161	PTR	1	0
1	G	1165	PTR	4	0
1	R	1161	PTR	4	0
1	I	1165	PTR	3	0
1	L	1161	PTR	4	0
1	H	1161	PTR	3	0
1	C	1165	PTR	3	0
1	J	1161	PTR	1	0
1	F	1166	PTR	1	0
1	K	1166	PTR	1	0
1	A	1166	PTR	2	0
1	M	1161	PTR	5	0
1	K	1165	PTR	2	0
1	C	1166	PTR	2	0
1	I	1161	PTR	4	0
1	L	1165	PTR	4	0
1	T	1161	PTR	5	0
1	G	1161	PTR	3	0
1	D	1161	PTR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1161	PTR	1	0
1	D	1165	PTR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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$
2	741	L	13	-	39,41,41	1.12	4 (10%)	47,56,56	2.48	15 (31%)
2	741	R	14	-	39,41,41	1.16	4 (10%)	47,56,56	2.21	13 (27%)
2	741	D	4	-	39,41,41	1.14	2 (5%)	47,56,56	2.15	15 (31%)
2	741	H	8	-	39,41,41	0.97	2 (5%)	47,56,56	2.24	14 (29%)
2	741	T	16	-	39,41,41	1.01	2 (5%)	47,56,56	2.57	14 (29%)
2	741	C	3	-	39,41,41	1.04	2 (5%)	47,56,56	2.18	13 (27%)
2	741	I	9	-	39,41,41	0.95	2 (5%)	47,56,56	2.37	13 (27%)
2	741	G	7	-	39,41,41	0.97	2 (5%)	47,56,56	2.33	15 (31%)
2	741	B	2	-	39,41,41	1.01	2 (5%)	47,56,56	2.49	14 (29%)
2	741	K	11	-	39,41,41	0.99	1 (2%)	47,56,56	2.40	14 (29%)
2	741	M	12	-	39,41,41	1.01	2 (5%)	47,56,56	2.14	11 (23%)
2	741	S	15	-	39,41,41	0.98	2 (5%)	47,56,56	2.43	18 (38%)
2	741	F	6	-	39,41,41	1.05	3 (7%)	47,56,56	2.29	16 (34%)
2	741	A	1	-	39,41,41	1.05	3 (7%)	47,56,56	2.25	14 (29%)
2	741	E	5	-	39,41,41	1.10	2 (5%)	47,56,56	2.33	13 (27%)
2	741	J	10	-	39,41,41	1.13	3 (7%)	47,56,56	2.23	15 (31%)

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
2	741	L	13	-	-	10/20/22/22	0/4/4/4
2	741	R	14	-	-	7/20/22/22	0/4/4/4
2	741	D	4	-	-	7/20/22/22	0/4/4/4
2	741	H	8	-	-	8/20/22/22	0/4/4/4
2	741	T	16	-	-	8/20/22/22	0/4/4/4
2	741	C	3	-	-	9/20/22/22	0/4/4/4
2	741	I	9	-	-	5/20/22/22	0/4/4/4
2	741	G	7	-	-	12/20/22/22	0/4/4/4
2	741	B	2	-	-	8/20/22/22	0/4/4/4
2	741	K	11	-	-	6/20/22/22	0/4/4/4
2	741	M	12	-	-	5/20/22/22	0/4/4/4
2	741	S	15	-	-	11/20/22/22	0/4/4/4
2	741	F	6	-	-	7/20/22/22	0/4/4/4
2	741	A	1	-	-	11/20/22/22	0/4/4/4
2	741	E	5	-	-	6/20/22/22	0/4/4/4
2	741	J	10	-	-	7/20/22/22	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	13	741	C3-C2	2.88	1.41	1.36
2	C	3	741	C3-C2	2.87	1.41	1.36
2	D	4	741	C3-C2	2.80	1.41	1.36
2	R	14	741	C3-C2	2.79	1.41	1.36
2	L	13	741	C6-C1	2.72	1.41	1.36
2	M	12	741	C3-C2	2.71	1.41	1.36
2	A	1	741	C3-C2	2.69	1.41	1.36
2	D	4	741	C6-C1	2.68	1.41	1.36
2	C	3	741	C6-C1	2.67	1.41	1.36
2	F	6	741	C6-C1	2.66	1.41	1.36
2	R	14	741	C6-C1	2.65	1.41	1.36
2	E	5	741	C6-C1	2.63	1.41	1.36
2	E	5	741	C3-C2	2.62	1.41	1.36
2	J	10	741	C3-C2	2.62	1.41	1.36
2	M	12	741	C6-C1	2.54	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	741	C3-C2	2.51	1.41	1.36
2	A	1	741	C6-C1	2.50	1.41	1.36
2	K	11	741	C3-C2	2.46	1.41	1.36
2	G	7	741	C6-C1	2.41	1.40	1.36
2	J	10	741	C5-C4	2.41	1.46	1.42
2	H	8	741	C6-C1	2.38	1.40	1.36
2	A	1	741	C26-N30	-2.38	1.34	1.36
2	B	2	741	C6-C1	2.35	1.40	1.36
2	J	10	741	C6-C1	2.34	1.40	1.36
2	I	9	741	C3-C2	2.31	1.40	1.36
2	I	9	741	C6-C1	2.27	1.40	1.36
2	S	15	741	C6-C1	2.27	1.40	1.36
2	S	15	741	C3-C2	2.26	1.40	1.36
2	G	7	741	C3-C2	2.25	1.40	1.36
2	T	16	741	C6-C1	2.23	1.40	1.36
2	F	6	741	C3-C2	2.20	1.40	1.36
2	T	16	741	C3-C2	2.20	1.40	1.36
2	R	14	741	C23-C22	2.19	1.42	1.38
2	H	8	741	C3-C2	2.16	1.40	1.36
2	R	14	741	C5-C4	2.16	1.46	1.42
2	L	13	741	O12-C2	2.10	1.41	1.37
2	L	13	741	O11-C1	2.05	1.40	1.37
2	F	6	741	C5-C4	2.01	1.45	1.42

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	16	741	O11-C1-C6	-8.35	114.45	125.24
2	J	10	741	O11-C1-C6	-6.97	116.22	125.24
2	L	13	741	O11-C1-C6	-6.90	116.31	125.24
2	B	2	741	O11-C1-C6	-6.90	116.32	125.24
2	E	5	741	C29-N30-C26	-6.87	102.03	108.56
2	M	12	741	C29-N30-C26	-6.80	102.10	108.56
2	C	3	741	C29-N30-C26	-6.78	102.11	108.56
2	A	1	741	O11-C1-C6	-6.75	116.51	125.24
2	K	11	741	C29-N30-C26	-6.73	102.16	108.56
2	G	7	741	C29-N30-C26	-6.69	102.20	108.56
2	S	15	741	C29-N30-C26	-6.68	102.21	108.56
2	I	9	741	C29-N30-C26	-6.62	102.27	108.56
2	T	16	741	O11-C1-C2	6.59	124.59	115.41
2	T	16	741	C29-N30-C26	-6.58	102.31	108.56
2	H	8	741	C29-N30-C26	-6.57	102.32	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	741	C29-N30-C26	-6.56	102.32	108.56
2	D	4	741	C29-N30-C26	-6.50	102.39	108.56
2	G	7	741	O11-C1-C6	-6.44	116.91	125.24
2	F	6	741	C29-N30-C26	-6.40	102.48	108.56
2	R	14	741	C29-N30-C26	-6.33	102.54	108.56
2	B	2	741	C29-N30-C26	-6.28	102.59	108.56
2	K	11	741	O11-C1-C6	-6.25	117.16	125.24
2	L	13	741	C29-N30-C26	-6.22	102.65	108.56
2	F	6	741	O11-C1-C6	-5.96	117.54	125.24
2	B	2	741	C16-O11-C1	-5.87	108.68	117.53
2	J	10	741	C29-N30-C26	-5.78	103.07	108.56
2	I	9	741	O11-C1-C6	-5.65	117.93	125.24
2	K	11	741	C16-O11-C1	-5.63	109.03	117.53
2	E	5	741	C9-C8-N7	-5.63	121.49	125.68
2	I	9	741	C9-C8-N7	-5.60	121.52	125.68
2	S	15	741	O11-C1-C6	-5.55	118.06	125.24
2	A	1	741	O11-C1-C2	5.53	123.11	115.41
2	E	5	741	O11-C1-C6	-5.49	118.14	125.24
2	T	16	741	C9-C8-N7	-5.45	121.63	125.68
2	S	15	741	C16-O11-C1	-5.29	109.54	117.53
2	L	13	741	C26-S25-C21	5.24	110.70	101.87
2	H	8	741	O11-C1-C6	-5.14	118.59	125.24
2	B	2	741	C26-S25-C21	5.09	110.44	101.87
2	D	4	741	O11-C1-C6	-5.07	118.69	125.24
2	M	12	741	C31-N30-C26	5.05	130.42	125.62
2	S	15	741	C9-C8-N7	-5.01	121.95	125.68
2	C	3	741	C9-C8-N7	-5.01	121.96	125.68
2	R	14	741	O11-C1-C6	-5.00	118.78	125.24
2	G	7	741	C31-N30-C26	4.93	130.31	125.62
2	K	11	741	C9-C8-N7	-4.89	122.04	125.68
2	L	13	741	C9-C8-N7	-4.86	122.07	125.68
2	M	12	741	C9-C8-N7	-4.81	122.10	125.68
2	R	14	741	C9-C8-N7	-4.80	122.11	125.68
2	M	12	741	O11-C1-C6	-4.73	119.12	125.24
2	L	13	741	O11-C1-C2	4.69	121.95	115.41
2	B	2	741	C9-C8-N7	-4.65	122.22	125.68
2	D	4	741	C9-C8-N7	-4.63	122.24	125.68
2	B	2	741	O11-C1-C2	4.62	121.85	115.41
2	I	9	741	C16-O11-C1	-4.49	110.76	117.53
2	F	6	741	C9-C8-N7	-4.48	122.35	125.68
2	C	3	741	O11-C1-C6	-4.44	119.49	125.24
2	E	5	741	C31-N30-C26	4.42	129.83	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7	741	C16-O11-C1	-4.40	110.89	117.53
2	J	10	741	C9-C8-N7	-4.31	122.47	125.68
2	F	6	741	C31-N30-C26	4.24	129.66	125.62
2	H	8	741	C31-N30-C26	4.24	129.65	125.62
2	J	10	741	O11-C1-C2	4.22	121.28	115.41
2	G	7	741	O11-C1-C2	4.19	121.24	115.41
2	L	13	741	C13-O12-C2	4.15	127.84	117.69
2	A	1	741	C9-C8-N7	-4.15	122.59	125.68
2	G	7	741	C9-C8-N7	-4.09	122.64	125.68
2	K	11	741	O11-C1-C2	4.06	121.07	115.41
2	E	5	741	C13-O12-C2	4.04	127.58	117.69
2	H	8	741	C15-C14-C13	4.01	127.53	112.93
2	I	9	741	C31-N30-C26	4.00	129.43	125.62
2	S	15	741	C15-C14-C13	4.00	127.50	112.93
2	E	5	741	C8-N7-C4	3.97	121.69	116.91
2	R	14	741	C16-O11-C1	-3.93	111.60	117.53
2	L	13	741	C8-N7-C4	3.92	121.62	116.91
2	R	14	741	C31-N30-C26	3.89	129.32	125.62
2	J	10	741	C15-C14-C13	3.88	127.07	112.93
2	J	10	741	C13-O12-C2	3.87	127.15	117.69
2	R	14	741	C8-N7-C4	3.86	121.55	116.91
2	I	9	741	C8-N7-C4	3.82	121.50	116.91
2	I	9	741	C13-O12-C2	3.80	126.98	117.69
2	K	11	741	C31-N30-C26	3.77	129.20	125.62
2	B	2	741	C8-N7-C4	3.77	121.44	116.91
2	S	15	741	C31-N30-C26	3.75	129.19	125.62
2	F	6	741	O11-C1-C2	3.75	120.63	115.41
2	S	15	741	C13-O12-C2	3.73	126.82	117.69
2	C	3	741	C8-N7-C4	3.73	121.40	116.91
2	F	6	741	C16-O11-C1	-3.73	111.91	117.53
2	L	13	741	C31-N30-C26	3.71	129.15	125.62
2	H	8	741	C9-C8-N7	-3.70	122.93	125.68
2	E	5	741	O11-C1-C2	3.69	120.55	115.41
2	H	8	741	C13-O12-C2	3.68	126.69	117.69
2	F	6	741	C13-O12-C2	3.68	126.69	117.69
2	B	2	741	C5-C4-N7	-3.67	118.92	122.83
2	R	14	741	C5-C4-N7	-3.65	118.94	122.83
2	C	3	741	C31-N30-C26	3.65	129.09	125.62
2	C	3	741	C13-O12-C2	3.63	126.57	117.69
2	T	16	741	C8-N7-C4	3.60	121.25	116.91
2	S	15	741	C8-N7-C4	3.55	121.19	116.91
2	E	5	741	C5-C4-N7	-3.54	119.06	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	741	C15-C14-C13	3.52	125.77	112.93
2	I	9	741	C5-C4-N7	-3.51	119.09	122.83
2	H	8	741	C5-C4-N7	-3.47	119.13	122.83
2	L	13	741	C16-O11-C1	-3.45	112.32	117.53
2	H	8	741	O11-C1-C2	3.45	120.21	115.41
2	T	16	741	C15-C14-C13	3.42	125.39	112.93
2	K	11	741	C15-C14-C13	3.42	125.38	112.93
2	M	12	741	C8-N7-C4	3.38	120.98	116.91
2	E	5	741	C15-C14-C13	3.37	125.21	112.93
2	T	16	741	C26-S25-C21	3.36	107.53	101.87
2	J	10	741	C16-O11-C1	-3.36	112.46	117.53
2	L	13	741	C5-C4-N7	-3.32	119.30	122.83
2	R	14	741	C13-O12-C2	3.31	125.79	117.69
2	C	3	741	C16-O11-C1	-3.29	112.56	117.53
2	R	14	741	C15-C14-C13	3.28	124.87	112.93
2	C	3	741	C5-C4-N7	-3.28	119.34	122.83
2	F	6	741	C8-N7-C4	3.27	120.84	116.91
2	K	11	741	C13-O12-C2	3.24	125.62	117.69
2	H	8	741	C8-N7-C4	3.24	120.81	116.91
2	D	4	741	C13-O12-C2	3.21	125.55	117.69
2	C	3	741	C15-C14-C13	3.21	124.63	112.93
2	T	16	741	C5-C4-N7	-3.21	119.41	122.83
2	F	6	741	C5-C4-N7	-3.16	119.46	122.83
2	T	16	741	C13-O12-C2	3.15	125.39	117.69
2	M	12	741	C16-O11-C1	-3.13	112.80	117.53
2	D	4	741	C8-N7-C4	3.10	120.64	116.91
2	M	12	741	C15-C14-C13	3.06	124.07	112.93
2	K	11	741	C5-C4-N7	-3.03	119.60	122.83
2	T	16	741	C31-N30-C26	3.03	128.50	125.62
2	S	15	741	C14-C15-N34	-3.02	104.86	113.79
2	M	12	741	C14-C15-N34	-3.00	104.93	113.79
2	I	9	741	C15-C14-C13	2.98	123.81	112.93
2	D	4	741	C15-C14-C13	2.98	123.78	112.93
2	D	4	741	C5-C4-N7	-2.97	119.67	122.83
2	M	12	741	C5-C4-N7	-2.96	119.68	122.83
2	D	4	741	O11-C1-C2	2.95	119.52	115.41
2	A	1	741	C14-C15-N34	-2.95	105.09	113.79
2	D	4	741	C26-S25-C21	2.92	106.79	101.87
2	B	2	741	C15-C14-C13	2.90	123.51	112.93
2	G	7	741	C13-O12-C2	2.88	124.73	117.69
2	K	11	741	C8-N7-C4	2.88	120.38	116.91
2	A	1	741	C15-C14-C13	2.87	123.40	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	10	741	C5-C4-N7	-2.86	119.79	122.83
2	M	12	741	O11-C1-C2	2.82	119.33	115.41
2	S	15	741	C5-C4-N7	-2.80	119.85	122.83
2	D	4	741	C16-O11-C1	-2.80	113.31	117.53
2	G	7	741	C8-N7-C4	2.79	120.27	116.91
2	I	9	741	O11-C1-C2	2.77	119.27	115.41
2	A	1	741	C9-C32-N33	-2.77	173.31	177.88
2	A	1	741	C13-O12-C2	2.74	124.39	117.69
2	D	4	741	C8-C9-C32	-2.73	113.40	119.10
2	H	8	741	C14-C15-N34	-2.73	105.73	113.79
2	A	1	741	C8-N7-C4	2.72	120.19	116.91
2	B	2	741	C31-N30-C26	2.71	128.20	125.62
2	S	15	741	O11-C1-C2	2.69	119.15	115.41
2	S	15	741	C6-C1-C2	2.68	122.71	120.07
2	C	3	741	O11-C1-C2	2.67	119.13	115.41
2	B	2	741	C13-O12-C2	2.67	124.22	117.69
2	G	7	741	C15-C14-C13	2.66	122.64	112.93
2	I	9	741	C26-S25-C21	2.66	106.34	101.87
2	H	8	741	O12-C13-C14	-2.65	98.50	108.33
2	G	7	741	C5-C4-N7	-2.65	120.01	122.83
2	I	9	741	C6-C1-C2	2.64	122.68	120.07
2	E	5	741	C16-O11-C1	-2.64	113.54	117.53
2	C	3	741	C14-C15-N34	-2.62	106.04	113.79
2	G	7	741	C14-C15-N34	-2.61	106.09	113.79
2	H	8	741	C16-O11-C1	-2.60	113.61	117.53
2	R	14	741	O11-C1-C2	2.59	119.02	115.41
2	I	9	741	C9-C32-N33	-2.59	173.62	177.88
2	A	1	741	C31-N30-C29	2.57	129.77	124.89
2	E	5	741	C20-C19-C18	2.53	123.22	120.30
2	R	14	741	C26-S25-C21	2.53	106.13	101.87
2	K	11	741	C6-C5-C10	-2.52	120.12	123.22
2	D	4	741	C31-N30-C26	2.51	128.01	125.62
2	L	13	741	C14-C15-N34	-2.50	106.40	113.79
2	F	6	741	C26-S25-C21	2.49	106.07	101.87
2	D	4	741	C31-N30-C29	2.46	129.57	124.89
2	H	8	741	C8-C9-C32	-2.45	113.98	119.10
2	M	12	741	C13-O12-C2	2.44	123.67	117.69
2	J	10	741	C31-N30-C29	2.42	129.49	124.89
2	S	15	741	C23-C22-CL24	2.39	122.35	118.49
2	S	15	741	C8-C9-C32	-2.39	114.13	119.10
2	A	1	741	C5-C4-N7	-2.38	120.29	122.83
2	J	10	741	C6-C1-C2	2.38	122.42	120.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8	741	C26-S25-C21	2.38	105.87	101.87
2	L	13	741	O12-C2-C3	-2.38	121.17	125.19
2	D	4	741	C9-C32-N33	-2.37	173.97	177.88
2	A	1	741	C31-N30-C26	2.37	127.88	125.62
2	G	7	741	C8-C9-C32	-2.35	114.20	119.10
2	L	13	741	C15-C14-C13	2.35	121.48	112.93
2	R	14	741	C14-C15-N34	-2.34	106.88	113.79
2	J	10	741	C8-C9-C32	-2.32	114.27	119.10
2	E	5	741	C26-S25-C21	2.29	105.73	101.87
2	G	7	741	C23-C22-CL24	2.27	122.15	118.49
2	S	15	741	C20-C21-C22	2.26	120.53	117.52
2	B	2	741	C31-N30-C29	2.25	129.17	124.89
2	S	15	741	O12-C13-C14	-2.25	99.98	108.33
2	T	16	741	C20-C19-C18	2.25	122.89	120.30
2	T	16	741	C31-N30-C29	2.24	129.16	124.89
2	T	16	741	C23-C22-CL24	2.22	122.08	118.49
2	K	11	741	C10-C5-C4	2.22	120.54	117.30
2	J	10	741	C8-N7-C4	2.22	119.58	116.91
2	G	7	741	C21-C22-CL24	-2.22	115.79	119.69
2	J	10	741	C26-S25-C21	2.17	105.53	101.87
2	R	14	741	C6-C1-C2	2.17	122.21	120.07
2	F	6	741	O12-C13-C14	-2.16	100.31	108.33
2	D	4	741	C14-C15-N34	-2.16	107.42	113.79
2	G	7	741	C26-S25-C21	2.15	105.50	101.87
2	B	2	741	C14-C15-N34	-2.15	107.44	113.79
2	S	15	741	C36-N34-C15	2.14	116.46	110.62
2	F	6	741	C14-C15-N34	-2.14	107.48	113.79
2	S	15	741	C9-C32-N33	-2.11	174.40	177.88
2	J	10	741	O12-C13-C14	-2.10	100.55	108.33
2	L	13	741	C8-C9-C32	-2.09	114.75	119.10
2	F	6	741	C20-C19-C18	2.09	122.71	120.30
2	C	3	741	C36-N34-C15	2.05	116.23	110.62
2	L	13	741	O12-C2-C1	2.05	119.97	115.73
2	B	2	741	C9-C32-N33	-2.05	174.50	177.88
2	C	3	741	C31-N30-C29	2.04	128.76	124.89
2	J	10	741	C14-C15-N34	-2.03	107.81	113.79
2	K	11	741	C26-S25-C21	2.03	105.28	101.87
2	A	1	741	C36-N34-C15	2.02	116.14	110.62
2	E	5	741	C19-C18-C23	-2.02	117.26	119.65
2	A	1	741	O12-C13-C14	-2.01	100.86	108.33
2	T	16	741	C21-C22-CL24	-2.01	116.16	119.69
2	K	11	741	C23-C22-CL24	2.01	121.73	118.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	741	C8-C9-C32	-2.00	114.92	119.10
2	F	6	741	C10-C5-C4	2.00	120.22	117.30

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	13	741	C13-C14-C15-N34
2	L	13	741	N34-C35-C37-O38
2	S	15	741	N33-C32-C9-C10
2	S	15	741	C14-C15-N34-C36
2	S	15	741	C22-C21-S25-C26
2	S	15	741	C37-C35-N34-C36
2	D	4	741	N33-C32-C9-C10
2	D	4	741	C14-C15-N34-C36
2	D	4	741	N34-C35-C37-O38
2	I	9	741	C22-C21-S25-C26
2	H	8	741	N33-C32-C9-C8
2	H	8	741	N33-C32-C9-C10
2	H	8	741	C14-C15-N34-C36
2	T	16	741	C14-C15-N34-C36
2	T	16	741	C22-C21-S25-C26
2	C	3	741	N33-C32-C9-C8
2	C	3	741	N33-C32-C9-C10
2	C	3	741	C13-C14-C15-N34
2	C	3	741	C37-C35-N34-C36
2	G	7	741	N33-C32-C9-C10
2	G	7	741	C14-C15-N34-C35
2	G	7	741	C22-C21-S25-C26
2	F	6	741	N33-C32-C9-C8
2	F	6	741	C37-C35-N34-C36
2	J	10	741	N33-C32-C9-C10
2	J	10	741	C14-C15-N34-C36
2	J	10	741	C22-C21-S25-C26
2	E	5	741	N33-C32-C9-C10
2	B	2	741	C14-C15-N34-C35
2	B	2	741	N34-C35-C37-O38
2	L	13	741	C3-C2-O12-C13
2	L	13	741	C1-C2-O12-C13
2	A	1	741	C6-C1-O11-C16
2	T	16	741	C2-C1-O11-C16
2	T	16	741	C6-C1-O11-C16

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Mol	Chain	Res	Type	Atoms
2	A	1	741	C2-C1-O11-C16
2	B	2	741	C6-C1-O11-C16
2	R	14	741	O12-C13-C14-C15
2	I	9	741	O12-C13-C14-C15
2	F	6	741	O12-C13-C14-C15
2	G	7	741	C6-C1-O11-C16
2	K	11	741	C6-C1-O11-C16
2	S	15	741	N34-C35-C37-O38
2	I	9	741	N34-C35-C37-O38
2	G	7	741	N34-C35-C37-O38
2	E	5	741	N34-C35-C37-O38
2	C	3	741	O12-C13-C14-C15
2	B	2	741	C2-C1-O11-C16
2	S	15	741	C6-C1-O11-C16
2	G	7	741	C2-C1-O11-C16
2	M	12	741	O12-C13-C14-C15
2	T	16	741	C14-C15-N34-C35
2	S	15	741	C2-C1-O11-C16
2	K	11	741	C2-C1-O11-C16
2	A	1	741	O12-C13-C14-C15
2	G	7	741	O12-C13-C14-C15
2	E	5	741	C14-C13-O12-C2
2	L	13	741	C37-C35-N34-C36
2	R	14	741	C37-C35-N34-C36
2	D	4	741	C37-C35-N34-C36
2	H	8	741	C37-C35-N34-C36
2	A	1	741	C37-C35-N34-C36
2	J	10	741	C37-C35-N34-C36
2	B	2	741	C37-C35-N34-C36
2	R	14	741	C14-C13-O12-C2
2	C	3	741	C37-C35-N34-C15
2	A	1	741	C14-C13-O12-C2
2	J	10	741	C14-C15-N34-C35
2	H	8	741	C14-C13-O12-C2
2	A	1	741	C13-C14-C15-N34
2	G	7	741	C14-C13-O12-C2
2	J	10	741	O12-C13-C14-C15
2	L	13	741	C22-C21-S25-C26
2	R	14	741	C22-C21-S25-C26
2	D	4	741	C22-C21-S25-C26
2	H	8	741	C22-C21-S25-C26
2	C	3	741	C22-C21-S25-C26

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Mol	Chain	Res	Type	Atoms
2	A	1	741	C22-C21-S25-C26
2	F	6	741	C22-C21-S25-C26
2	K	11	741	C22-C21-S25-C26
2	M	12	741	C22-C21-S25-C26
2	E	5	741	C22-C21-S25-C26
2	B	2	741	C22-C21-S25-C26
2	R	14	741	C14-C15-N34-C36
2	A	1	741	C14-C15-N34-C35
2	T	16	741	C14-C13-O12-C2
2	D	4	741	C14-C13-O12-C2
2	S	15	741	C13-C14-C15-N34
2	G	7	741	C13-C14-C15-N34
2	H	8	741	C2-C1-O11-C16
2	L	13	741	O12-C13-C14-C15
2	K	11	741	C14-C13-O12-C2
2	L	13	741	C14-C13-O12-C2
2	F	6	741	C14-C13-O12-C2
2	G	7	741	C14-C15-N34-C36
2	K	11	741	N34-C35-C37-O38
2	C	3	741	C14-C13-O12-C2
2	E	5	741	C13-C14-C15-N34
2	F	6	741	C14-C15-N34-C35
2	M	12	741	C14-C15-N34-C35
2	L	13	741	C9-C10-N17-C18
2	I	9	741	C9-C10-N17-C18
2	M	12	741	C37-C35-N34-C15
2	S	15	741	N33-C32-C9-C8
2	D	4	741	N33-C32-C9-C8
2	T	16	741	N33-C32-C9-C8
2	A	1	741	N33-C32-C9-C8
2	G	7	741	N33-C32-C9-C8
2	K	11	741	N33-C32-C9-C8
2	M	12	741	N33-C32-C9-C8
2	B	2	741	N33-C32-C9-C8
2	L	13	741	C19-C18-N17-C10
2	S	15	741	C9-C10-N17-C18
2	S	15	741	C20-C21-S25-C26
2	R	14	741	C9-C10-N17-C18
2	F	6	741	C9-C10-N17-C18
2	R	14	741	N33-C32-C9-C10
2	I	9	741	N33-C32-C9-C10
2	H	8	741	C9-C10-N17-C18

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Mol	Chain	Res	Type	Atoms
2	T	16	741	C9-C10-N17-C18
2	A	1	741	N33-C32-C9-C10
2	A	1	741	C9-C10-N17-C18
2	C	3	741	C9-C10-N17-C18
2	G	7	741	C9-C10-N17-C18
2	J	10	741	C9-C10-N17-C18
2	E	5	741	C9-C10-N17-C18
2	B	2	741	C9-C10-N17-C18

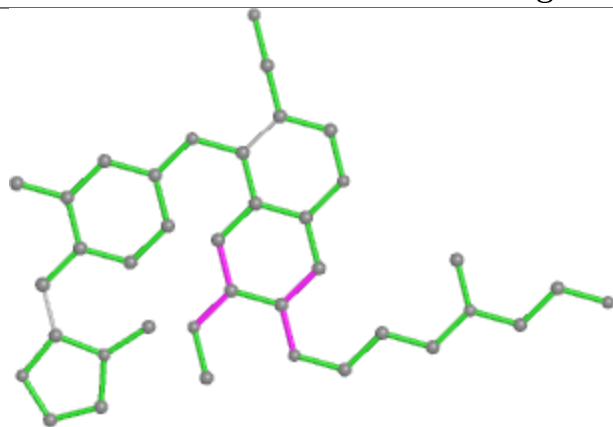
There are no ring outliers.

16 monomers are involved in 57 short contacts:

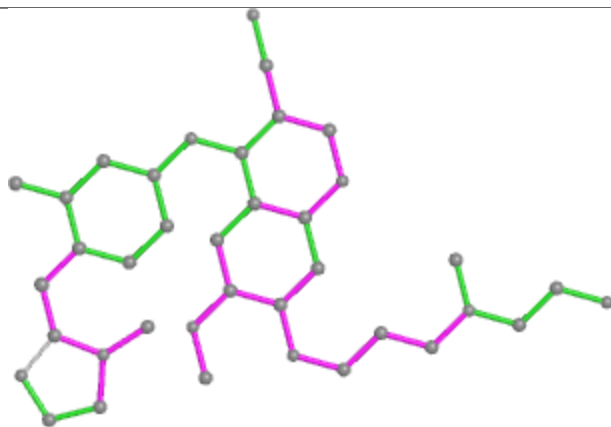
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	13	741	3	0
2	R	14	741	6	0
2	D	4	741	1	0
2	H	8	741	4	0
2	T	16	741	3	0
2	C	3	741	2	0
2	I	9	741	9	0
2	G	7	741	2	0
2	B	2	741	3	0
2	K	11	741	2	0
2	M	12	741	1	0
2	S	15	741	4	0
2	F	6	741	5	0
2	A	1	741	5	0
2	E	5	741	5	0
2	J	10	741	2	0

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.

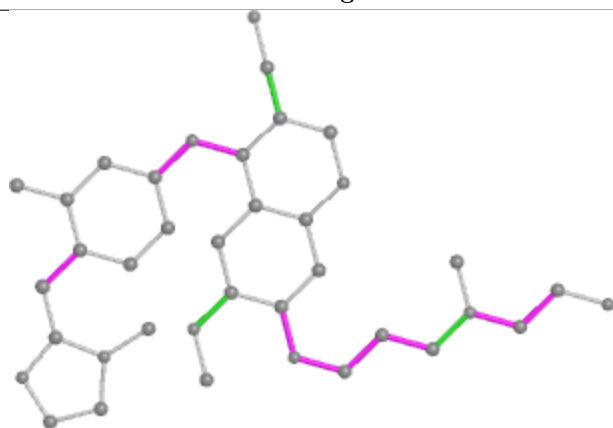
Ligand 741 L 13



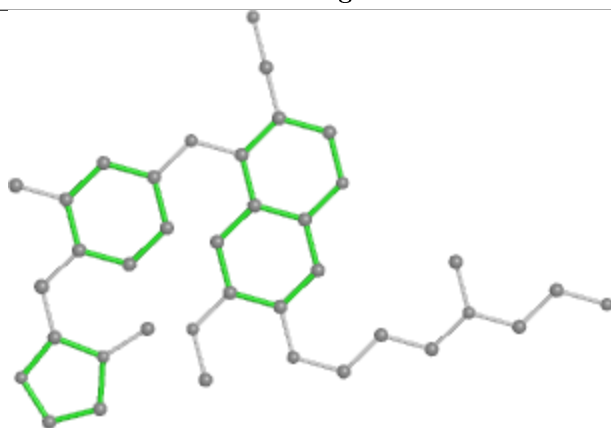
Bond lengths



Bond angles

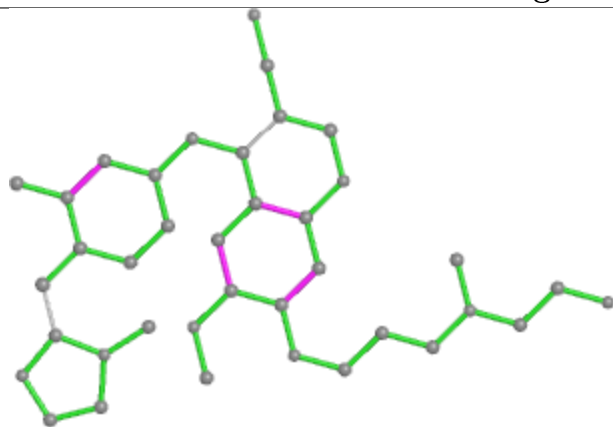


Torsions

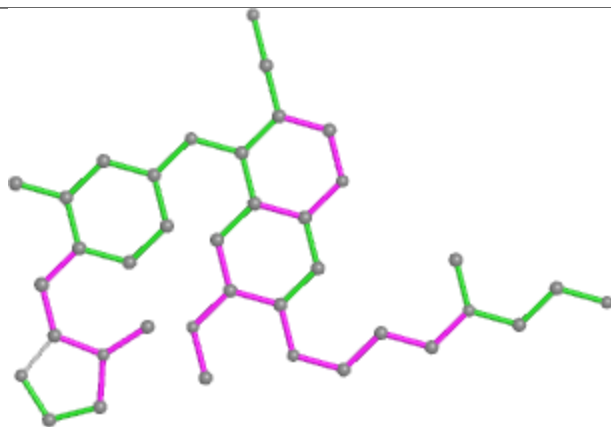


Rings

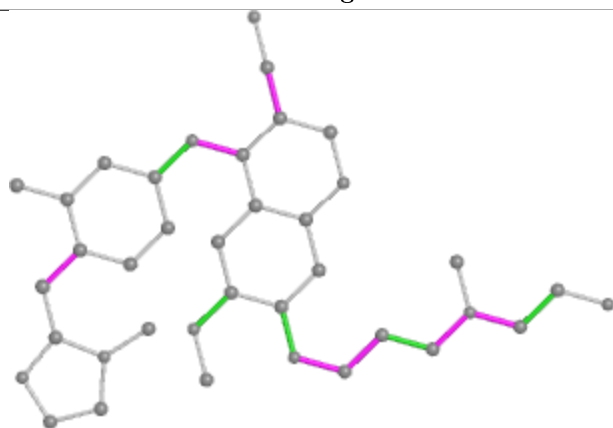
Ligand 741 R 14



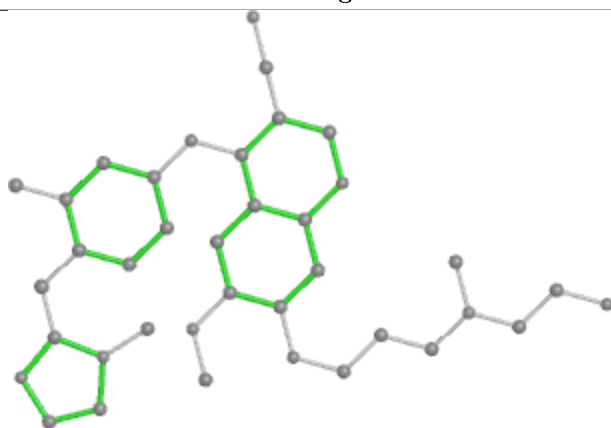
Bond lengths



Bond angles

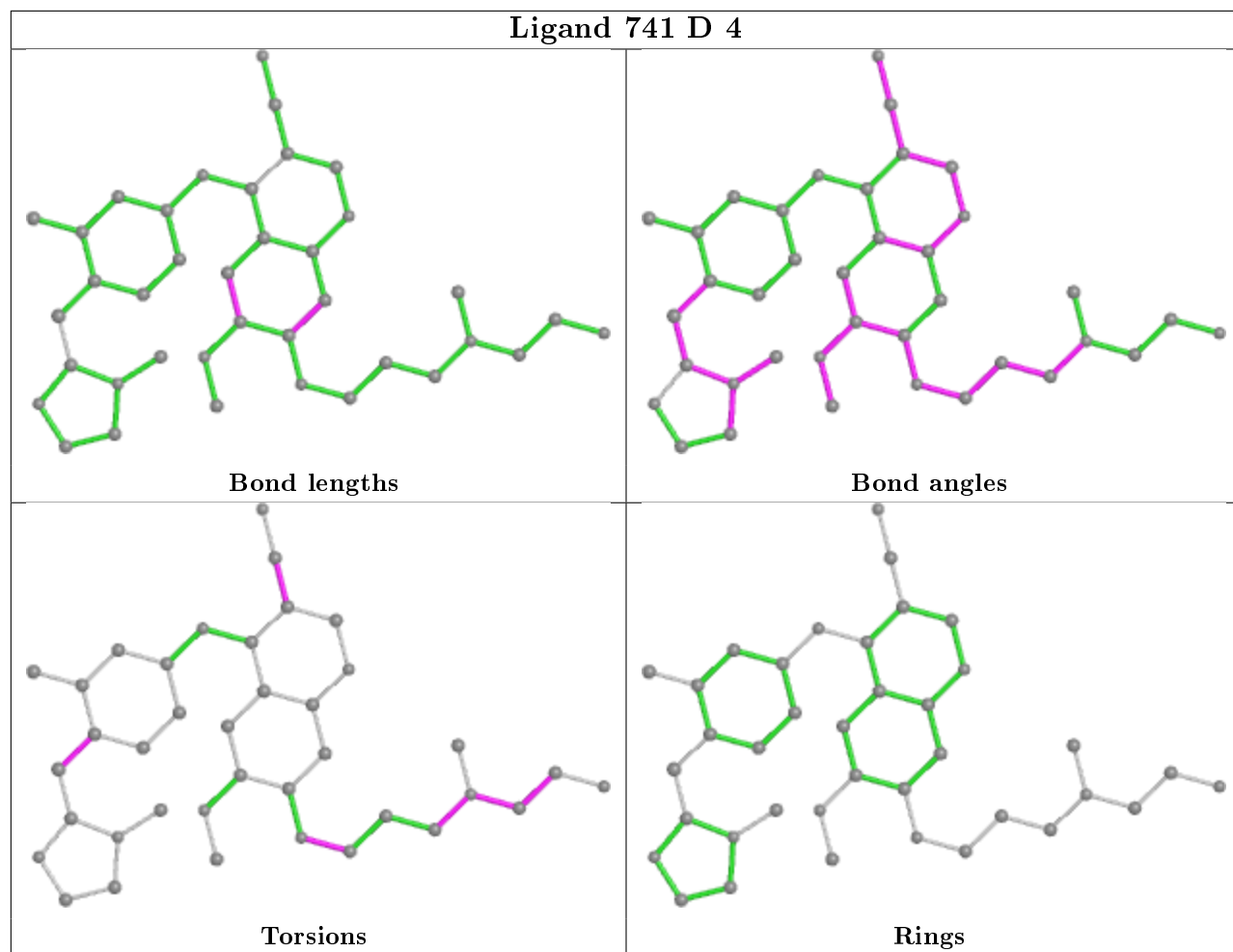


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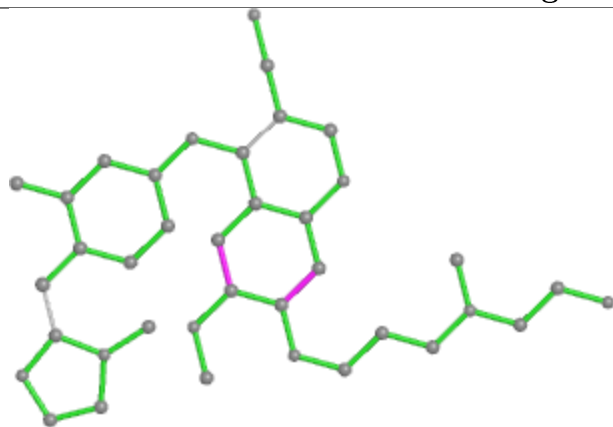


Rings

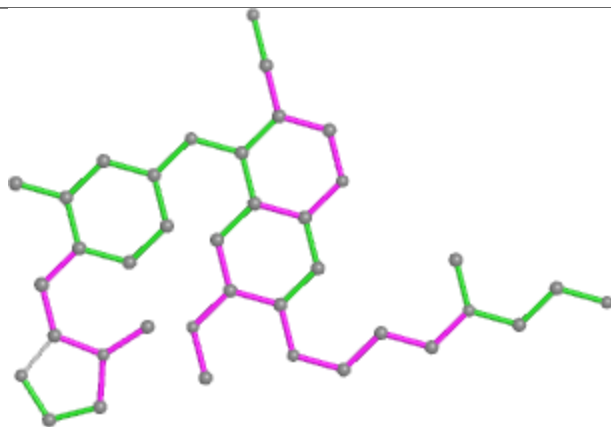
Ligand 741 D 4



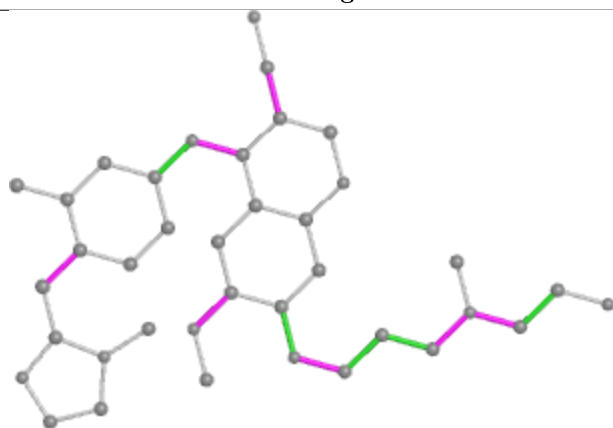
Ligand 741 H 8



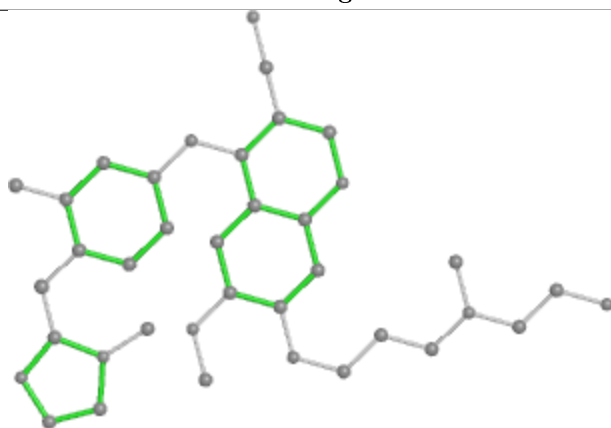
Bond lengths



Bond angles

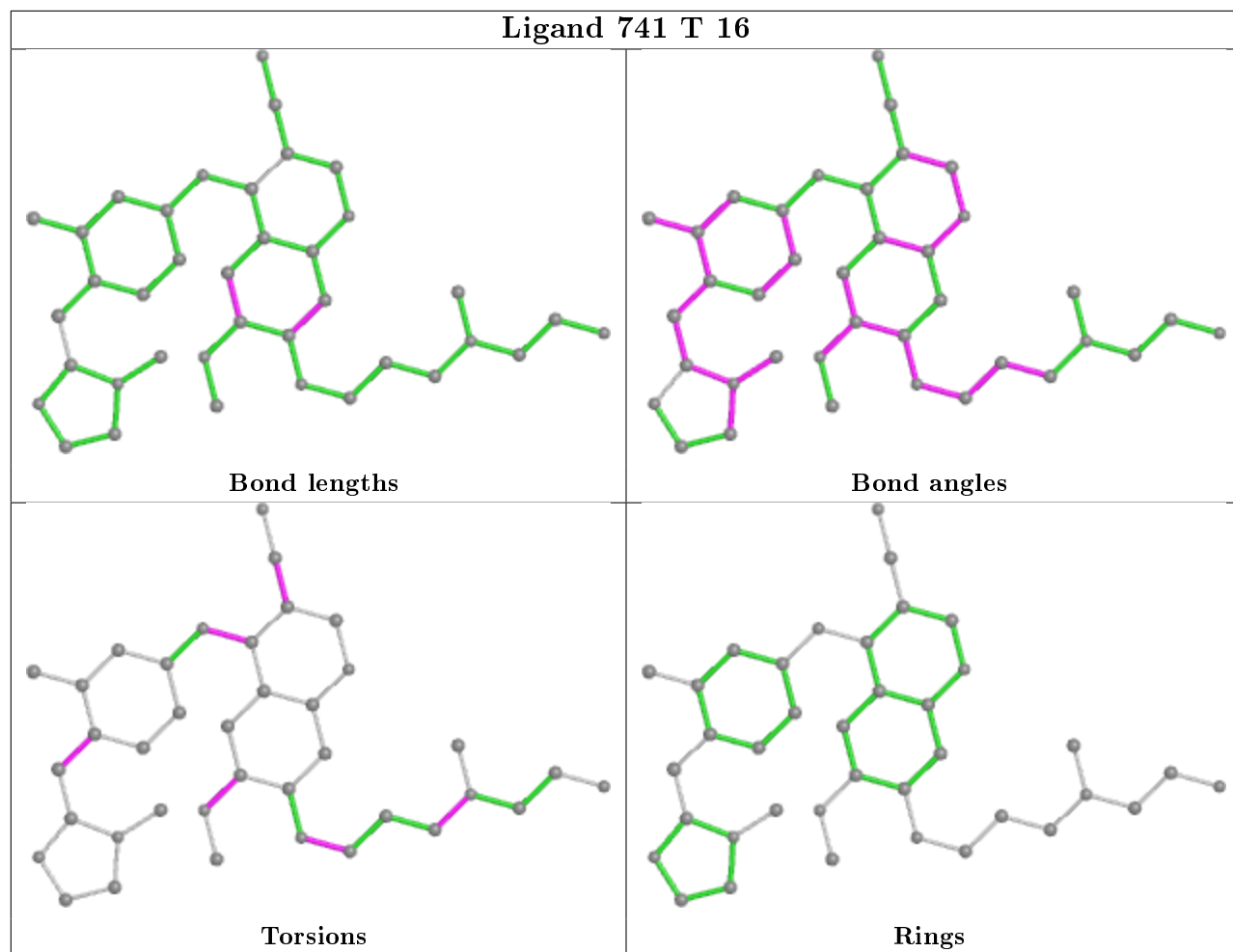


Torsions

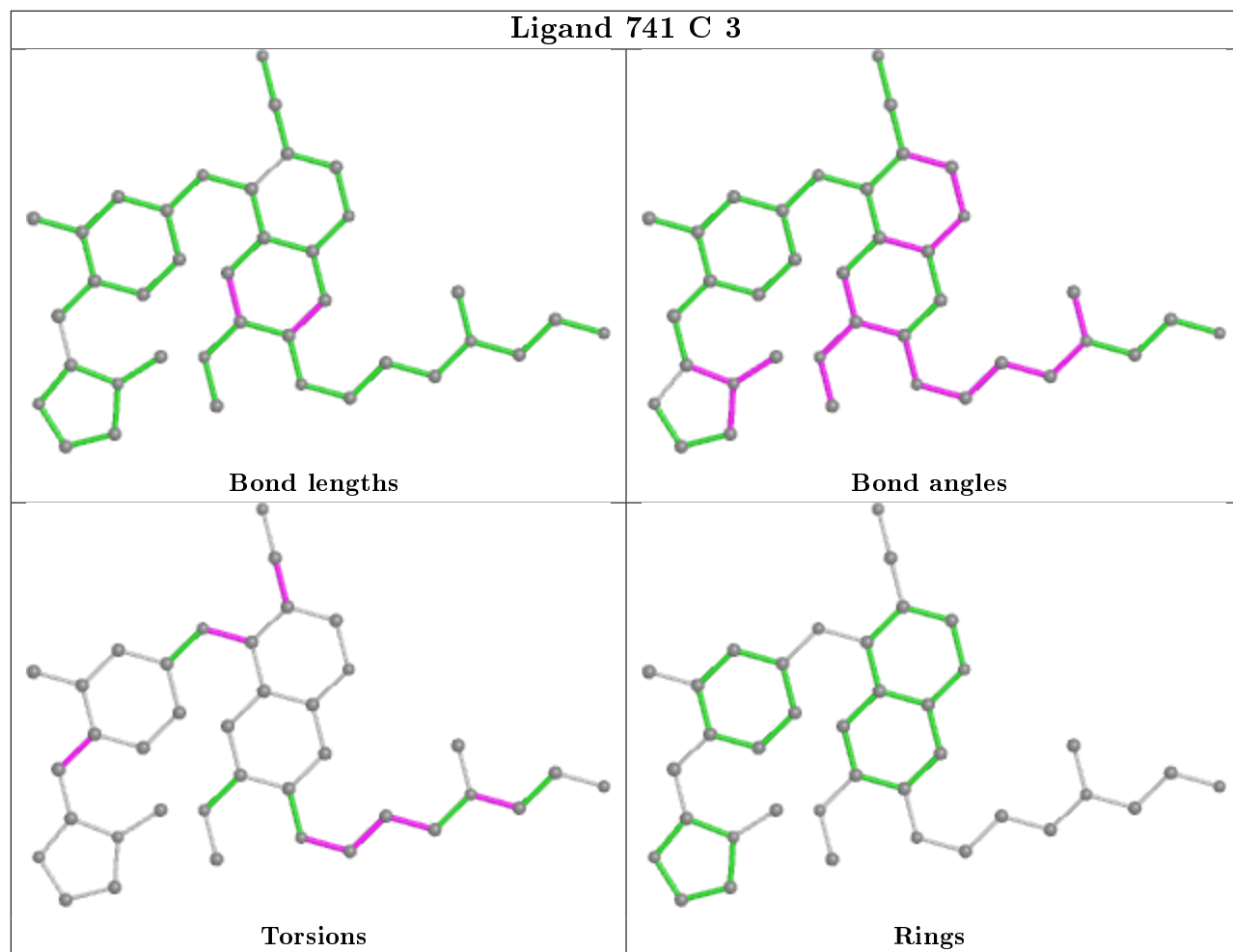


Rings

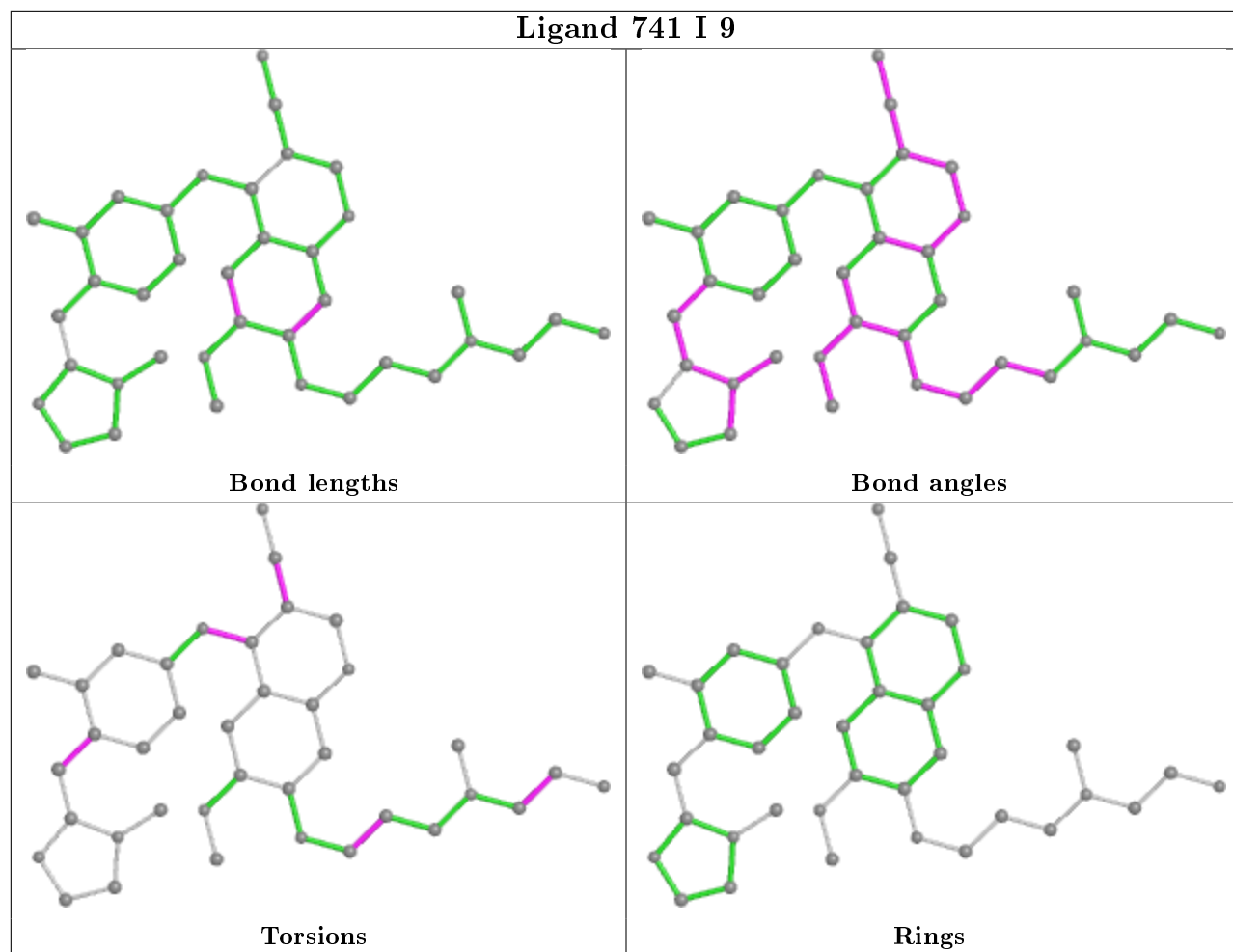
Ligand 741 T 16



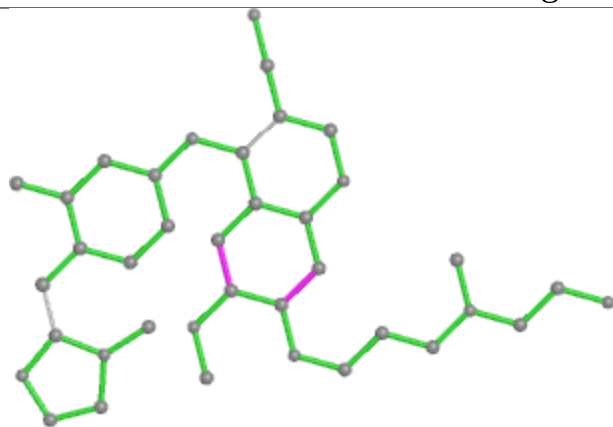
Ligand 741 C 3



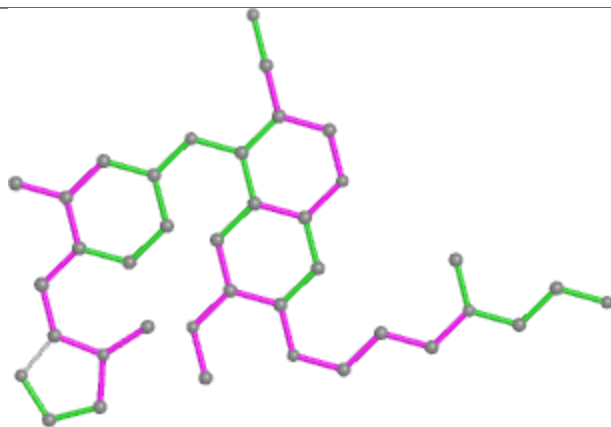
Ligand 741 I 9



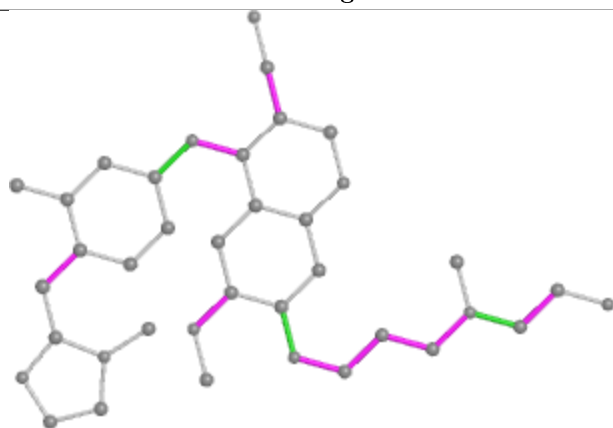
Ligand 741 G 7



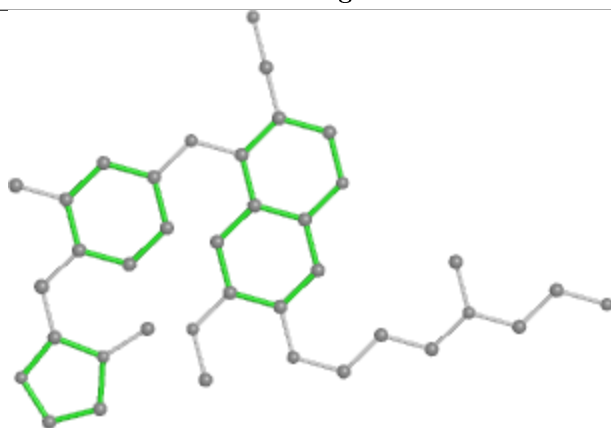
Bond lengths



Bond angles

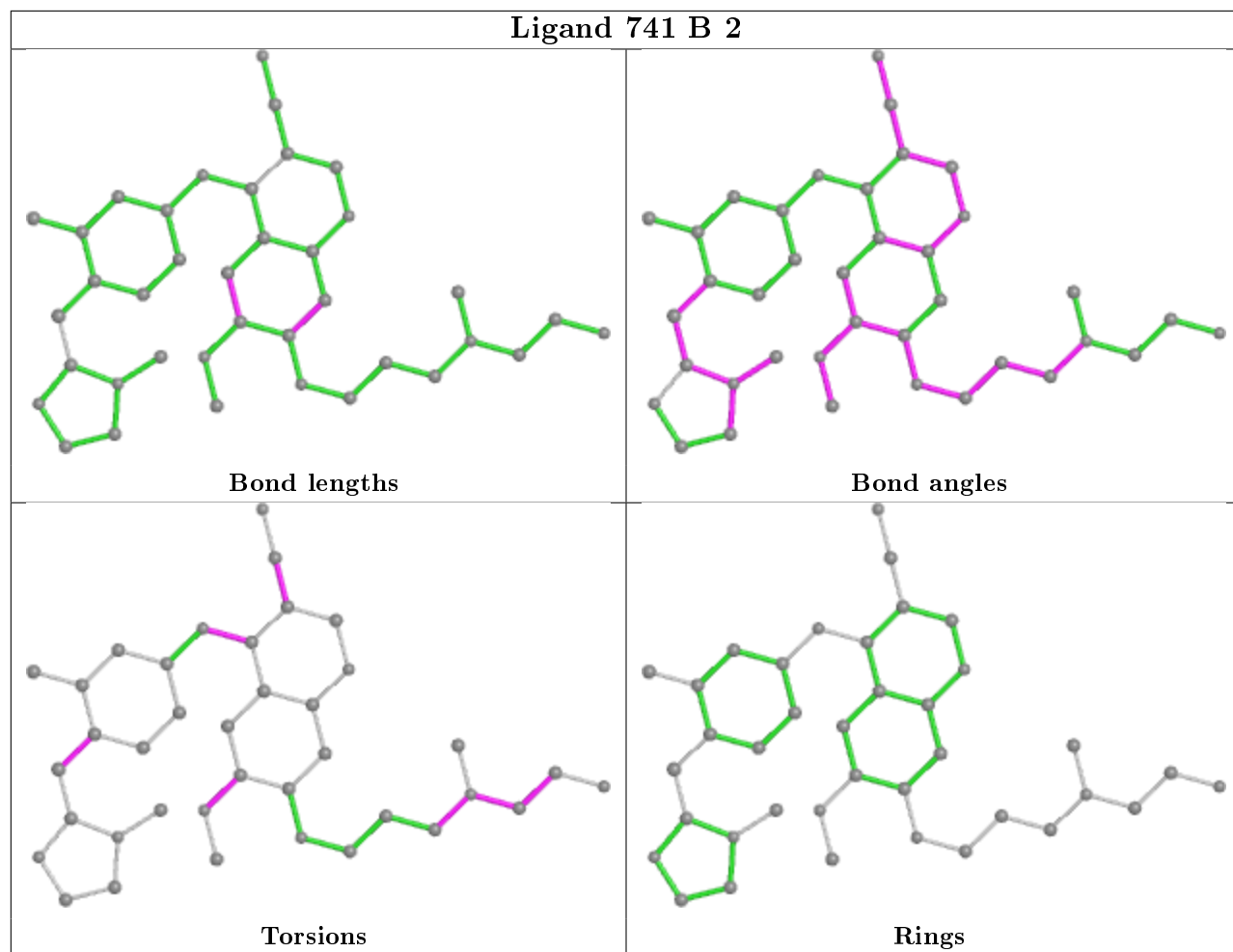


Torsions

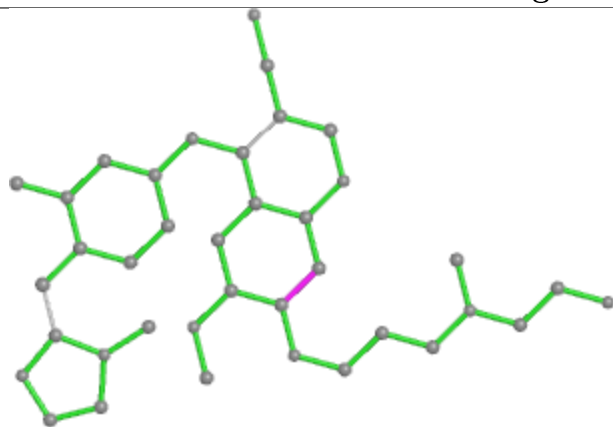


Rings

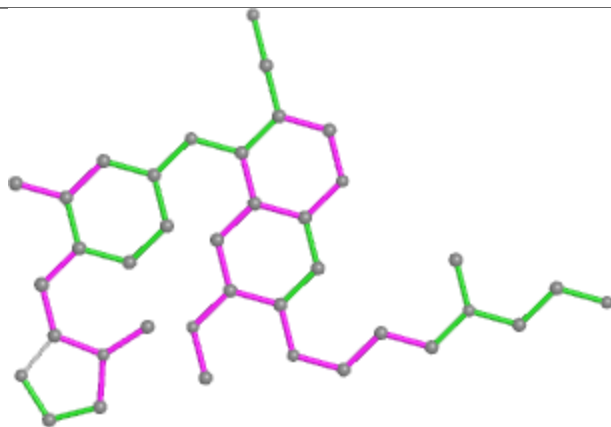
Ligand 741 B 2



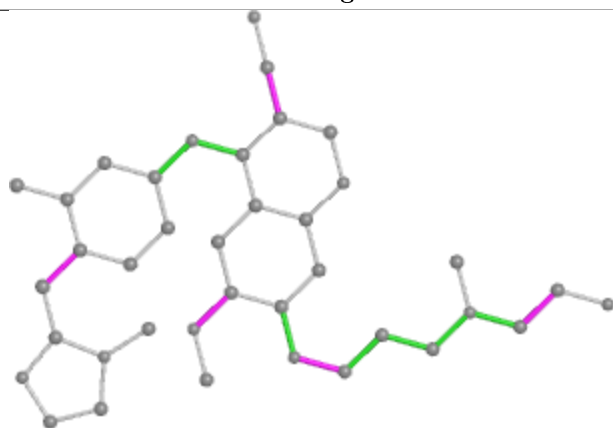
Ligand 741 K 11



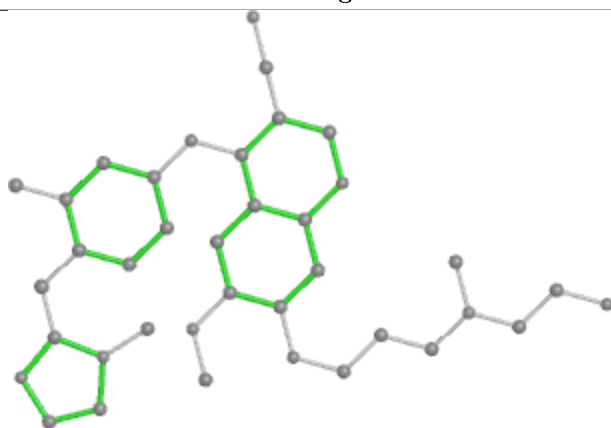
Bond lengths



Bond angles

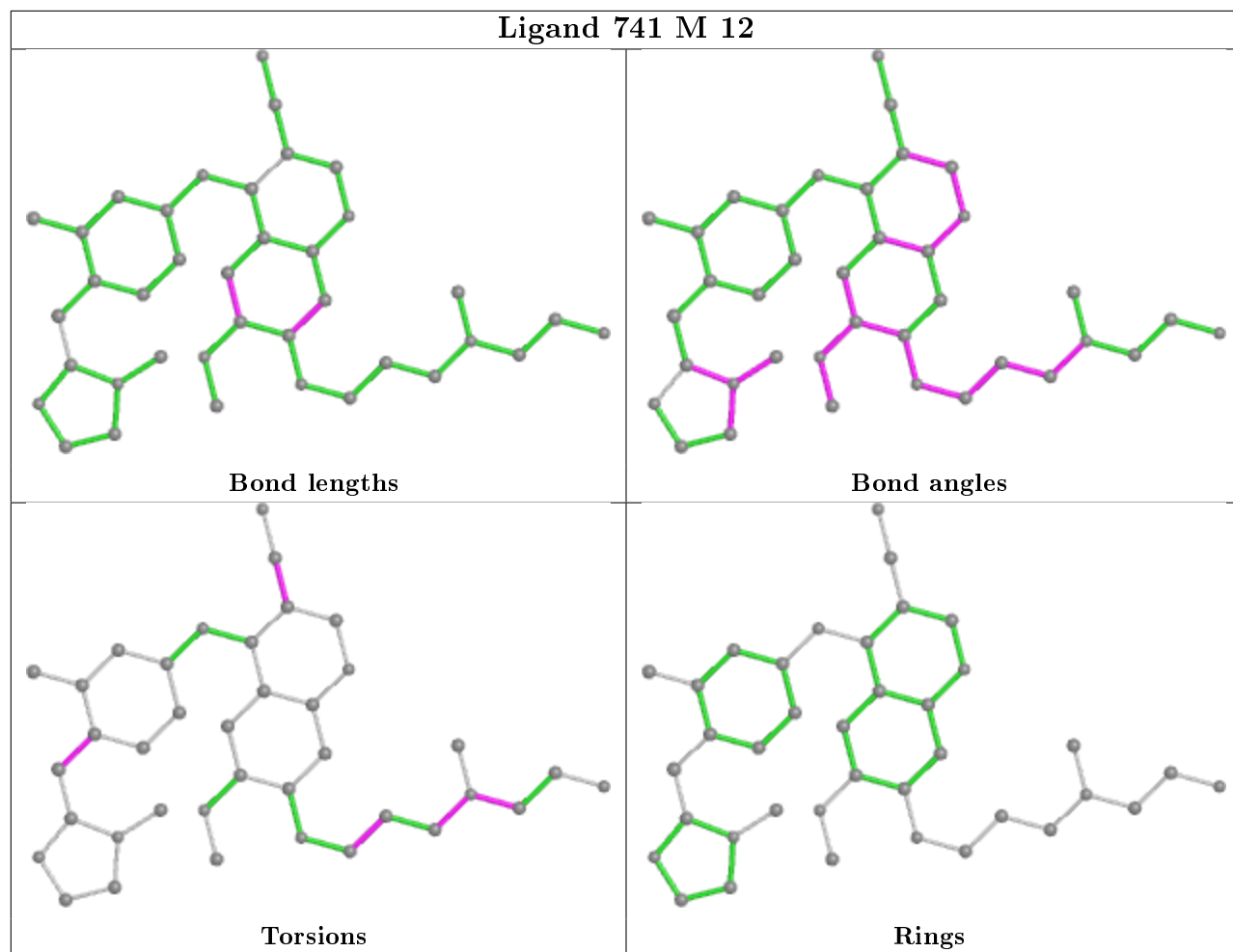


Torsions

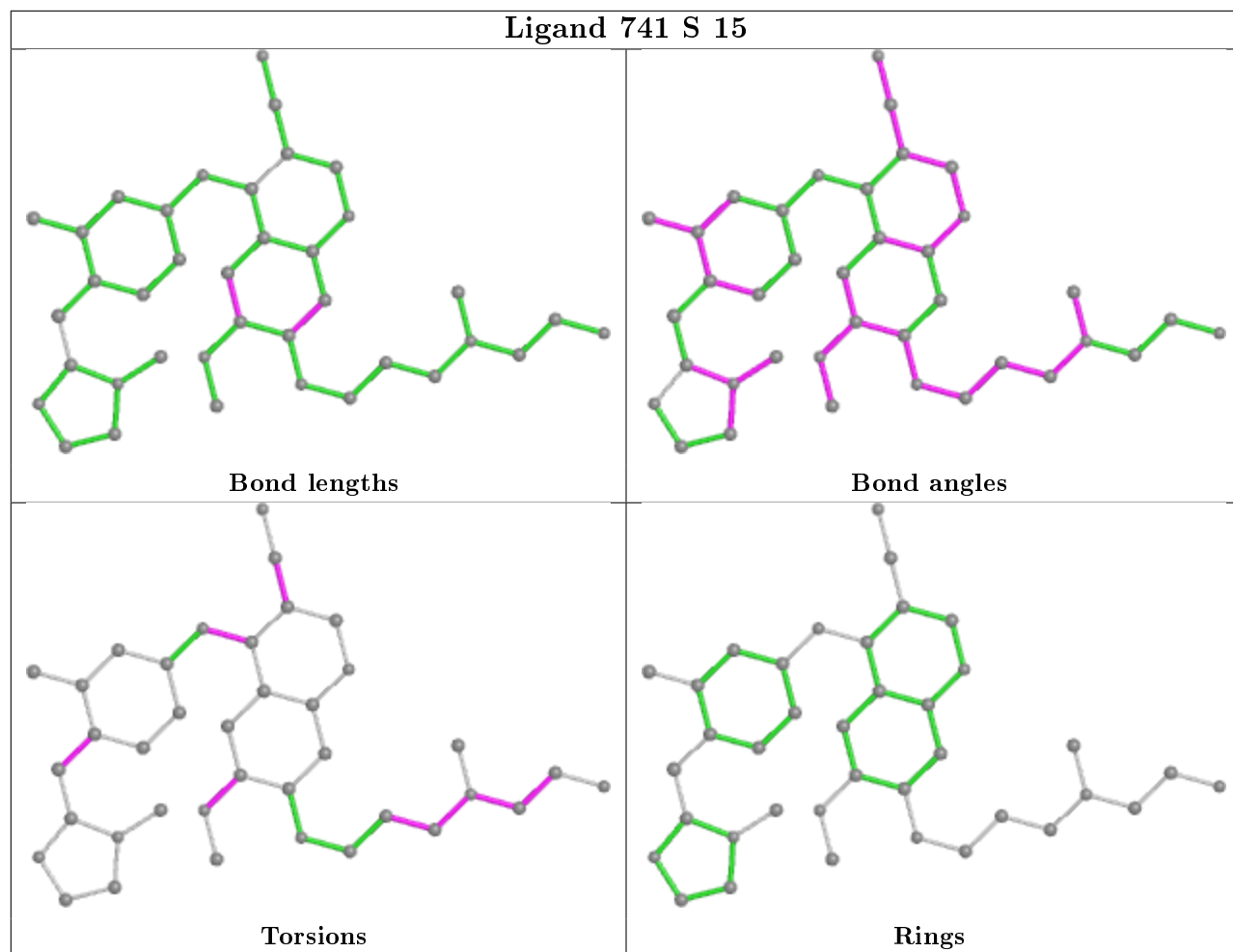


Rings

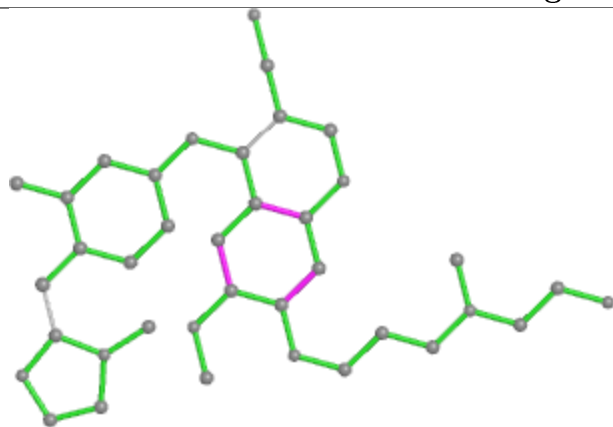
Ligand 741 M 12



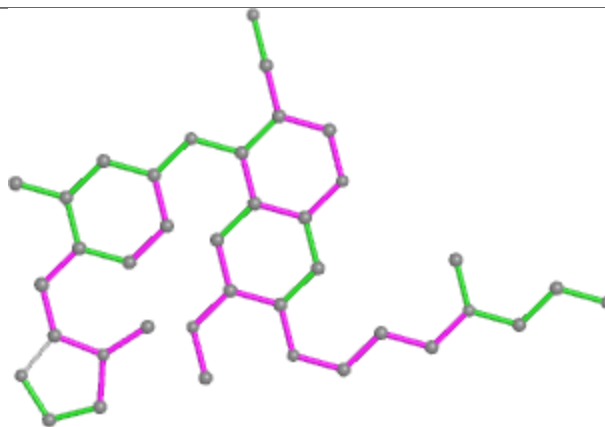
Ligand 741 S 15



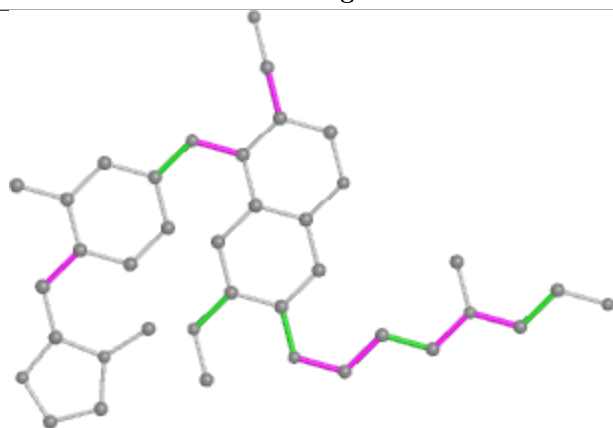
Ligand 741 F 6



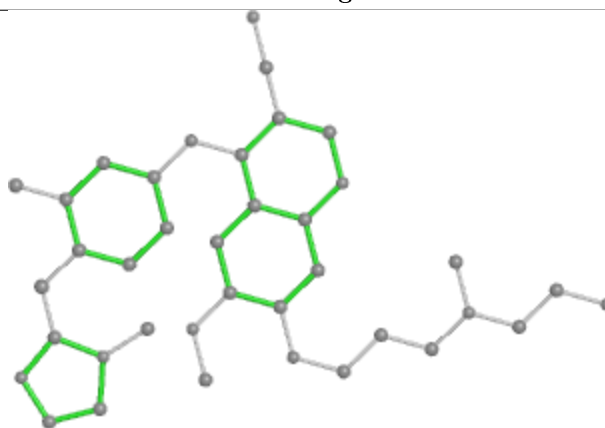
Bond lengths



Bond angles

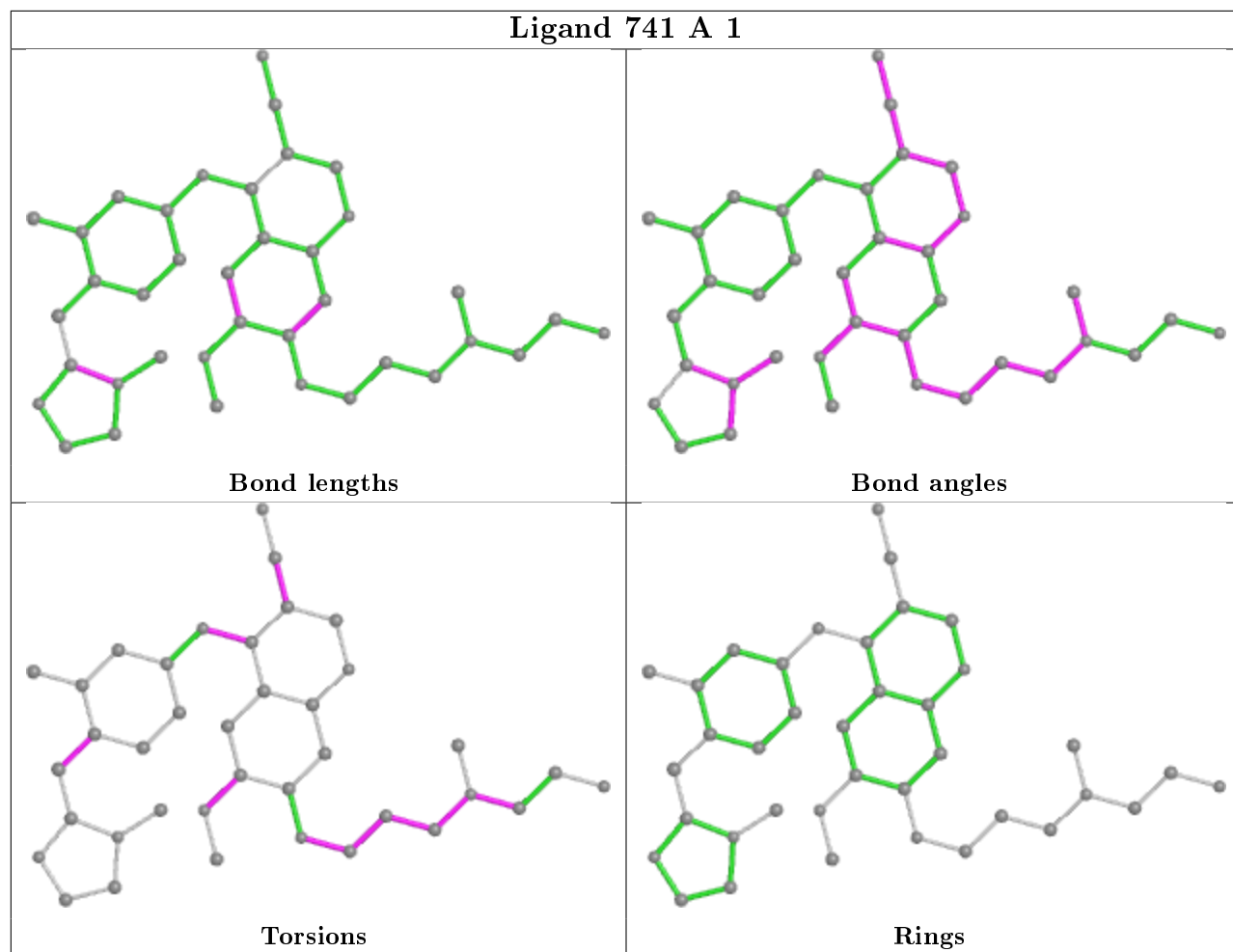


Torsions

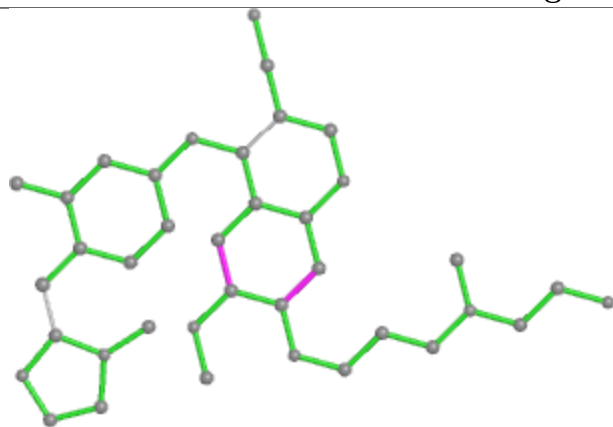


Rings

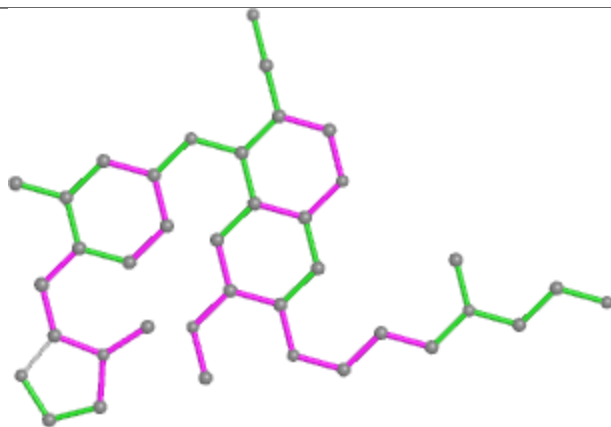
Ligand 741 A 1



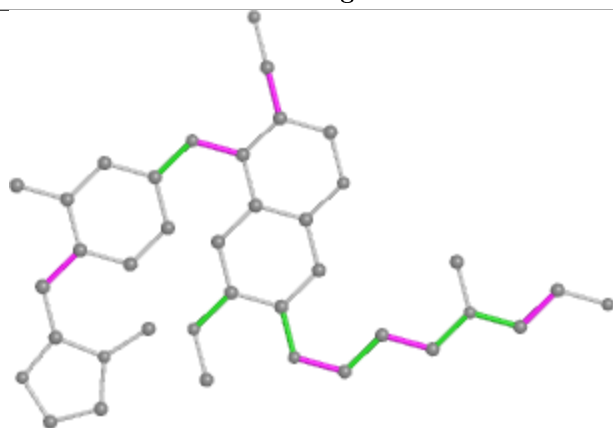
Ligand 741 E 5



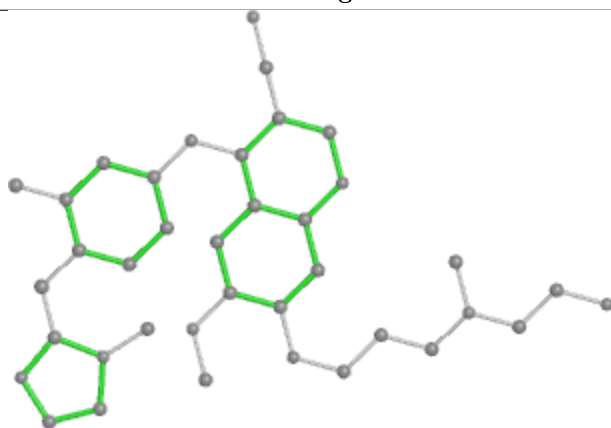
Bond lengths



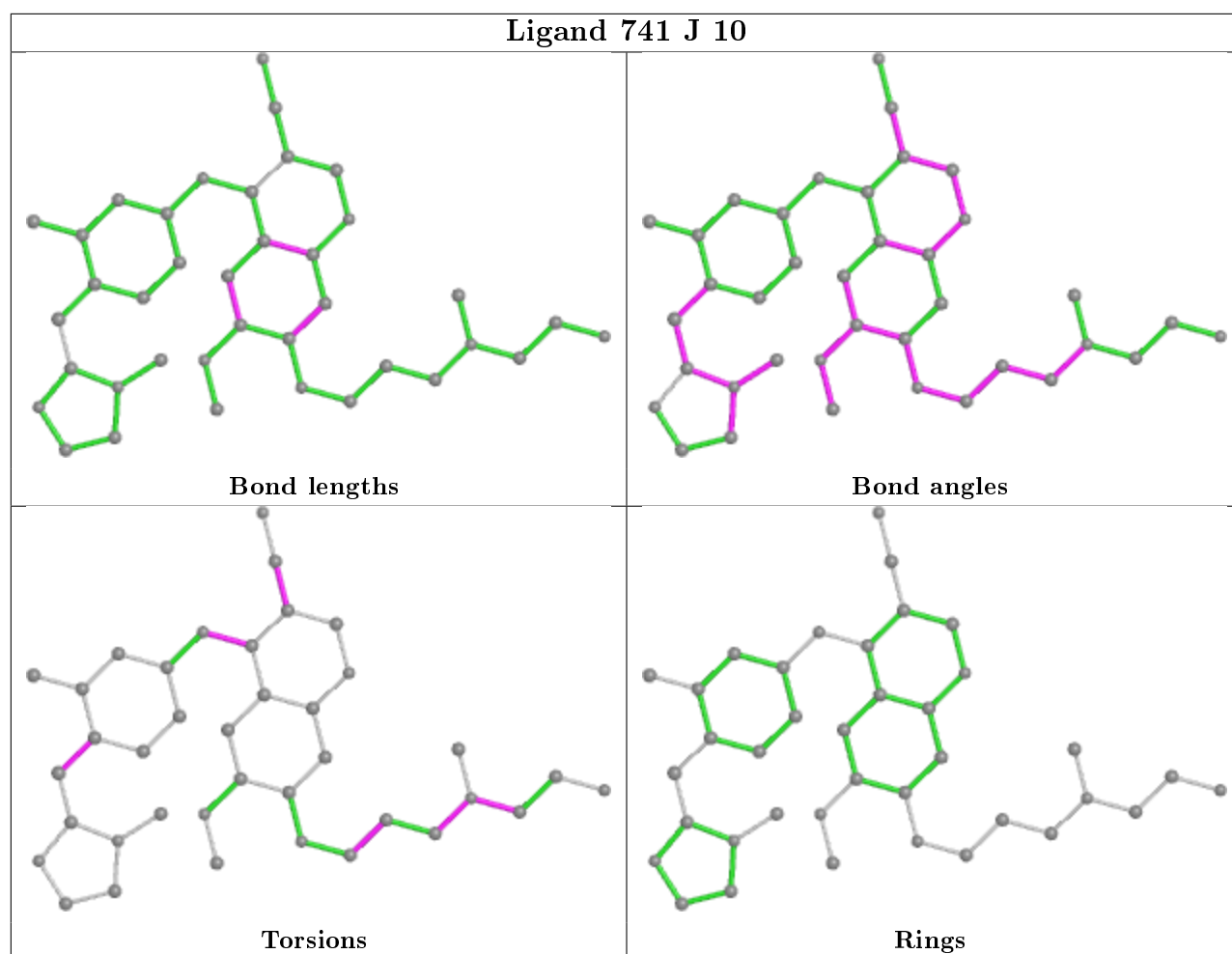
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/308 (97%)	-0.24	5 (1%) 70 69	18, 36, 79, 100	0
1	B	298/308 (96%)	-0.23	4 (1%) 77 77	22, 39, 78, 98	0
1	C	301/308 (97%)	-0.16	9 (2%) 50 45	20, 42, 82, 108	0
1	D	297/308 (96%)	-0.18	6 (2%) 65 63	23, 41, 79, 106	0
1	E	299/308 (97%)	-0.05	11 (3%) 41 37	26, 45, 84, 105	0
1	F	299/308 (97%)	-0.11	11 (3%) 41 37	22, 43, 88, 108	0
1	G	299/308 (97%)	-0.23	4 (1%) 77 77	23, 41, 76, 100	0
1	H	299/308 (97%)	-0.13	10 (3%) 46 41	24, 43, 85, 107	0
1	I	294/308 (95%)	-0.31	4 (1%) 75 75	18, 31, 60, 84	0
1	J	293/308 (95%)	-0.29	3 (1%) 82 82	26, 39, 69, 92	0
1	K	293/308 (95%)	-0.19	3 (1%) 82 82	26, 41, 72, 93	0
1	L	293/308 (95%)	-0.23	7 (2%) 59 56	24, 41, 75, 92	0
1	M	295/308 (95%)	-0.24	2 (0%) 87 87	25, 40, 72, 88	0
1	R	294/308 (95%)	-0.29	2 (0%) 87 87	19, 38, 73, 94	0
1	S	295/308 (95%)	-0.07	8 (2%) 54 50	29, 46, 79, 110	0
1	T	295/308 (95%)	-0.17	6 (2%) 65 63	23, 40, 71, 86	0
All	All	4743/4928 (96%)	-0.19	95 (2%) 65 63	18, 41, 77, 110	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	1073	GLN	6.5
1	K	1073	GLN	6.1
1	D	1037	GLU	4.7
1	S	1073	GLN	4.5
1	E	1009	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	M	1073	GLN	4.3
1	D	1073	GLN	4.3
1	R	1073	GLN	4.2
1	M	1106	PRO	4.0
1	T	1106	PRO	3.9
1	C	1073	GLN	3.8
1	C	1038	ALA	3.8
1	F	1037	GLU	3.8
1	F	1024	ASP	3.7
1	C	1037	GLU	3.6
1	H	1022	VAL	3.6
1	E	1272	PRO	3.5
1	G	1024	ASP	3.5
1	I	1073	GLN	3.4
1	A	1098	MET	3.4
1	T	1286	LYS	3.3
1	C	1024	ASP	3.3
1	E	990	ASP	3.3
1	F	990	ASP	3.3
1	L	990	ASP	3.2
1	G	1073	GLN	3.2
1	E	1073	GLN	3.2
1	F	1038	ALA	3.1
1	F	1073	GLN	3.1
1	A	1037	GLU	3.1
1	L	1096	PRO	3.1
1	B	1073	GLN	3.0
1	L	1073	GLN	3.0
1	H	1073	GLN	2.9
1	F	997	GLU	2.8
1	B	1038	ALA	2.8
1	F	992	TRP	2.8
1	S	1024	ASP	2.7
1	F	1007	GLN	2.7
1	D	1056	GLU	2.6
1	F	1023	LYS	2.6
1	I	990	ASP	2.6
1	S	1286	LYS	2.6
1	E	1007	GLN	2.6
1	E	1021	VAL	2.6
1	T	1023	LYS	2.6
1	H	1024	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	1023	LYS	2.5
1	G	1023	LYS	2.5
1	L	997	GLU	2.4
1	H	1098	MET	2.4
1	L	1235	ASP	2.4
1	D	1283	GLU	2.4
1	K	1096	PRO	2.4
1	R	1024	ASP	2.4
1	D	1024	ASP	2.4
1	H	1286	LYS	2.4
1	J	1096	PRO	2.4
1	C	1235	ASP	2.4
1	G	1037	GLU	2.4
1	S	1106	PRO	2.4
1	H	1009	SER	2.4
1	H	1037	GLU	2.3
1	A	1235	ASP	2.3
1	B	1286	LYS	2.3
1	H	1019	LYS	2.3
1	C	1007	GLN	2.3
1	C	1097	GLU	2.3
1	E	1025	GLU	2.3
1	A	1052	SER	2.3
1	B	1283	GLU	2.3
1	E	1026	PRO	2.3
1	T	997	GLU	2.3
1	S	1096	PRO	2.3
1	C	997	GLU	2.2
1	E	997	GLU	2.2
1	F	1040	SER	2.2
1	H	1038	ALA	2.2
1	F	1009	SER	2.2
1	D	1002	SER	2.2
1	E	1037	GLU	2.2
1	J	1003	ARG	2.2
1	A	1286	LYS	2.2
1	S	1235	ASP	2.2
1	L	1283	GLU	2.2
1	I	1096	PRO	2.2
1	E	1283	GLU	2.1
1	S	1023	LYS	2.1
1	L	1162	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	1284	GLU	2.1
1	J	1073	GLN	2.0
1	C	1023	LYS	2.0
1	I	1024	ASP	2.0
1	K	997	GLU	2.0
1	T	1162	GLU	2.0

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

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
1	PTR	K	1161	12/17	0.72	0.27	43,69,87,92	0
1	PTR	L	1161	12/17	0.75	0.30	50,67,82,86	0
1	PTR	M	1161	12/17	0.75	0.26	49,64,81,84	0
1	PTR	C	1161	12/17	0.77	0.37	50,67,81,88	0
1	PTR	B	1161	12/17	0.81	0.30	44,69,80,81	0
1	PTR	I	1161	12/17	0.82	0.24	39,64,80,83	0
1	PTR	T	1161	12/17	0.82	0.25	47,71,82,84	0
1	PTR	D	1161	12/17	0.82	0.35	58,65,81,83	0
1	PTR	A	1161	16/17	0.82	0.30	46,81,114,234	0
1	PTR	H	1161	12/17	0.84	0.27	53,70,78,81	0
1	PTR	F	1161	12/17	0.85	0.28	58,72,85,88	0
1	PTR	G	1161	12/17	0.85	0.31	49,60,71,73	0
1	PTR	S	1161	12/17	0.86	0.20	51,61,68,68	0
1	PTR	R	1161	12/17	0.86	0.26	45,59,74,76	0
1	PTR	J	1161	12/17	0.86	0.28	46,64,81,87	0
1	PTR	E	1161	12/17	0.88	0.23	53,68,76,81	0
1	PTR	F	1165	16/17	0.90	0.21	40,50,73,73	0
1	PTR	C	1165	16/17	0.91	0.19	32,46,60,63	0
1	PTR	E	1165	16/17	0.91	0.19	38,46,51,61	0
1	PTR	B	1165	16/17	0.91	0.18	34,44,63,68	0
1	PTR	M	1166	16/17	0.91	0.18	32,39,69,78	0
1	PTR	L	1165	16/17	0.92	0.20	40,47,66,72	0
1	PTR	S	1165	16/17	0.92	0.26	36,47,64,66	0
1	PTR	I	1165	16/17	0.92	0.20	32,44,64,66	0
1	PTR	M	1165	16/17	0.92	0.20	37,48,61,64	0
1	PTR	T	1165	16/17	0.92	0.23	37,53,63,67	0
1	PTR	D	1165	16/17	0.92	0.19	42,51,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	PTR	A	1165	16/17	0.93	0.20	37,44,59,61	0
1	PTR	H	1165	16/17	0.93	0.20	40,48,55,56	0
1	PTR	K	1165	16/17	0.93	0.18	35,45,53,57	0
1	PTR	R	1165	16/17	0.94	0.18	33,44,64,64	0
1	PTR	G	1165	16/17	0.94	0.18	40,48,56,57	0
1	PTR	J	1165	16/17	0.94	0.19	32,45,57,64	0
1	PTR	I	1166	16/17	0.96	0.15	27,33,45,48	0
1	PTR	F	1166	16/17	0.96	0.14	36,38,50,53	0
1	PTR	T	1166	16/17	0.96	0.14	38,44,54,55	0
1	PTR	K	1166	16/17	0.96	0.14	29,38,47,48	0
1	PTR	B	1166	16/17	0.96	0.12	32,35,46,48	0
1	PTR	E	1166	16/17	0.97	0.11	27,31,39,43	0
1	PTR	J	1166	16/17	0.97	0.13	26,31,44,44	0
1	PTR	S	1166	16/17	0.97	0.13	33,38,52,55	0
1	PTR	H	1166	16/17	0.97	0.10	29,34,41,49	0
1	PTR	L	1166	16/17	0.97	0.14	36,39,55,56	0
1	PTR	D	1166	16/17	0.97	0.10	31,37,47,56	0
1	PTR	G	1166	16/17	0.98	0.11	30,37,45,48	0
1	PTR	C	1166	16/17	0.98	0.10	30,33,38,42	0
1	PTR	A	1166	16/17	0.98	0.09	28,32,40,49	0
1	PTR	R	1166	16/17	0.98	0.11	29,34,44,48	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	741	R	14	38/38	0.84	0.22	24,34,59,304	0
2	741	E	5	38/38	0.88	0.20	40,45,57,58	0
2	741	D	4	38/38	0.90	0.21	31,41,57,78	0
2	741	H	8	38/38	0.91	0.20	33,44,53,60	0
2	741	B	2	38/38	0.92	0.19	31,36,59,84	0
2	741	G	7	38/38	0.93	0.17	31,38,48,54	0
2	741	S	15	38/38	0.94	0.15	27,42,67,77	0

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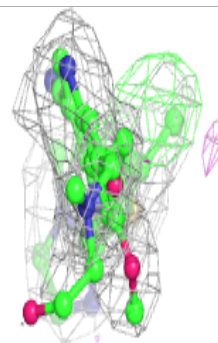
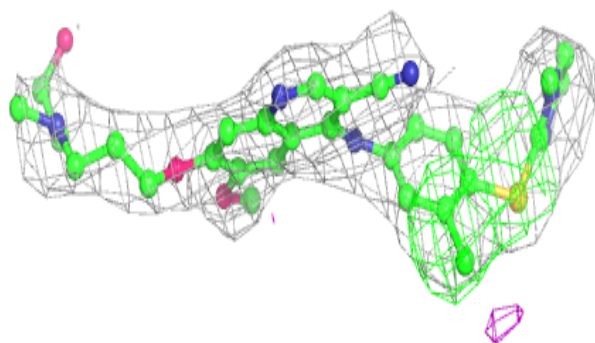
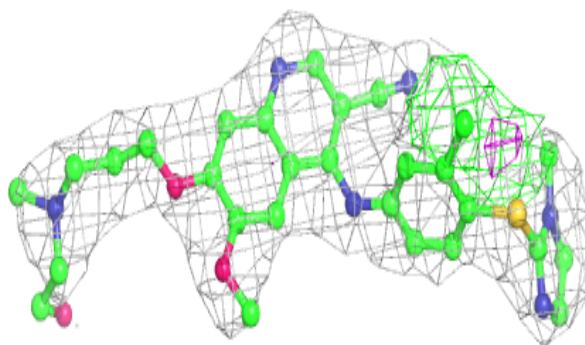
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	741	F	6	38/38	0.94	0.17	33,41,55,58	0
2	741	K	11	38/38	0.94	0.15	29,36,52,59	0
2	741	J	10	38/38	0.94	0.17	20,30,48,69	0
2	741	C	3	38/38	0.94	0.17	32,39,55,84	0
2	741	A	1	38/38	0.94	0.18	24,33,51,60	0
2	741	M	12	38/38	0.95	0.15	23,27,58,64	0
2	741	T	16	38/38	0.95	0.14	22,28,43,56	0
2	741	I	9	38/38	0.95	0.14	17,21,34,53	0
2	741	L	13	38/38	0.95	0.14	24,30,44,51	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.

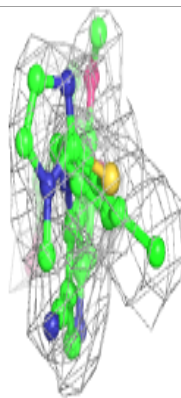
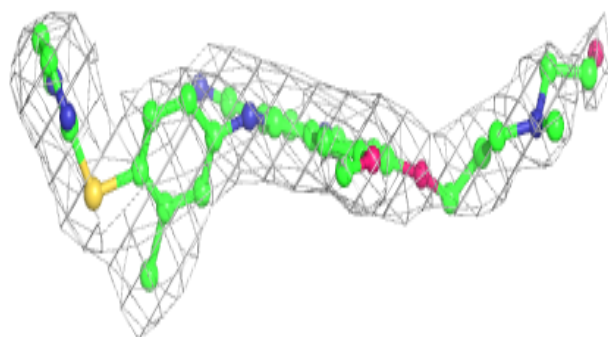
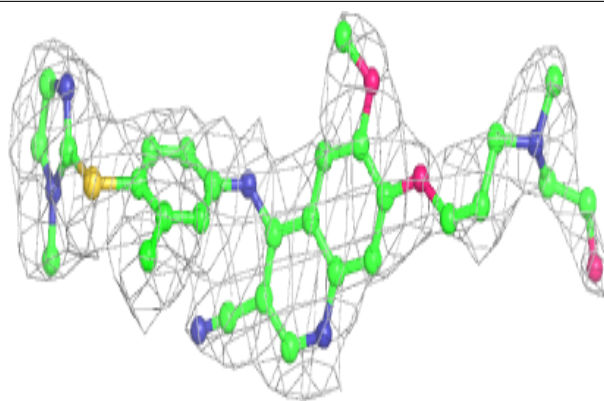
Electron density around 741 R 14:

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

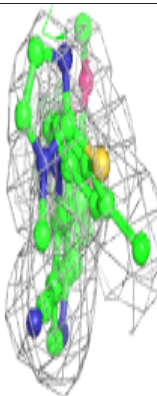
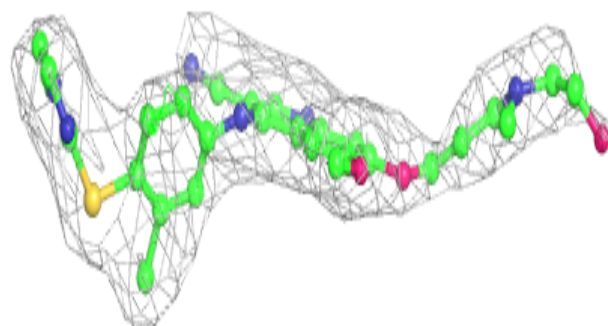
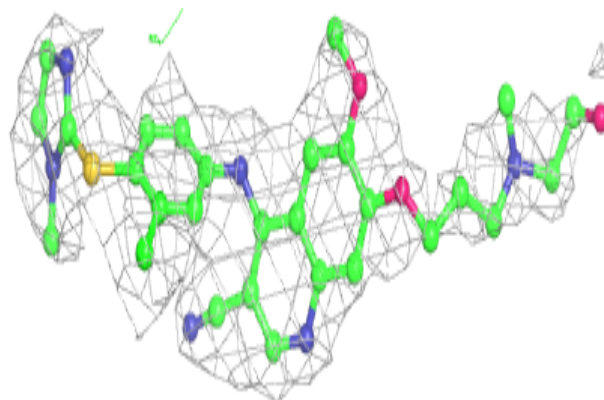


Electron density around 741 E 5:

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

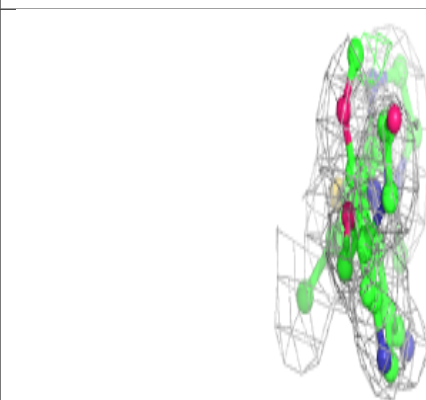
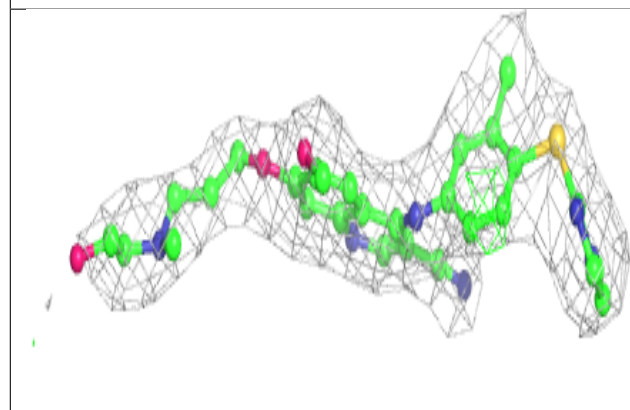
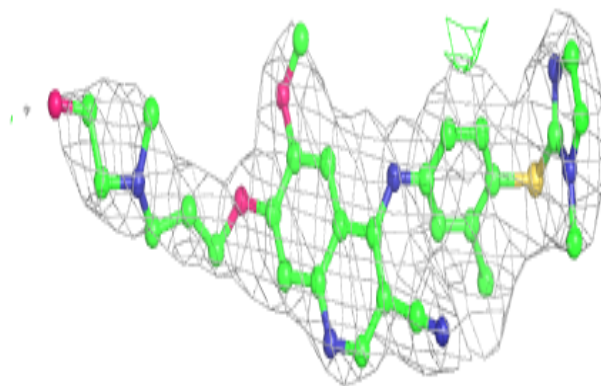
**Electron density around 741 D 4:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

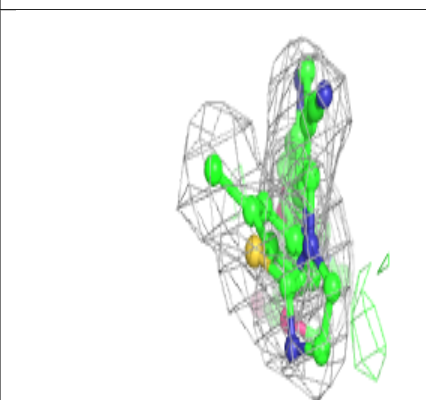
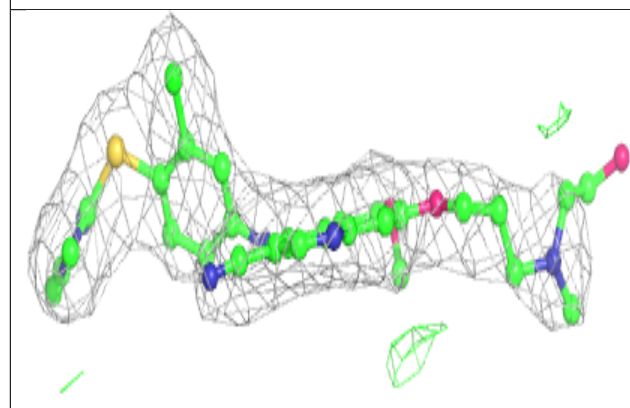
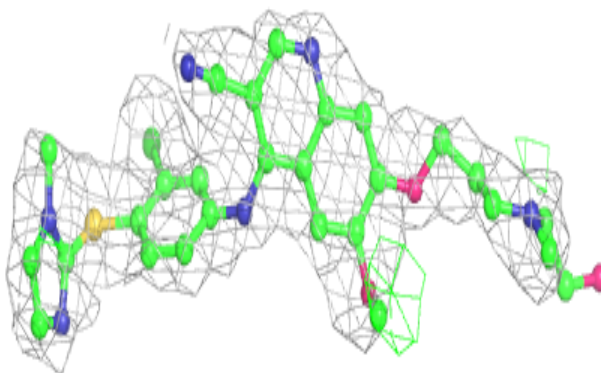


Electron density around 741 H 8:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

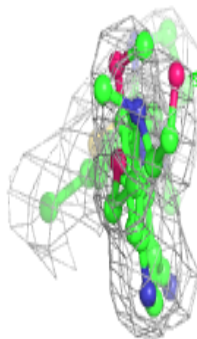
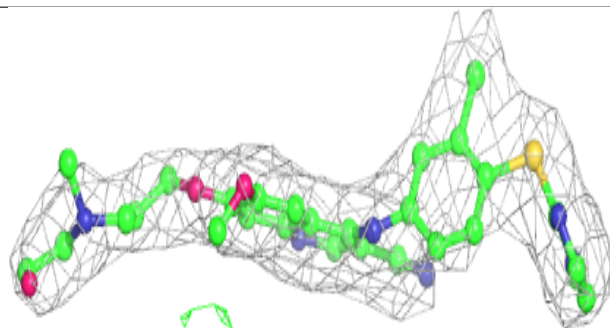
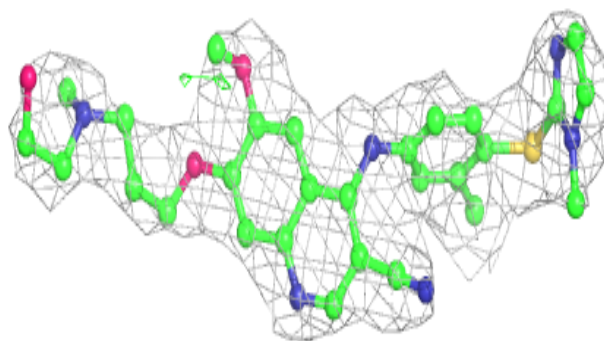
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

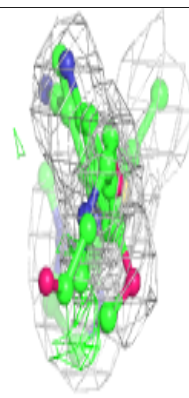
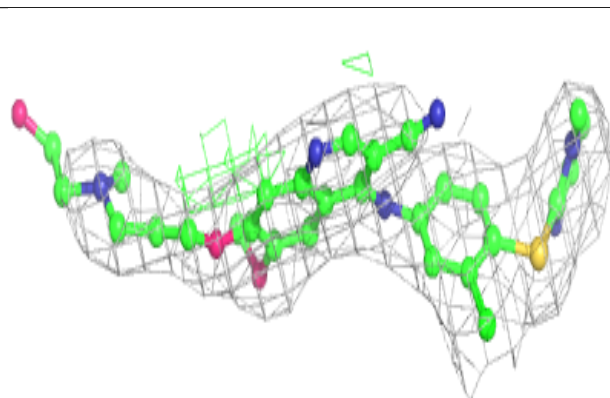
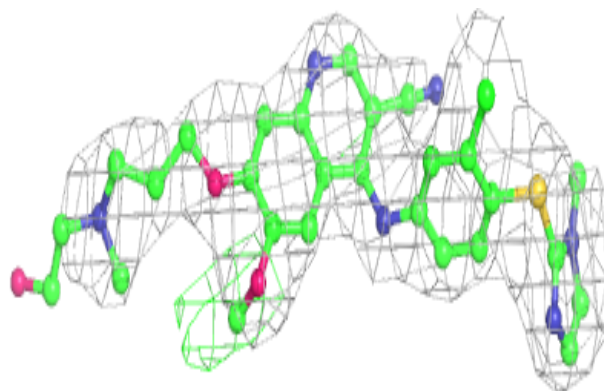


Electron density around 741 G 7:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

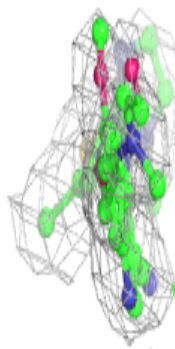
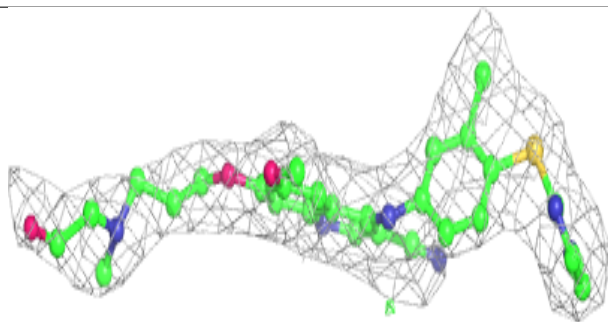
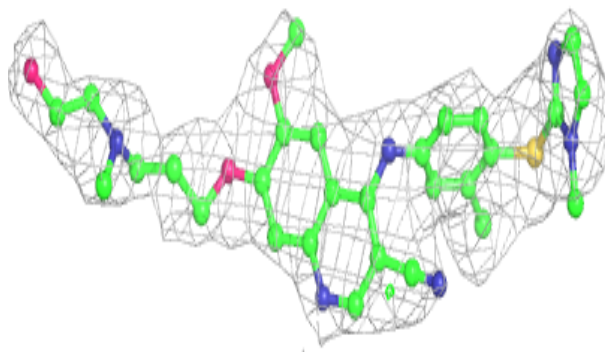
**Electron density around 741 S 15:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

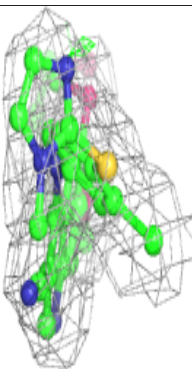
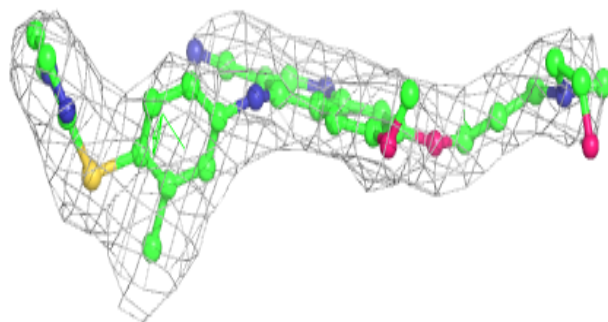
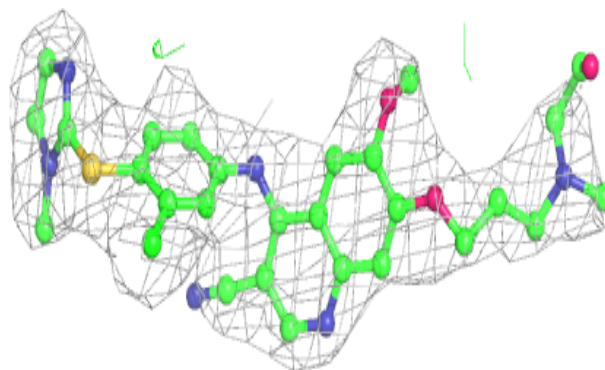


Electron density around 741 F 6:

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and green (positive)

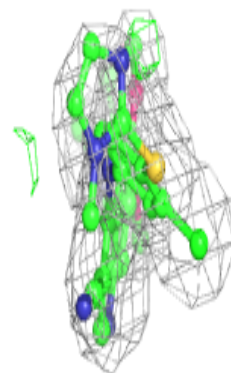
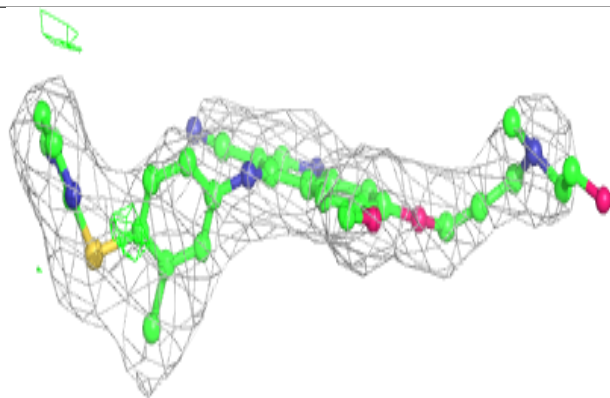
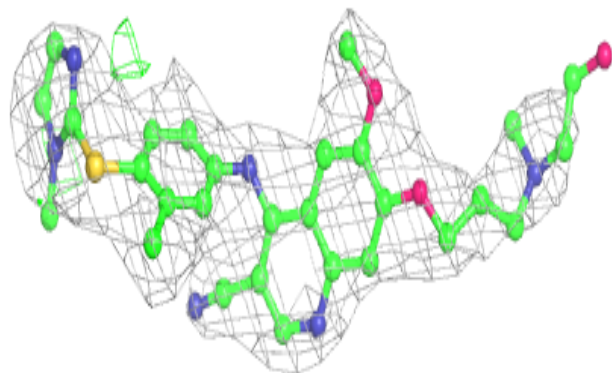
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and green (positive)

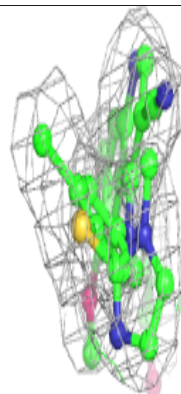
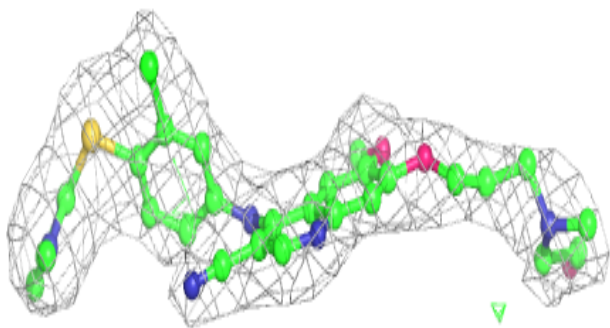
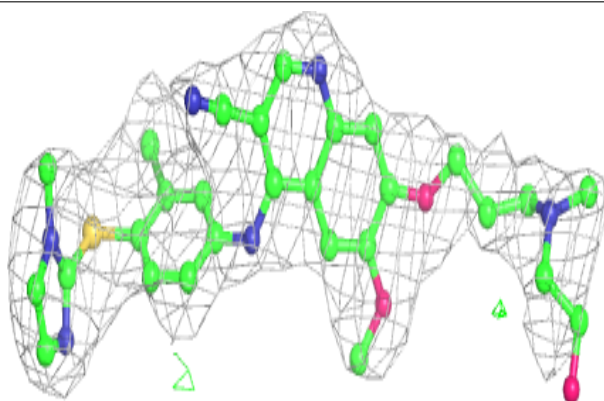


Electron density around 741 J 10:

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and green (positive)

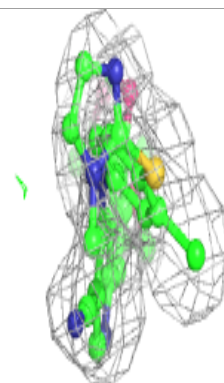
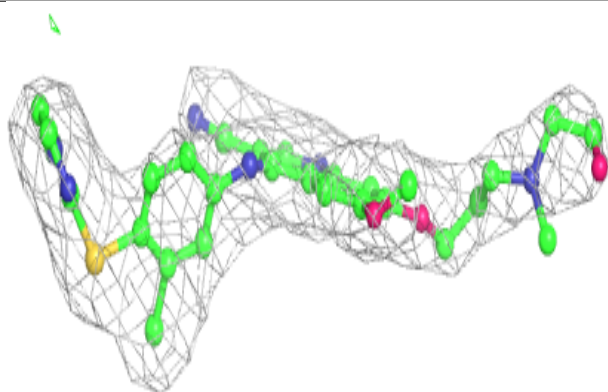
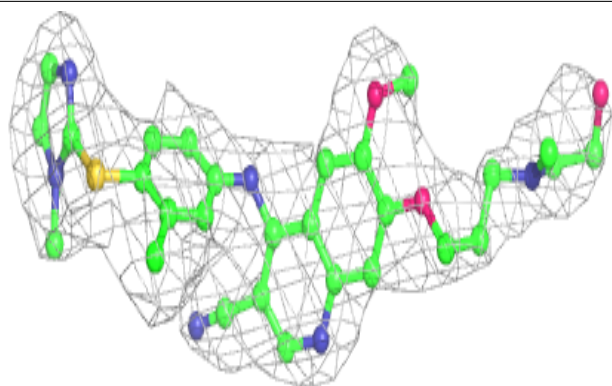
**Electron density around 741 C 3:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

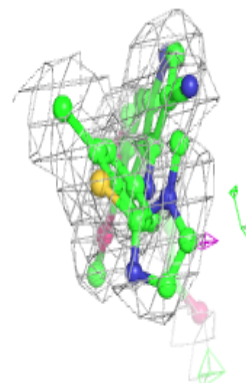
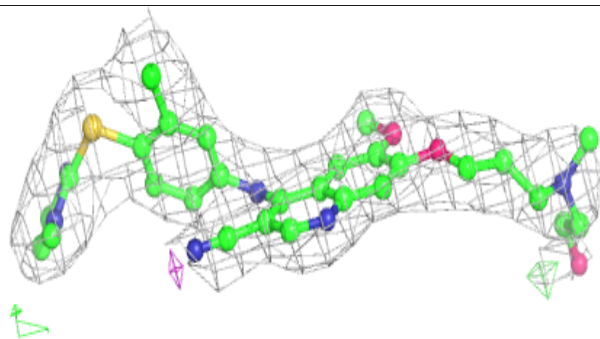
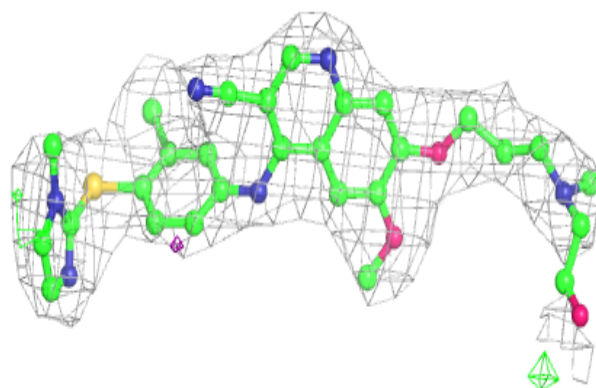


Electron density around 741 A 1:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

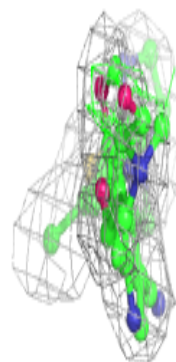
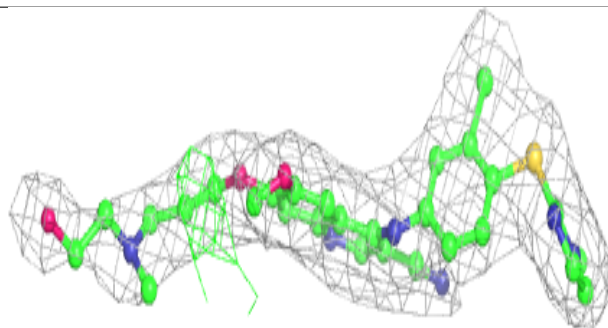
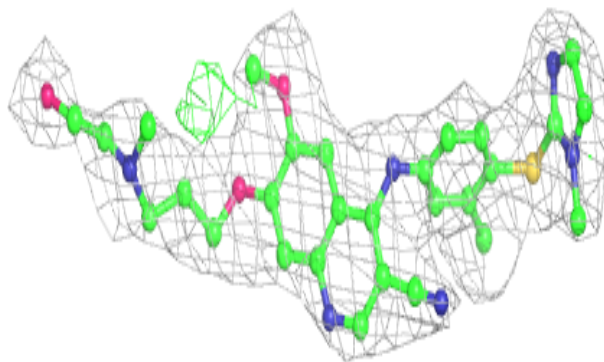
**Electron density around 741 M 12:**

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

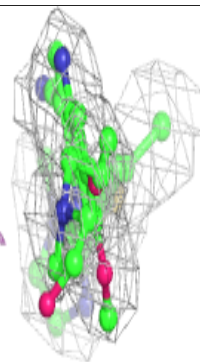
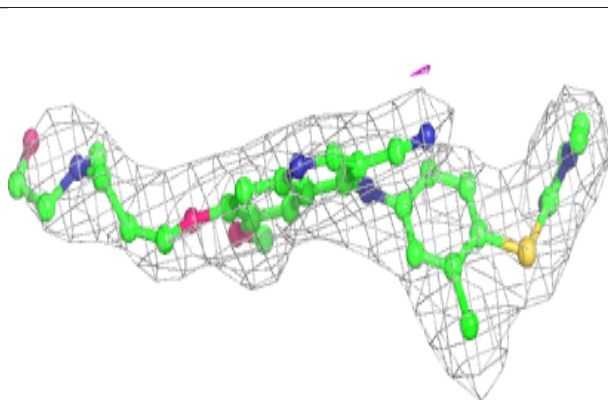
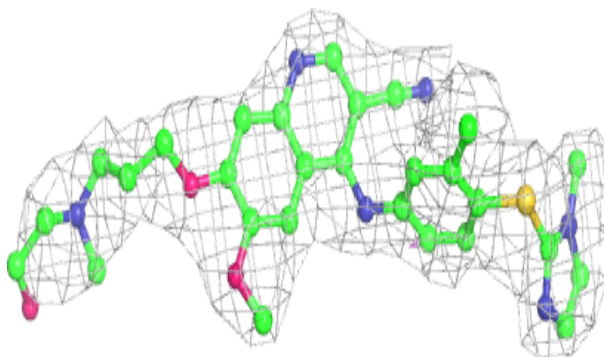


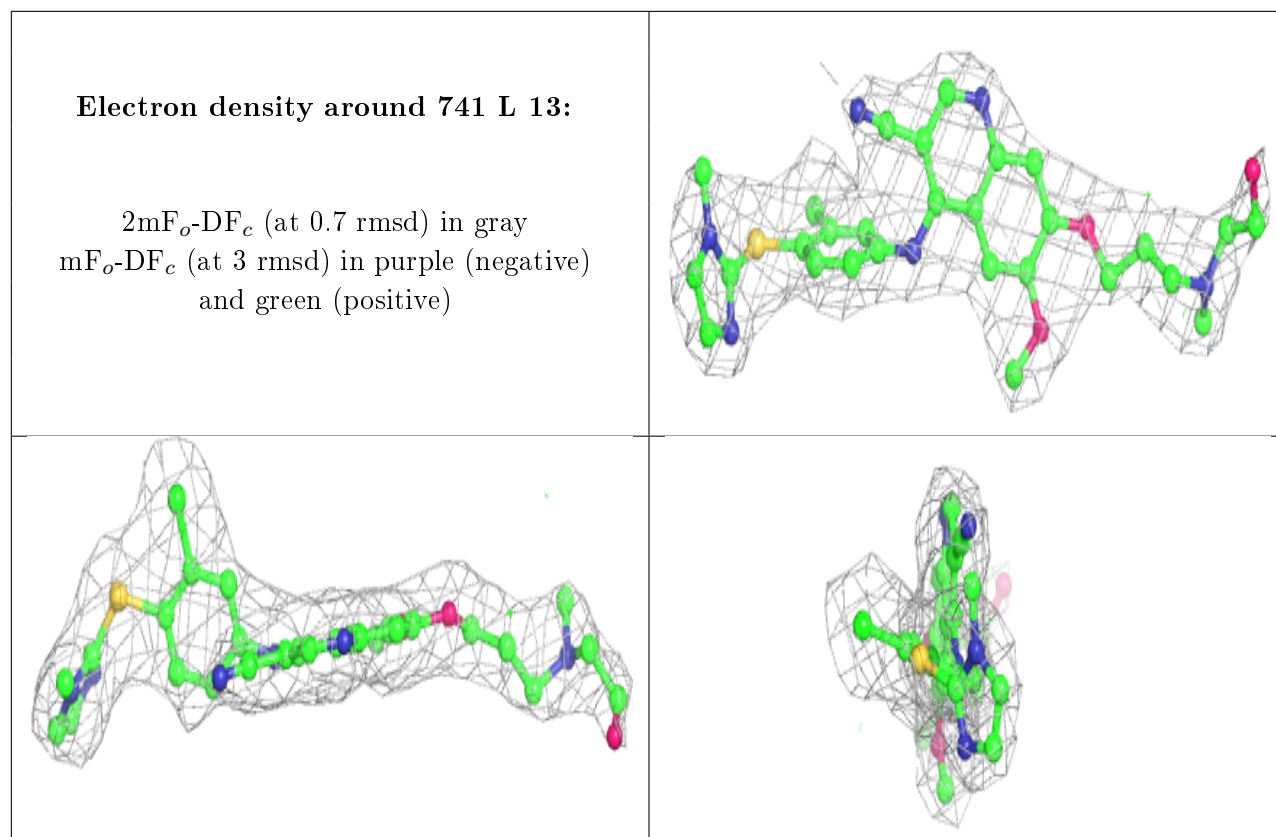
Electron density around 741 T 16:

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

**Electron density around 741 I 9:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.