Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 12:45 am BST

PDB ID	:	3H06
Title	:	Crystal structure of the binding domain of the AMPA subunit GluR2 bound to the willardiine antagonist, UBP282
Authors	:	Ahmed, A.H.; Oswald, R.E.
Deposited on	:	2009-04-08
Resolution	:	2.80 Å(reported)

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

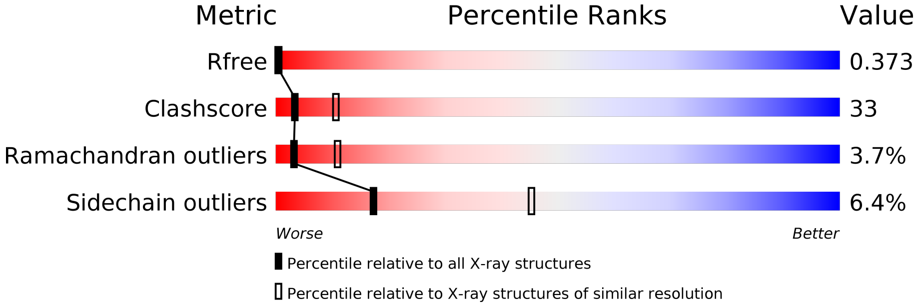
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	B	258	
1	E	258	
1	G	258	
1	H	258	
1	J	258	
1	L	258	
1	N	258	

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Mol	Chain	Length	Quality of chain
1	P	258	

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
2	VBP	B	807	X	-	-	-
2	VBP	E	808	X	-	-	-
2	VBP	G	803	X	-	-	-
2	VBP	H	806	X	-	-	-
2	VBP	J	804	X	-	-	-
2	VBP	L	801	X	-	-	-
2	VBP	N	802	X	-	-	-
2	VBP	P	805	X	-	-	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 16564 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	257	Total 2010	C 1280	N 334	O 382	S 14	0	0	0
1	B	257	Total 2010	C 1280	N 334	O 382	S 14	0	0	0
1	E	257	Total 2010	C 1280	N 334	O 382	S 14	0	0	0
1	H	257	Total 2010	C 1280	N 334	O 382	S 14	0	0	0
1	J	257	Total 2010	C 1280	N 334	O 382	S 14	0	0	0
1	L	257	Total 2010	C 1280	N 334	O 382	S 14	0	0	0
1	N	257	Total 2010	C 1280	N 334	O 382	S 14	0	0	0
1	P	257	Total 2010	C 1280	N 334	O 382	S 14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	118	GLY	-	LINKER	UNP P19491
G	119	THR	-	LINKER	UNP P19491
B	118	GLY	-	LINKER	UNP P19491
B	119	THR	-	LINKER	UNP P19491
E	118	GLY	-	LINKER	UNP P19491
E	119	THR	-	LINKER	UNP P19491
H	118	GLY	-	LINKER	UNP P19491
H	119	THR	-	LINKER	UNP P19491
J	118	GLY	-	LINKER	UNP P19491
J	119	THR	-	LINKER	UNP P19491
L	118	GLY	-	LINKER	UNP P19491
L	119	THR	-	LINKER	UNP P19491
N	118	GLY	-	LINKER	UNP P19491

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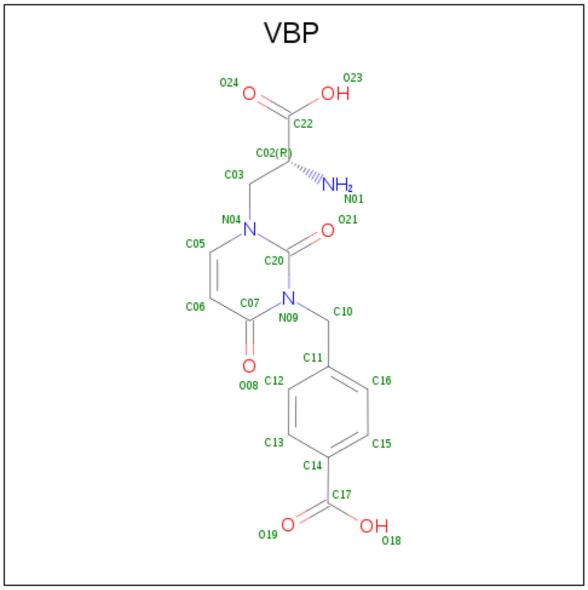
Chain	Residue	Modelled	Actual	Comment	Reference
N	119	THR	-	LINKER	UNP P19491
P	118	GLY	-	LINKER	UNP P19491
P	119	THR	-	LINKER	UNP P19491

- Molecule 2 is 4-({3-[(2R)-2-amino-2-carboxyethyl]-2,6-dioxo-3,6-dihydropyrimidin-1(2H)-yl} methyl)benzoic acid (three-letter code: VBP) (formula: $C_{15}H_{15}N_3O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C N O 24 15 3 6	0	0
2	B	1	Total C N O 24 15 3 6	0	0
2	E	1	Total C N O 24 15 3 6	0	0
2	H	1	Total C N O 24 15 3 6	0	0
2	J	1	Total C N O 24 15 3 6	0	0
2	L	1	Total C N O 24 15 3 6	0	0
2	N	1	Total C N O 24 15 3 6	0	0
2	P	1	Total C N O 24 15 3 6	0	0

- Molecule 3 is water.

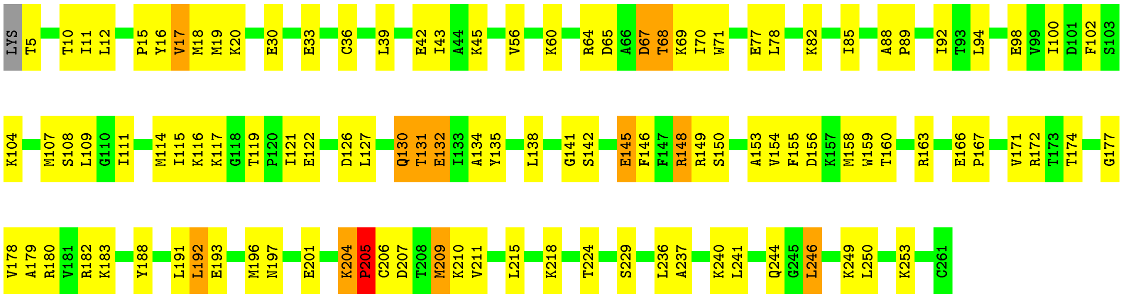
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	39	Total O 39 39	0	0
3	B	42	Total O 42 42	0	0
3	E	30	Total O 30 30	0	0
3	H	30	Total O 30 30	0	0
3	J	43	Total O 43 43	0	0
3	L	34	Total O 34 34	0	0
3	N	39	Total O 39 39	0	0
3	P	35	Total O 35 35	0	0

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. 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. 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: Glutamate receptor 2

Chain G:

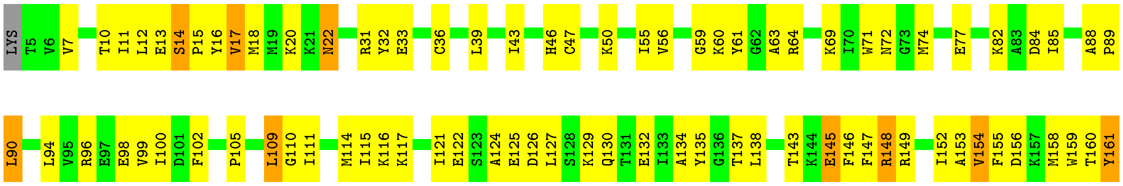


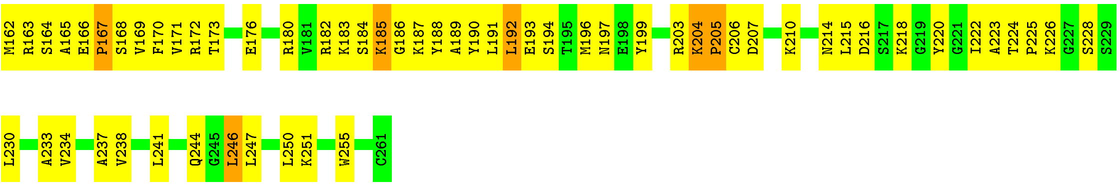
- Molecule 1: Glutamate receptor 2

Chain B:

- Molecule 1: Glutamate receptor 2

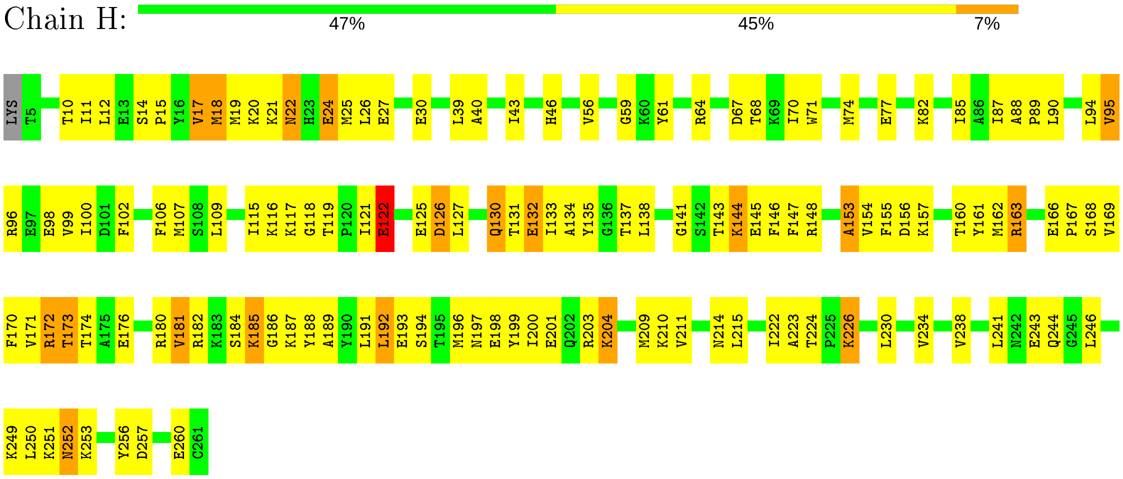
Chain E:





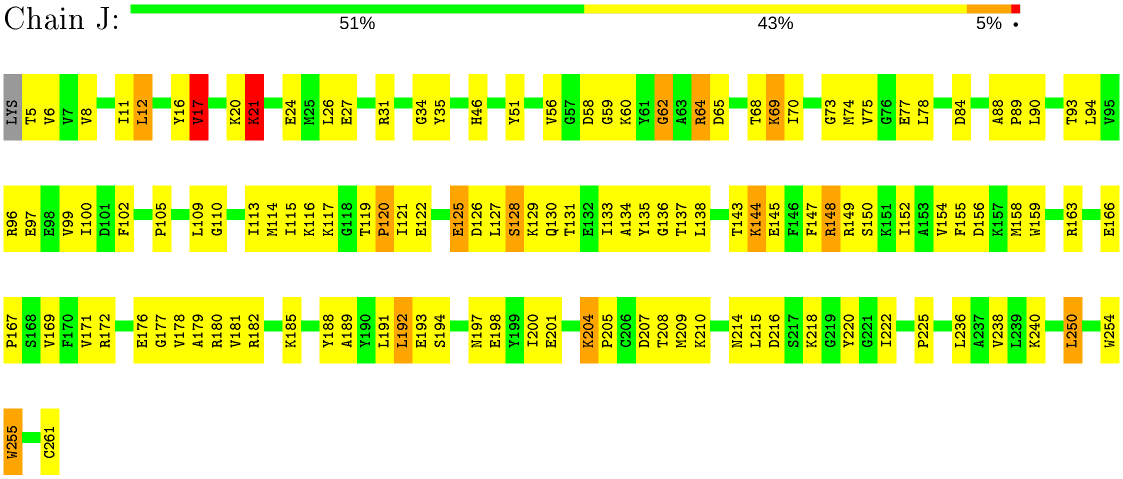
- Molecule 1: Glutamate receptor 2

Chain H:



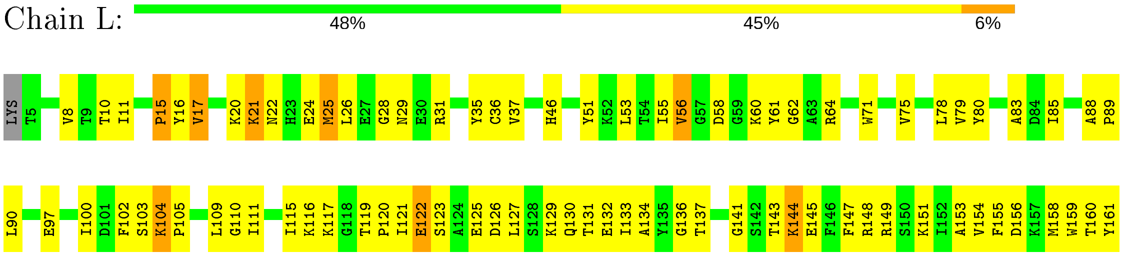
- Molecule 1: Glutamate receptor 2

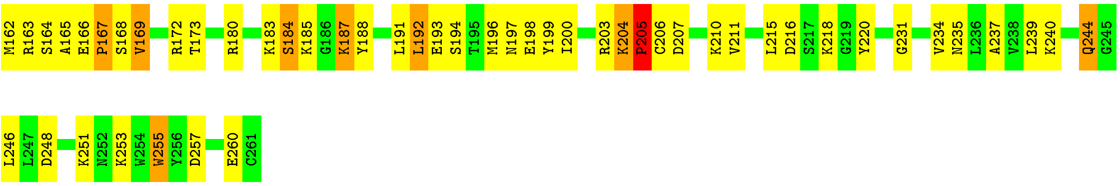
Chain J:



- Molecule 1: Glutamate receptor 2

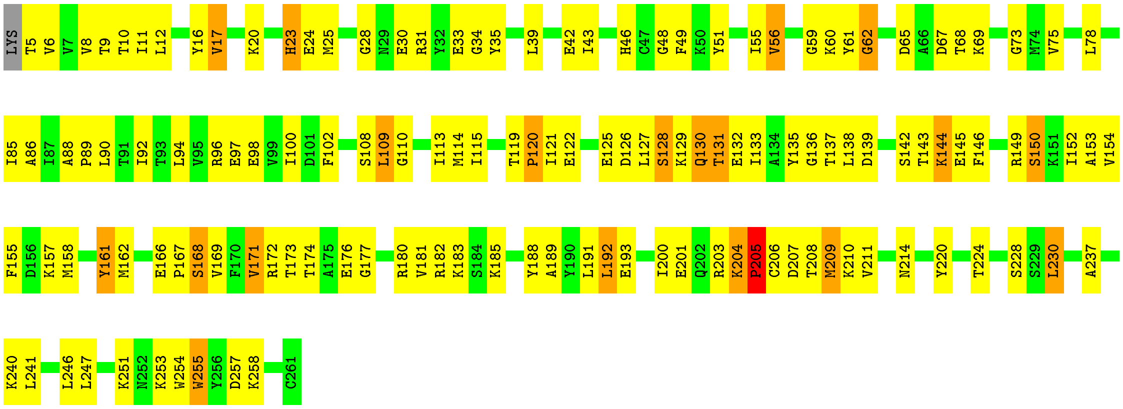
Chain L:





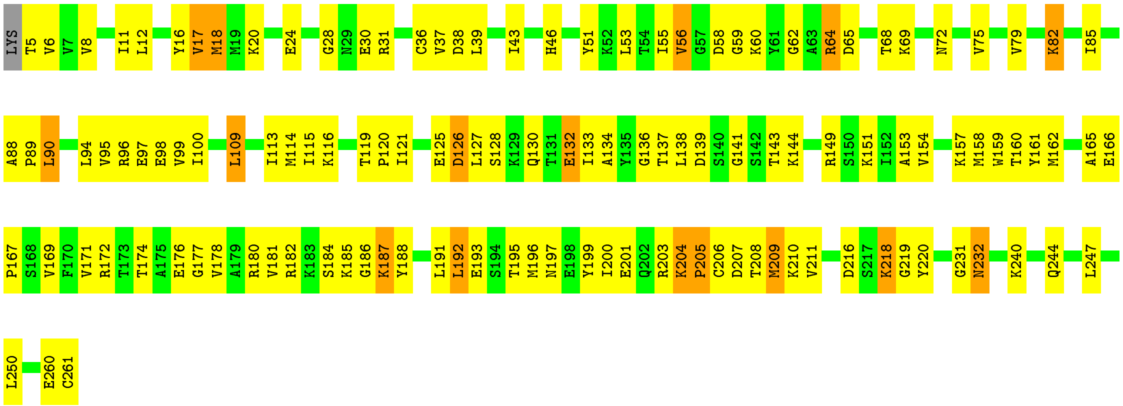
- Molecule 1: Glutamate receptor 2

Chain N:



- Molecule 1: Glutamate receptor 2

Chain P:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	91.01Å 90.92Å 92.51Å 85.61° 85.52° 72.40°	Depositor
Resolution (Å)	39.71 – 2.80 39.71 – 2.78	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.71-2.80) 90.8 (39.71-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	64.73 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.295 0.376 , 0.373	Depositor DCC
R_{free} test set	3259 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 16.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.62$, $< L^2 > = 0.49$	Xtriage
Estimated twinning fraction	0.349 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	16564	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	B	0.41	0/2046	0.64	0/2751
1	E	0.41	0/2046	0.63	0/2751
1	G	0.41	0/2046	0.65	0/2751
1	H	0.41	0/2046	0.61	0/2751
1	J	0.40	0/2046	0.62	0/2751
1	L	0.41	0/2046	0.62	0/2751
1	N	0.39	0/2046	0.62	0/2751
1	P	0.40	0/2046	0.64	0/2751
All	All	0.40	0/16368	0.63	0/22008

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2010	0	2037	133	0
1	E	2010	0	2037	140	0
1	G	2010	0	2037	116	0
1	H	2010	0	2037	139	0
1	J	2010	0	2037	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2010	0	2037	137	0
1	N	2010	0	2037	129	0
1	P	2010	0	2037	155	0
2	B	24	0	13	3	0
2	E	24	0	13	4	0
2	G	24	0	13	5	0
2	H	24	0	13	3	0
2	J	24	0	13	4	0
2	L	24	0	13	2	0
2	N	24	0	13	3	0
2	P	24	0	13	5	0
3	B	42	0	0	8	0
3	E	30	0	0	6	0
3	G	39	0	0	4	0
3	H	30	0	0	6	0
3	J	43	0	0	9	0
3	L	34	0	0	1	0
3	N	39	0	0	7	0
3	P	35	0	0	10	0
All	All	16564	0	16400	1065	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 33.

All (1065) 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:E:204:LYS:HB3	1:E:205:PRO:HD2	1.12	1.11
1:L:204:LYS:HB3	1:L:205:PRO:HD2	1.09	1.09
1:P:204:LYS:HB3	1:P:205:PRO:HD2	1.31	1.09
1:H:173:THR:HG23	1:H:176:GLU:HB2	1.36	1.07
1:G:204:LYS:HB3	1:G:205:PRO:HD2	1.11	1.06
1:N:204:LYS:HB3	1:N:205:PRO:HD2	1.07	1.04
1:N:204:LYS:HB3	1:N:205:PRO:CD	1.91	1.01
1:J:21:LYS:HD3	1:J:21:LYS:H	1.28	0.99
1:B:95:VAL:HG11	1:E:69:LYS:HD3	1.42	0.99
1:L:104:LYS:H	1:L:104:LYS:NZ	1.61	0.97
1:L:104:LYS:HZ3	1:L:104:LYS:H	1.01	0.96
1:L:104:LYS:N	1:L:104:LYS:HZ3	1.62	0.96
1:G:117:LYS:HE2	1:G:209:MET:HE3	1.49	0.94
1:E:185:LYS:HB2	1:E:187:LYS:HE2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:LYS:HB3	1:E:205:PRO:CD	1.99	0.92
1:L:204:LYS:HB3	1:L:205:PRO:CD	1.98	0.91
1:L:130:GLN:HE21	1:L:132:GLU:HB3	1.36	0.91
1:G:114:MET:HE1	1:G:178:VAL:HG13	1.52	0.90
1:H:116:LYS:HE2	1:N:25:MET:O	1.72	0.89
1:L:204:LYS:CB	1:L:205:PRO:HD2	2.01	0.89
1:J:21:LYS:CD	1:J:21:LYS:H	1.83	0.89
1:B:121:ILE:HD13	1:B:127:LEU:HD21	1.56	0.88
1:J:117:LYS:HA	1:J:209:MET:HE3	1.53	0.88
1:L:187:LYS:HE3	1:L:188:TYR:N	1.89	0.87
1:G:204:LYS:HB3	1:G:205:PRO:CD	2.01	0.87
1:N:150:SER:HA	3:N:285:HOH:O	1.75	0.86
1:E:204:LYS:CB	1:E:205:PRO:HD2	2.01	0.85
1:N:130:GLN:NE2	1:N:132:GLU:HB3	1.89	0.85
1:P:116:LYS:HE3	1:P:207:ASP:HB2	1.56	0.84
1:G:89:PRO:HB2	2:G:803:VBP:H05	1.56	0.83
1:E:172:ARG:HB3	1:E:176:GLU:OE1	1.78	0.83
1:P:204:LYS:CB	1:P:205:PRO:HD2	2.08	0.82
1:G:204:LYS:CB	1:G:205:PRO:HD2	2.03	0.82
1:B:39:LEU:O	1:B:43:ILE:HG12	1.78	0.82
1:H:64:ARG:NH1	1:H:71:TRP:HE1	1.78	0.81
1:J:204:LYS:HB3	1:J:205:PRO:HD3	1.63	0.81
1:B:122:GLU:HA	1:B:211:VAL:HG21	1.63	0.80
1:B:89:PRO:HB2	2:B:807:VBP:H05	1.63	0.80
1:E:99:VAL:HG23	1:E:100:ILE:HG23	1.63	0.80
1:G:130:GLN:OE1	1:G:132:GLU:HB3	1.82	0.79
1:P:204:LYS:HB3	1:P:205:PRO:CD	2.12	0.79
1:E:88:ALA:HB1	1:E:89:PRO:HD2	1.62	0.79
1:H:160:THR:HA	1:H:163:ARG:NH1	1.97	0.79
1:E:152:ILE:HG22	1:E:154:VAL:HG23	1.63	0.78
1:E:10:THR:HA	1:E:74:MET:HE1	1.64	0.78
1:N:130:GLN:HE21	1:N:132:GLU:HB3	1.48	0.78
1:B:159:TRP:O	1:B:163:ARG:HB2	1.83	0.78
1:J:182:ARG:HH12	1:J:205:PRO:HB2	1.48	0.77
1:J:89:PRO:HB2	2:J:804:VBP:H05	1.66	0.76
1:P:82:LYS:NZ	1:P:82:LYS:HA	2.00	0.76
1:L:100:ILE:HD12	1:L:100:ILE:O	1.86	0.76
1:P:94:LEU:O	1:P:98:GLU:HG3	1.85	0.76
1:H:153:ALA:HA	3:H:289:HOH:O	1.85	0.76
1:E:22:ASN:H	1:E:22:ASN:HD22	1.31	0.75
1:L:22:ASN:HB2	1:L:25:MET:HG3	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:166:GLU:HA	1:J:167:PRO:C	2.07	0.75
1:G:122:GLU:HA	1:G:211:VAL:HG21	1.65	0.75
1:N:128:SER:OG	1:N:154:VAL:HG13	1.86	0.75
1:H:64:ARG:HH11	1:H:71:TRP:HE1	1.35	0.75
1:G:122:GLU:HG2	1:G:126:ASP:OD2	1.87	0.74
1:N:56:VAL:HG13	1:N:59:GLY:HA2	1.69	0.74
1:H:15:PRO:HA	1:H:18:MET:HE3	1.70	0.74
1:H:130:GLN:HE21	1:H:132:GLU:N	1.85	0.74
1:P:232:ASN:HD22	1:P:232:ASN:N	1.82	0.74
1:P:58:ASP:O	1:P:60:LYS:HG3	1.88	0.73
1:E:39:LEU:O	1:E:43:ILE:HG12	1.89	0.73
1:H:56:VAL:HG13	1:H:59:GLY:HA2	1.70	0.73
1:B:114:MET:HE1	1:B:178:VAL:HG13	1.70	0.73
1:N:115:ILE:HD13	1:N:211:VAL:HG11	1.71	0.73
1:B:140:SER:HA	1:B:144:LYS:NZ	2.03	0.73
1:H:88:ALA:HB1	1:H:89:PRO:HD2	1.69	0.73
1:L:46:HIS:CD2	1:L:240:LYS:HD2	2.24	0.73
1:P:46:HIS:CD2	1:P:240:LYS:HD2	2.24	0.73
1:B:166:GLU:HA	1:B:167:PRO:C	2.08	0.72
1:L:154:VAL:O	1:L:158:MET:HG3	1.88	0.72
1:E:224:THR:HG23	3:E:268:HOH:O	1.89	0.72
1:N:204:LYS:CB	1:N:205:PRO:HD2	2.02	0.72
1:J:148:ARG:HG3	1:J:149:ARG:N	2.04	0.72
1:B:144:LYS:HE3	1:B:148:ARG:HH22	1.54	0.71
1:L:160:THR:HA	1:L:163:ARG:NH1	2.05	0.71
1:G:68:THR:OG1	1:G:70:ILE:HB	1.91	0.71
1:H:181:VAL:O	1:H:181:VAL:HG12	1.90	0.71
1:L:111:ILE:HD11	1:L:143:THR:HA	1.73	0.71
1:E:216:ASP:OD1	1:E:218:LYS:HE3	1.91	0.71
1:G:159:TRP:O	1:G:163:ARG:HB2	1.90	0.71
1:G:138:LEU:HD22	2:G:803:VBP:H15	1.73	0.71
1:H:135:TYR:HB3	1:H:189:ALA:HB3	1.72	0.71
1:L:156:ASP:O	1:L:160:THR:HG23	1.90	0.71
1:B:241:LEU:HD22	1:B:246:LEU:CD2	2.21	0.70
1:L:21:LYS:H	1:L:21:LYS:HD3	1.56	0.70
1:B:241:LEU:HD22	1:B:246:LEU:HD23	1.74	0.70
1:E:20:LYS:HG2	1:E:31:ARG:O	1.91	0.70
1:B:20:LYS:HG2	1:B:33:GLU:CD	2.12	0.70
1:N:154:VAL:O	1:N:158:MET:HG3	1.91	0.70
1:G:145:GLU:HA	1:G:148:ARG:HG2	1.73	0.70
1:H:141:GLY:O	1:H:145:GLU:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:166:GLU:HA	1:L:167:PRO:C	2.12	0.70
1:L:192:LEU:H	1:L:192:LEU:HD12	1.57	0.70
1:P:134:ALA:N	1:P:187:LYS:O	2.25	0.70
1:E:230:LEU:O	1:E:234:VAL:HG23	1.91	0.70
1:E:50:LYS:HE2	1:E:50:LYS:HA	1.73	0.70
1:N:162:MET:HE1	1:N:191:LEU:HD12	1.73	0.70
1:J:261:CYS:HB3	3:J:300:HOH:O	1.92	0.70
1:N:135:TYR:HB3	1:N:189:ALA:HB3	1.74	0.69
1:H:10:THR:HA	1:H:74:MET:HE1	1.74	0.69
1:L:184:SER:O	1:L:187:LYS:HE2	1.92	0.69
1:P:121:ILE:HG22	1:P:126:ASP:HB3	1.73	0.69
1:E:193:GLU:HG3	3:E:279:HOH:O	1.92	0.69
1:L:187:LYS:NZ	1:L:188:TYR:HB3	2.08	0.69
1:N:137:THR:HG22	1:N:191:LEU:HB2	1.75	0.69
1:H:39:LEU:O	1:H:43:ILE:HG12	1.93	0.69
1:B:204:LYS:HB2	3:B:300:HOH:O	1.92	0.69
1:B:210:LYS:HD2	3:B:298:HOH:O	1.93	0.69
1:B:251:LYS:HE3	3:B:293:HOH:O	1.93	0.69
1:L:104:LYS:CE	1:L:104:LYS:H	2.04	0.68
1:J:134:ALA:O	1:J:188:TYR:HA	1.94	0.68
1:P:64:ARG:HD3	1:P:69:LYS:HA	1.76	0.68
1:E:172:ARG:HG2	1:E:173:THR:HG23	1.76	0.68
1:G:130:GLN:HA	1:G:130:GLN:HE21	1.58	0.68
1:L:130:GLN:NE2	1:L:133:ILE:HG13	2.07	0.68
1:H:230:LEU:O	1:H:234:VAL:HG23	1.94	0.68
1:J:185:LYS:HD2	1:J:185:LYS:N	2.09	0.67
1:L:125:GLU:OE2	1:L:154:VAL:HG21	1.93	0.67
1:N:89:PRO:HB2	2:N:802:VBP:H05	1.76	0.67
1:P:16:TYR:CD1	1:P:89:PRO:HG3	2.28	0.67
1:J:46:HIS:CD2	1:J:240:LYS:HD2	2.29	0.67
1:E:205:PRO:O	1:E:207:ASP:N	2.26	0.67
1:G:16:TYR:CD1	1:G:89:PRO:HG3	2.29	0.67
1:J:129:LYS:O	1:J:131:THR:N	2.28	0.67
1:G:193:GLU:HG3	3:G:264:HOH:O	1.94	0.66
1:E:156:ASP:O	1:E:160:THR:HG23	1.96	0.66
1:E:203:ARG:O	1:E:204:LYS:O	2.13	0.66
1:L:115:ILE:HG21	1:L:121:ILE:CD1	2.26	0.66
1:H:117:LYS:HA	1:H:209:MET:HE2	1.78	0.66
1:J:69:LYS:NZ	1:J:69:LYS:HB2	2.10	0.66
1:P:114:MET:HE1	1:P:178:VAL:HA	1.77	0.66
1:B:145:GLU:HG2	1:B:148:ARG:HH21	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:ILE:HG23	1:H:133:ILE:HD12	1.77	0.66
1:J:149:ARG:HG2	3:J:265:HOH:O	1.95	0.66
1:P:169:VAL:HA	1:P:180:ARG:HH12	1.61	0.66
1:P:193:GLU:H	2:P:805:VBP:H13	1.61	0.66
1:J:152:ILE:HB	1:J:155:PHE:HD2	1.60	0.66
1:E:14:SER:O	1:E:18:MET:SD	2.54	0.65
1:G:166:GLU:HA	1:G:167:PRO:C	2.17	0.65
1:G:180:ARG:HD2	1:G:188:TYR:CZ	2.31	0.65
1:L:203:ARG:O	1:L:204:LYS:O	2.15	0.65
1:L:244:GLN:HB3	1:L:246:LEU:HD13	1.79	0.65
1:N:110:GLY:HA3	1:N:214:ASN:HB3	1.78	0.65
1:N:152:ILE:HG22	3:N:280:HOH:O	1.95	0.65
1:J:35:TYR:CE1	1:J:250:LEU:HB3	2.30	0.65
1:B:251:LYS:O	1:B:255:TRP:HB2	1.97	0.65
1:N:121:ILE:HD13	1:N:127:LEU:CD2	2.27	0.65
1:B:95:VAL:HG11	1:E:69:LYS:CD	2.25	0.65
1:J:64:ARG:HD3	1:J:69:LYS:HA	1.78	0.65
1:L:164:SER:O	1:L:165:ALA:HB3	1.97	0.65
1:H:11:ILE:HG13	3:H:268:HOH:O	1.97	0.65
1:J:6:VAL:O	1:J:51:TYR:HA	1.97	0.65
1:B:154:VAL:O	1:B:158:MET:HG3	1.97	0.65
1:L:89:PRO:HB2	2:L:801:VBP:H05	1.79	0.65
1:H:197:ASN:ND2	1:H:210:LYS:HG3	2.12	0.64
1:E:154:VAL:O	1:E:158:MET:HG3	1.97	0.64
1:H:130:GLN:HG2	1:H:131:THR:N	2.11	0.64
1:H:144:LYS:HE3	1:H:148:ARG:NH2	2.13	0.64
1:J:148:ARG:HA	1:J:159:TRP:CD1	2.31	0.64
1:B:172:ARG:HB3	1:B:172:ARG:NH1	2.12	0.64
1:G:193:GLU:OE1	1:G:218:LYS:NZ	2.29	0.64
1:G:205:PRO:O	1:G:207:ASP:N	2.30	0.64
1:J:178:VAL:HG12	1:J:182:ARG:HE	1.61	0.64
1:P:138:LEU:HD11	1:P:172:ARG:O	1.97	0.64
1:G:193:GLU:HG2	2:G:803:VBP:H13	1.80	0.64
1:N:20:LYS:HG2	1:N:31:ARG:O	1.97	0.64
1:H:224:THR:HG23	3:H:287:HOH:O	1.98	0.64
1:L:10:THR:OG1	1:L:17:VAL:HG11	1.97	0.64
1:N:158:MET:O	1:N:162:MET:HG3	1.98	0.64
1:H:166:GLU:HA	1:H:167:PRO:C	2.18	0.63
1:P:116:LYS:HG3	1:P:207:ASP:O	1.98	0.63
1:B:92:ILE:HG23	1:B:102:PHE:CD2	2.32	0.63
1:J:90:LEU:O	1:J:220:TYR:HA	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:177:GLY:O	1:J:181:VAL:HG23	1.97	0.63
1:B:16:TYR:CD1	1:B:89:PRO:HG3	2.34	0.63
1:E:64:ARG:NH1	1:E:71:TRP:HE1	1.96	0.63
1:G:197:ASN:ND2	1:G:210:LYS:HG3	2.14	0.63
1:P:115:ILE:HB	1:P:119:THR:HB	1.81	0.63
1:B:19:MET:HG3	3:J:289:HOH:O	1.98	0.63
1:H:134:ALA:HB3	1:H:187:LYS:O	1.99	0.63
1:N:157:LYS:HE3	1:N:161:TYR:CE1	2.34	0.63
1:N:180:ARG:O	1:N:188:TYR:HD2	1.82	0.63
1:E:166:GLU:HA	1:E:167:PRO:C	2.20	0.62
1:G:183:LYS:H	1:G:183:LYS:HD2	1.64	0.62
1:L:103:SER:HB2	1:L:104:LYS:HZ1	1.64	0.62
1:N:16:TYR:CD1	1:N:89:PRO:HG3	2.34	0.62
1:P:199:TYR:HE1	1:P:203:ARG:NH1	1.96	0.62
1:H:163:ARG:HH11	1:H:163:ARG:CB	2.12	0.62
1:L:8:VAL:HG22	1:L:85:ILE:CG2	2.29	0.62
1:L:104:LYS:HE3	1:L:239:LEU:HG	1.81	0.62
1:H:180:ARG:HG2	1:H:188:TYR:CD2	2.34	0.62
1:L:192:LEU:HD13	1:L:197:ASN:HB2	1.82	0.62
1:B:191:LEU:N	1:B:191:LEU:HD12	2.15	0.62
1:L:137:THR:HG22	1:L:191:LEU:HB2	1.82	0.62
1:N:144:LYS:HB3	1:N:144:LYS:NZ	2.15	0.62
1:B:100:ILE:HD12	1:B:223:ALA:HB1	1.80	0.62
1:B:42:GLU:HG3	1:B:246:LEU:HD21	1.81	0.62
1:L:16:TYR:CD1	1:L:89:PRO:HG3	2.34	0.62
1:P:201:GLU:HG3	1:P:209:MET:HA	1.82	0.62
1:E:100:ILE:HD13	1:E:223:ALA:HB1	1.82	0.62
1:H:117:LYS:HG3	1:H:209:MET:HE2	1.82	0.62
1:J:110:GLY:HA3	1:J:214:ASN:HB3	1.82	0.62
1:N:251:LYS:HD2	1:N:255:TRP:CE3	2.34	0.62
1:E:138:LEU:HD22	2:E:808:VBP:H15	1.81	0.62
1:J:20:LYS:HB2	1:J:31:ARG:O	1.99	0.62
1:L:172:ARG:HG2	1:L:173:THR:HG23	1.81	0.62
1:L:24:GLU:H	1:L:24:GLU:CD	2.04	0.62
1:L:58:ASP:O	1:L:60:LYS:HG3	2.00	0.62
1:N:152:ILE:HB	1:N:155:PHE:CD2	2.35	0.62
1:P:171:VAL:HB	1:P:176:GLU:HB3	1.81	0.62
1:H:137:THR:HG22	1:H:191:LEU:HB2	1.80	0.61
1:L:104:LYS:HD2	1:L:239:LEU:HD21	1.81	0.61
1:E:183:LYS:HB2	1:E:183:LYS:NZ	2.15	0.61
1:E:204:LYS:O	1:E:205:PRO:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:TRP:HE1	1:G:163:ARG:NH1	1.97	0.61
1:H:157:LYS:HE2	1:H:161:TYR:CE1	2.35	0.61
1:B:144:LYS:HE3	1:B:148:ARG:HH12	1.65	0.61
1:E:125:GLU:N	1:E:125:GLU:OE1	2.25	0.61
1:E:169:VAL:HA	1:E:180:ARG:HH12	1.65	0.61
1:B:92:ILE:HA	1:B:102:PHE:CE2	2.35	0.61
1:H:172:ARG:HB3	1:H:176:GLU:OE1	2.00	0.61
1:N:130:GLN:HG3	1:N:133:ILE:H	1.64	0.61
1:G:240:LYS:O	1:G:244:GLN:HG3	1.99	0.61
1:P:232:ASN:N	1:P:232:ASN:ND2	2.48	0.61
1:J:148:ARG:HB2	1:J:148:ARG:HH11	1.66	0.61
1:P:79:VAL:HG22	1:P:99:VAL:HG12	1.82	0.61
1:G:172:ARG:NH1	1:G:172:ARG:HB3	2.16	0.61
1:J:222:ILE:HD13	1:J:238:VAL:HG21	1.83	0.61
1:H:10:THR:HA	1:H:74:MET:CE	2.30	0.60
1:J:121:ILE:HG13	1:J:126:ASP:HB3	1.83	0.60
1:E:155:PHE:CE1	1:E:215:LEU:HD13	2.37	0.60
1:H:147:PHE:CE2	1:H:191:LEU:HD13	2.37	0.60
1:N:166:GLU:HA	1:N:167:PRO:C	2.22	0.60
1:B:144:LYS:NZ	3:B:273:HOH:O	2.32	0.60
1:P:125:GLU:OE1	1:P:154:VAL:HG11	2.02	0.60
1:J:152:ILE:HB	1:J:155:PHE:CD2	2.36	0.60
1:P:154:VAL:O	1:P:158:MET:HG3	2.02	0.60
1:B:11:ILE:O	1:B:17:VAL:HG13	2.02	0.60
1:H:130:GLN:NE2	1:H:132:GLU:N	2.49	0.59
1:P:203:ARG:O	1:P:204:LYS:O	2.19	0.59
1:H:134:ALA:O	1:H:188:TYR:HA	2.03	0.59
1:J:114:MET:HE1	1:J:178:VAL:HA	1.84	0.59
1:L:192:LEU:N	1:L:192:LEU:HD12	2.15	0.59
1:N:130:GLN:HE21	1:N:133:ILE:H	1.50	0.59
1:B:42:GLU:CG	1:B:246:LEU:HD21	2.33	0.59
1:E:11:ILE:O	1:E:17:VAL:CG1	2.50	0.59
1:H:26:LEU:HD22	1:H:30:GLU:OE2	2.03	0.59
1:L:78:LEU:HD23	1:L:83:ALA:HB3	1.84	0.59
1:P:172:ARG:HB2	1:P:172:ARG:NH1	2.18	0.59
1:E:147:PHE:CE2	1:E:191:LEU:HD13	2.37	0.59
1:H:133:ILE:HG23	1:H:186:GLY:O	2.02	0.59
1:B:62:GLY:HA3	1:B:75:VAL:HG23	1.84	0.59
1:G:109:LEU:HD12	1:G:193:GLU:HB3	1.83	0.59
1:L:163:ARG:HG3	1:L:164:SER:N	2.17	0.59
1:L:199:TYR:O	1:L:203:ARG:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:VAL:HG23	1:H:100:ILE:HG23	1.84	0.59
1:L:21:LYS:HG2	1:L:22:ASN:H	1.67	0.59
1:J:121:ILE:HD13	1:J:133:ILE:HD12	1.85	0.59
1:J:125:GLU:HA	1:J:128:SER:OG	2.03	0.59
1:J:194:SER:O	1:J:198:GLU:HG3	2.01	0.59
1:L:183:LYS:O	1:L:184:SER:HB3	2.02	0.59
1:L:20:LYS:HD2	1:L:26:LEU:HD12	1.85	0.59
1:E:10:THR:HA	1:E:74:MET:CE	2.31	0.59
1:E:121:ILE:HD13	1:E:127:LEU:HD21	1.85	0.59
1:L:121:ILE:HG22	1:L:126:ASP:HB3	1.85	0.59
1:N:253:LYS:HE2	1:N:258:LYS:NZ	2.18	0.59
1:P:11:ILE:O	1:P:17:VAL:HG13	2.02	0.59
1:B:115:ILE:CG2	1:B:121:ILE:HD11	2.33	0.59
1:B:144:LYS:HE3	1:B:148:ARG:NH2	2.17	0.59
1:G:171:VAL:HG11	1:G:177:GLY:HA2	1.83	0.59
1:L:155:PHE:CE1	1:L:215:LEU:HD13	2.37	0.59
1:P:46:HIS:HD2	1:P:240:LYS:HD2	1.67	0.59
1:J:117:LYS:HG2	1:J:209:MET:CE	2.33	0.58
1:N:136:GLY:HA3	1:N:169:VAL:O	2.02	0.58
1:P:53:LEU:HD11	3:P:292:HOH:O	2.02	0.58
1:B:137:THR:HG22	1:B:191:LEU:HB2	1.85	0.58
1:G:100:ILE:HD12	1:G:100:ILE:C	2.23	0.58
1:B:20:LYS:HD3	1:B:33:GLU:HB3	1.85	0.58
1:H:130:GLN:NE2	1:H:133:ILE:N	2.51	0.58
1:H:163:ARG:HB2	1:H:163:ARG:HH11	1.67	0.58
1:P:203:ARG:HD3	1:P:260:GLU:HG2	1.85	0.58
1:P:37:VAL:HG13	3:P:292:HOH:O	2.02	0.58
1:P:56:VAL:HG13	1:P:59:GLY:HA2	1.85	0.58
1:B:134:ALA:O	1:B:188:TYR:HA	2.03	0.58
1:B:225:PRO:HD2	1:B:228:SER:HB2	1.84	0.58
1:H:77:GLU:HG2	1:H:82:LYS:HB2	1.84	0.58
1:L:172:ARG:HB2	1:L:172:ARG:HH11	1.66	0.58
1:L:197:ASN:HD21	1:L:210:LYS:HA	1.69	0.58
1:N:152:ILE:HB	1:N:155:PHE:HD2	1.69	0.58
1:E:134:ALA:HA	1:E:161:TYR:OH	2.04	0.58
1:G:130:GLN:HG3	1:G:131:THR:N	2.18	0.58
1:G:154:VAL:O	1:G:158:MET:HG3	2.04	0.58
1:G:172:ARG:CZ	1:G:172:ARG:HB3	2.31	0.58
1:E:152:ILE:O	1:E:156:ASP:N	2.34	0.58
1:L:104:LYS:HB3	1:L:105:PRO:HD2	1.84	0.58
1:L:141:GLY:O	1:L:145:GLU:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:LYS:H	1:L:21:LYS:CD	2.17	0.58
1:B:196:MET:HA	1:B:196:MET:CE	2.34	0.58
1:G:109:LEU:HD23	1:G:109:LEU:N	2.19	0.58
1:N:46:HIS:CD2	1:N:240:LYS:HD2	2.38	0.58
1:E:22:ASN:H	1:E:22:ASN:ND2	2.02	0.58
1:E:56:VAL:HG13	1:E:59:GLY:HA2	1.86	0.58
1:P:121:ILE:CG2	1:P:126:ASP:HB3	2.34	0.58
1:P:166:GLU:HA	1:P:167:PRO:C	2.23	0.58
1:G:119:THR:HG22	1:G:121:ILE:HG12	1.85	0.57
1:P:180:ARG:HD2	1:P:188:TYR:CD2	2.38	0.57
1:E:31:ARG:HH21	1:E:32:TYR:HE2	1.51	0.57
1:L:29:ASN:HB2	3:L:282:HOH:O	2.05	0.57
1:J:135:TYR:HB3	1:J:189:ALA:HB3	1.87	0.57
1:J:216:ASP:OD2	1:J:218:LYS:HE2	2.05	0.57
1:G:160:THR:O	1:G:163:ARG:HB3	2.04	0.57
1:L:11:ILE:O	1:L:17:VAL:HG13	2.04	0.57
1:N:20:LYS:HG3	1:N:30:GLU:O	2.04	0.57
1:B:192:LEU:H	1:B:192:LEU:HD12	1.69	0.57
1:E:153:ALA:HA	1:E:156:ASP:HB3	1.87	0.57
1:H:162:MET:HA	1:H:169:VAL:HG21	1.86	0.57
1:L:121:ILE:HG22	1:L:126:ASP:O	2.05	0.57
1:P:125:GLU:HA	1:P:128:SER:OG	2.04	0.57
1:P:193:GLU:OE1	1:P:218:LYS:HE2	2.04	0.57
1:E:125:GLU:O	1:E:129:LYS:HG2	2.04	0.57
1:E:192:LEU:HD13	1:E:197:ASN:HB2	1.85	0.57
1:H:160:THR:HA	1:H:163:ARG:HH11	1.67	0.57
1:N:180:ARG:HG2	1:N:188:TYR:CD2	2.40	0.57
1:N:204:LYS:O	1:N:205:PRO:C	2.42	0.57
1:N:172:ARG:HG2	1:N:173:THR:HG23	1.86	0.57
1:P:210:LYS:HE3	3:P:290:HOH:O	2.04	0.57
1:E:20:LYS:HD3	1:E:33:GLU:HB3	1.87	0.57
1:J:90:LEU:HD22	1:J:96:ARG:NH1	2.19	0.57
1:J:182:ARG:HH12	1:J:205:PRO:CB	2.16	0.56
1:N:130:GLN:O	1:N:130:GLN:HG3	2.05	0.56
1:E:152:ILE:CG2	1:E:154:VAL:HG23	2.34	0.56
1:G:246:LEU:O	1:G:250:LEU:HG	2.05	0.56
1:L:16:TYR:CG	1:L:89:PRO:HG3	2.39	0.56
1:H:130:GLN:HG2	1:H:131:THR:H	1.69	0.56
1:H:203:ARG:O	1:H:260:GLU:HB2	2.05	0.56
1:H:243:GLU:O	1:L:149:ARG:HD2	2.05	0.56
1:P:119:THR:HG22	1:P:121:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:182:ARG:HG2	1:J:207:ASP:OD2	2.05	0.56
1:J:8:VAL:HG23	1:J:51:TYR:HB2	1.87	0.56
1:G:92:ILE:HG23	1:G:102:PHE:CD2	2.40	0.56
1:G:179:ALA:O	1:G:183:LYS:HD3	2.06	0.56
1:L:21:LYS:HD3	1:L:21:LYS:N	2.20	0.56
1:P:121:ILE:HD12	1:P:127:LEU:CD2	2.35	0.56
1:P:157:LYS:HD3	1:P:157:LYS:O	2.05	0.56
1:B:155:PHE:CE1	1:B:215:LEU:HD13	2.40	0.56
1:P:182:ARG:HH21	1:P:200:ILE:CG2	2.18	0.56
1:N:139:ASP:HB2	1:N:171:VAL:O	2.06	0.56
1:P:28:GLY:HA2	1:P:31:ARG:HH21	1.69	0.56
1:J:58:ASP:OD1	1:J:73:GLY:HA2	2.05	0.56
1:P:141:GLY:HA3	3:P:262:HOH:O	2.06	0.56
1:P:151:LYS:HE2	1:P:151:LYS:HA	1.88	0.56
1:L:155:PHE:HE1	1:L:215:LEU:HD13	1.68	0.56
1:L:166:GLU:CA	1:L:167:PRO:C	2.73	0.56
1:P:109:LEU:CD2	1:P:219:GLY:HA2	2.36	0.56
1:J:138:LEU:HD22	2:J:804:VBP:H15	1.87	0.56
1:N:144:LYS:HE2	1:N:144:LYS:C	2.27	0.56
1:B:20:LYS:HE2	1:B:30:GLU:O	2.06	0.55
1:B:115:ILE:C	1:B:115:ILE:HD12	2.27	0.55
1:G:156:ASP:O	1:G:160:THR:HG23	2.05	0.55
1:H:196:MET:HE2	2:H:806:VBP:H10	1.87	0.55
1:G:148:ARG:HG3	1:G:149:ARG:HG3	1.88	0.55
1:H:148:ARG:NH2	3:H:269:HOH:O	2.32	0.55
1:J:155:PHE:HE1	1:J:215:LEU:HD22	1.70	0.55
1:J:192:LEU:HD12	1:J:192:LEU:N	2.20	0.55
1:P:82:LYS:HZ2	1:P:82:LYS:HA	1.71	0.55
1:G:183:LYS:N	1:G:183:LYS:HD2	2.21	0.55
1:N:24:GLU:H	1:N:24:GLU:CD	2.10	0.55
1:B:193:GLU:H	2:B:807:VBP:H13	1.71	0.55
1:G:122:GLU:O	1:G:211:VAL:HG22	2.06	0.55
1:B:140:SER:HA	1:B:144:LYS:CE	2.36	0.55
1:B:16:TYR:CG	1:B:89:PRO:HG3	2.42	0.55
1:L:172:ARG:NH1	1:L:172:ARG:HB2	2.22	0.55
1:H:19:MET:HG3	3:P:281:HOH:O	2.05	0.55
1:L:100:ILE:HD11	1:L:102:PHE:CE2	2.42	0.55
1:L:166:GLU:HB2	1:L:168:SER:N	2.22	0.55
1:P:125:GLU:C	1:P:127:LEU:H	2.09	0.55
1:B:136:GLY:O	1:B:191:LEU:HD13	2.06	0.55
1:H:138:LEU:HD22	2:H:806:VBP:H15	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:136:GLY:HA3	1:J:169:VAL:O	2.06	0.55
1:L:147:PHE:CZ	1:L:191:LEU:HD13	2.41	0.55
1:N:247:LEU:HB2	3:N:276:HOH:O	2.07	0.55
1:P:121:ILE:HD12	1:P:127:LEU:HD23	1.88	0.55
1:P:192:LEU:HD12	1:P:192:LEU:N	2.20	0.55
1:P:195:THR:HG21	1:P:220:TYR:HE2	1.71	0.55
1:B:122:GLU:HA	1:B:211:VAL:CG2	2.35	0.55
1:B:192:LEU:HD13	1:B:197:ASN:HB2	1.89	0.55
1:H:115:ILE:O	1:H:115:ILE:HD12	2.07	0.55
1:L:205:PRO:O	1:L:207:ASP:N	2.40	0.55
1:P:208:THR:O	1:P:209:MET:HB2	2.06	0.55
1:H:193:GLU:H	2:H:806:VBP:H13	1.72	0.55
1:H:201:GLU:HG3	1:H:209:MET:HA	1.89	0.55
1:B:95:VAL:HB	1:E:64:ARG:HH21	1.71	0.54
1:N:115:ILE:CD1	1:N:211:VAL:HG11	2.36	0.54
1:G:180:ARG:HD2	1:G:188:TYR:CE2	2.41	0.54
1:N:16:TYR:HA	1:N:35:TYR:HB3	1.89	0.54
1:E:226:LYS:HE3	3:P:285:HOH:O	2.08	0.54
1:G:39:LEU:O	1:G:43:ILE:HG12	2.07	0.54
1:L:121:ILE:HD12	1:L:121:ILE:O	2.08	0.54
1:L:194:SER:O	1:L:198:GLU:HG3	2.08	0.54
1:P:182:ARG:NH1	1:P:205:PRO:HB2	2.23	0.54
1:G:148:ARG:NH1	1:G:148:ARG:HB2	2.22	0.54
1:N:185:LYS:HD2	1:N:185:LYS:N	2.23	0.54
1:H:109:LEU:HD23	1:H:109:LEU:N	2.23	0.54
1:P:192:LEU:HD13	1:P:197:ASN:HB2	1.89	0.54
1:B:180:ARG:HG2	1:B:188:TYR:CD2	2.42	0.54
1:N:88:ALA:HB1	1:N:89:PRO:CD	2.38	0.54
1:P:115:ILE:HB	1:P:119:THR:CB	2.38	0.54
1:H:27:GLU:HG2	3:H:285:HOH:O	2.07	0.54
1:N:203:ARG:O	1:N:204:LYS:O	2.26	0.54
1:N:205:PRO:O	1:N:207:ASP:N	2.33	0.54
1:N:208:THR:O	1:N:209:MET:HB3	2.07	0.54
1:B:159:TRP:NE1	1:B:163:ARG:NH1	2.56	0.54
1:L:115:ILE:HG21	1:L:121:ILE:HD13	1.89	0.54
1:N:8:VAL:HG22	1:N:85:ILE:CG2	2.38	0.54
1:H:64:ARG:NH1	1:H:71:TRP:NE1	2.49	0.53
1:J:20:LYS:HG2	1:J:26:LEU:CD1	2.37	0.53
1:B:166:GLU:H	1:B:166:GLU:CD	2.11	0.53
1:H:156:ASP:HB3	3:H:289:HOH:O	2.07	0.53
1:L:97:GLU:OE2	1:L:102:PHE:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:82:LYS:HZ3	1:P:82:LYS:HA	1.72	0.53
1:G:18:MET:N	1:G:33:GLU:O	2.32	0.53
1:N:121:ILE:HD13	1:N:127:LEU:HD21	1.91	0.53
1:G:159:TRP:HE1	1:G:163:ARG:HH11	1.57	0.53
1:L:187:LYS:HZ2	1:L:188:TYR:HB3	1.72	0.53
1:B:90:LEU:HD22	1:B:96:ARG:NH1	2.23	0.53
1:G:92:ILE:HG12	1:G:102:PHE:CG	2.44	0.53
1:J:65:ASP:O	1:J:69:LYS:HA	2.09	0.53
1:N:119:THR:HG23	1:N:133:ILE:HD13	1.90	0.53
1:P:125:GLU:C	1:P:127:LEU:N	2.62	0.53
1:P:62:GLY:HA3	1:P:75:VAL:HG23	1.91	0.53
1:E:100:ILE:HD11	1:E:102:PHE:CE2	2.44	0.53
1:H:118:GLY:HA2	1:N:30:GLU:CG	2.39	0.53
1:H:192:LEU:HD13	1:H:197:ASN:HB2	1.91	0.53
1:N:20:LYS:O	1:N:23:HIS:HB3	2.07	0.53
1:G:94:LEU:HD12	1:J:236:LEU:HD22	1.91	0.53
1:N:237:ALA:O	1:N:241:LEU:HG	2.09	0.53
1:E:246:LEU:O	1:E:250:LEU:HG	2.09	0.52
1:G:197:ASN:HD22	1:G:210:LYS:HG3	1.73	0.52
1:B:62:GLY:HA2	1:B:72:ASN:O	2.09	0.52
1:E:127:LEU:HB3	1:E:135:TYR:CE2	2.44	0.52
1:E:64:ARG:NH1	1:E:71:TRP:NE1	2.57	0.52
1:J:21:LYS:HD3	1:J:21:LYS:N	2.10	0.52
1:P:89:PRO:HB2	2:P:805:VBP:H05	1.91	0.52
1:H:17:VAL:C	1:H:18:MET:HG3	2.28	0.52
1:L:36:CYS:SG	1:L:88:ALA:HA	2.49	0.52
1:B:20:LYS:CE	1:B:30:GLU:O	2.57	0.52
1:N:125:GLU:HA	1:N:125:GLU:OE1	2.09	0.52
1:J:115:ILE:HD13	1:J:121:ILE:O	2.10	0.52
1:J:148:ARG:HG3	1:J:149:ARG:H	1.74	0.52
1:L:134:ALA:O	1:L:188:TYR:HA	2.10	0.52
1:N:20:LYS:HD3	1:N:33:GLU:HB3	1.90	0.52
1:H:115:ILE:HD12	1:H:115:ILE:C	2.30	0.52
1:B:110:GLY:HA3	1:B:214:ASN:HB3	1.91	0.52
1:G:20:LYS:NZ	1:G:30:GLU:HG2	2.25	0.52
1:H:144:LYS:HE3	1:H:148:ARG:HH21	1.73	0.52
1:L:46:HIS:HD2	1:L:240:LYS:HD2	1.75	0.52
1:P:180:ARG:O	1:P:180:ARG:HG2	2.10	0.52
1:P:199:TYR:CE1	1:P:203:ARG:NH1	2.77	0.52
1:P:232:ASN:HA	3:P:289:HOH:O	2.09	0.52
1:G:114:MET:HE2	1:G:178:VAL:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:GLU:HG3	1:J:126:ASP:OD2	2.10	0.52
1:P:6:VAL:O	1:P:51:TYR:HA	2.09	0.52
1:G:201:GLU:HG2	1:G:201:GLU:O	2.09	0.52
1:P:109:LEU:HD23	1:P:219:GLY:HA2	1.91	0.52
1:B:112:SER:OG	1:B:194:SER:HA	2.10	0.52
1:H:173:THR:O	1:H:176:GLU:HB3	2.10	0.52
1:J:68:THR:HB	1:J:70:ILE:HG12	1.91	0.52
1:P:193:GLU:HG2	2:P:805:VBP:H13	1.92	0.52
1:H:252:ASN:ND2	1:H:256:TYR:HB2	2.25	0.51
1:H:24:GLU:HG2	1:H:25:MET:N	2.25	0.51
1:H:21:LYS:O	1:H:22:ASN:HB3	2.10	0.51
1:J:154:VAL:O	1:J:158:MET:HG3	2.11	0.51
1:N:200:ILE:HG22	1:N:208:THR:OG1	2.09	0.51
1:P:134:ALA:O	1:P:188:TYR:HA	2.11	0.51
1:E:11:ILE:HG12	1:E:12:LEU:N	2.25	0.51
1:P:113:ILE:HG12	1:P:191:LEU:HD21	1.92	0.51
1:G:191:LEU:HD12	1:G:191:LEU:N	2.25	0.51
1:L:134:ALA:N	1:L:187:LYS:O	2.41	0.51
1:N:16:TYR:CG	1:N:89:PRO:HG3	2.45	0.51
1:B:140:SER:HA	1:B:144:LYS:HZ3	1.73	0.51
1:B:114:MET:HE2	1:B:178:VAL:HA	1.91	0.51
1:H:109:LEU:HB2	1:H:194:SER:OG	2.10	0.51
1:N:171:VAL:HG22	1:N:176:GLU:HB3	1.93	0.51
1:N:121:ILE:HD13	1:N:127:LEU:HD23	1.92	0.51
1:E:130:GLN:OE1	1:E:132:GLU:N	2.44	0.51
1:E:22:ASN:N	1:E:22:ASN:ND2	2.59	0.51
1:H:234:VAL:O	1:H:238:VAL:HG23	2.11	0.51
1:P:196:MET:HE2	2:P:805:VBP:H10	1.93	0.51
1:B:19:MET:HB3	1:B:23:HIS:CD2	2.46	0.51
1:E:135:TYR:HB3	1:E:189:ALA:HB3	1.93	0.51
1:E:225:PRO:HD2	1:E:228:SER:HB2	1.93	0.51
1:J:117:LYS:HE3	3:J:279:HOH:O	2.11	0.51
1:J:56:VAL:HG13	1:J:59:GLY:HA2	1.92	0.51
1:L:111:ILE:CD1	1:L:143:THR:HA	2.40	0.51
1:B:89:PRO:HB2	2:B:807:VBP:C05	2.38	0.50
1:J:210:LYS:HE2	3:J:267:HOH:O	2.10	0.50
1:L:79:VAL:HG12	1:L:80:TYR:CD1	2.45	0.50
1:N:142:SER:HA	1:N:145:GLU:HB2	1.93	0.50
1:P:24:GLU:H	1:P:24:GLU:CD	2.14	0.50
1:B:159:TRP:HE1	1:B:163:ARG:NH1	2.08	0.50
1:E:153:ALA:O	1:E:154:VAL:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:GLN:HE21	1:H:131:THR:C	2.13	0.50
1:J:166:GLU:HA	1:J:167:PRO:O	2.12	0.50
1:J:180:ARG:HG2	1:J:188:TYR:CD2	2.46	0.50
1:J:46:HIS:NE2	1:J:240:LYS:HD2	2.26	0.50
1:B:144:LYS:HE3	1:B:148:ARG:NH1	2.25	0.50
1:B:95:VAL:HG13	3:B:270:HOH:O	2.11	0.50
1:J:114:MET:CE	1:J:178:VAL:HA	2.42	0.50
1:P:209:MET:HG2	1:P:210:LYS:O	2.11	0.50
1:P:39:LEU:O	1:P:43:ILE:HG12	2.12	0.50
1:B:92:ILE:HA	1:B:102:PHE:CZ	2.47	0.50
1:E:125:GLU:H	1:E:125:GLU:CD	2.13	0.50
1:E:11:ILE:O	1:E:17:VAL:HG11	2.10	0.50
1:E:64:ARG:HH12	1:E:71:TRP:HE1	1.59	0.50
1:G:127:LEU:HD22	1:G:135:TYR:CD2	2.47	0.50
1:L:180:ARG:HG2	1:L:188:TYR:CD2	2.46	0.50
1:N:129:LYS:O	1:N:131:THR:N	2.44	0.50
1:E:161:TYR:CD1	1:E:161:TYR:C	2.85	0.50
1:E:18:MET:HG2	1:E:33:GLU:O	2.11	0.50
1:E:90:LEU:HD23	1:E:96:ARG:NH1	2.27	0.50
1:G:42:GLU:OE2	1:G:246:LEU:HD22	2.12	0.50
1:E:218:LYS:HD3	3:E:280:HOH:O	2.12	0.50
1:G:88:ALA:HB1	1:G:89:PRO:CD	2.42	0.50
1:H:117:LYS:HG3	1:H:209:MET:CE	2.42	0.50
1:H:144:LYS:HD2	1:H:144:LYS:O	2.11	0.50
1:H:253:LYS:O	1:H:257:ASP:HB2	2.12	0.50
1:L:110:GLY:HA3	1:L:216:ASP:O	2.11	0.50
1:L:123:SER:HB3	1:L:126:ASP:OD1	2.12	0.50
1:L:204:LYS:O	1:L:205:PRO:C	2.50	0.50
1:E:32:TYR:HE2	3:E:287:HOH:O	1.94	0.50
1:H:143:THR:O	1:H:146:PHE:HB3	2.12	0.50
1:J:88:ALA:HB1	1:J:89:PRO:CD	2.42	0.50
1:E:196:MET:HG2	2:E:808:VBP:O08	2.12	0.49
1:H:130:GLN:OE1	1:H:133:ILE:HB	2.11	0.49
1:H:197:ASN:HD22	1:H:210:LYS:HG3	1.77	0.49
1:N:5:THR:O	1:N:5:THR:HG22	2.12	0.49
1:J:117:LYS:HG2	1:J:209:MET:HE3	1.93	0.49
1:L:103:SER:HB2	1:L:104:LYS:NZ	2.27	0.49
1:L:192:LEU:CD1	1:L:197:ASN:HB2	2.41	0.49
1:N:12:LEU:HD23	1:N:17:VAL:O	2.12	0.49
1:P:121:ILE:HG21	1:P:126:ASP:O	2.12	0.49
1:E:94:LEU:O	1:E:98:GLU:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:LYS:HE2	1:H:161:TYR:HE1	1.74	0.49
1:L:216:ASP:OD2	1:L:218:LYS:HE3	2.12	0.49
1:L:28:GLY:HA2	1:L:31:ARG:HH21	1.77	0.49
1:L:88:ALA:HB1	1:L:89:PRO:CD	2.43	0.49
1:P:172:ARG:HB2	1:P:172:ARG:HH11	1.78	0.49
1:P:210:LYS:HB3	1:P:210:LYS:NZ	2.28	0.49
1:B:117:LYS:HD3	1:B:209:MET:HE3	1.93	0.49
1:B:148:ARG:HG3	1:B:159:TRP:CZ2	2.47	0.49
1:J:222:ILE:N	1:J:222:ILE:HD12	2.28	0.49
1:L:160:THR:O	1:L:163:ARG:HG2	2.13	0.49
1:H:135:TYR:CB	1:H:189:ALA:HB3	2.42	0.49
1:J:185:LYS:N	1:J:185:LYS:CD	2.74	0.49
1:P:115:ILE:HG12	1:P:211:VAL:HG11	1.94	0.49
1:N:65:ASP:O	1:N:69:LYS:HA	2.12	0.49
1:N:6:VAL:O	1:N:51:TYR:HA	2.13	0.49
1:B:75:VAL:O	1:B:79:VAL:HG23	2.13	0.49
1:J:159:TRP:O	1:J:163:ARG:HB2	2.13	0.49
1:J:204:LYS:HB3	1:J:205:PRO:CD	2.38	0.49
1:B:171:VAL:HB	1:B:176:GLU:HG2	1.94	0.49
1:E:182:ARG:HG2	1:E:207:ASP:OD2	2.13	0.49
1:E:197:ASN:HD22	1:E:210:LYS:HG3	1.77	0.49
1:H:121:ILE:HD13	1:H:127:LEU:HG	1.94	0.49
1:N:108:SER:C	1:N:109:LEU:HD23	2.33	0.49
1:N:253:LYS:O	1:N:257:ASP:HB2	2.13	0.49
1:N:94:LEU:O	1:N:98:GLU:HG3	2.13	0.49
1:P:158:MET:O	1:P:162:MET:HG3	2.13	0.49
1:E:105:PRO:HA	1:E:220:TYR:O	2.13	0.49
1:E:244:GLN:HA	1:P:149:ARG:CD	2.43	0.49
1:H:122:GLU:OE1	1:H:126:ASP:OD2	2.31	0.49
1:H:99:VAL:O	1:H:226:LYS:HD3	2.13	0.49
1:J:148:ARG:HB2	1:J:148:ARG:NH1	2.26	0.49
1:B:122:GLU:O	1:B:211:VAL:HG22	2.13	0.48
1:B:241:LEU:HD22	1:B:246:LEU:HD22	1.95	0.48
1:E:159:TRP:O	1:E:163:ARG:HB2	2.13	0.48
1:B:95:VAL:CB	1:E:64:ARG:HH21	2.25	0.48
1:N:143:THR:HG21	3:N:266:HOH:O	2.13	0.48
1:P:114:MET:CE	1:P:208:THR:HG21	2.43	0.48
1:E:148:ARG:CG	1:E:148:ARG:O	2.61	0.48
1:E:77:GLU:HG2	1:E:82:LYS:HB2	1.95	0.48
1:G:11:ILE:HG13	3:G:290:HOH:O	2.12	0.48
1:L:100:ILE:HD12	1:L:100:ILE:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:125:GLU:O	1:P:127:LEU:N	2.46	0.48
1:P:97:GLU:HG3	1:P:97:GLU:O	2.13	0.48
1:E:137:THR:HG22	1:E:191:LEU:HB2	1.95	0.48
1:G:36:CYS:SG	1:G:88:ALA:HA	2.53	0.48
1:H:144:LYS:CE	1:H:148:ARG:NH2	2.76	0.48
1:J:27:GLU:HA	1:J:27:GLU:OE1	2.14	0.48
1:P:143:THR:HB	3:P:262:HOH:O	2.13	0.48
1:B:88:ALA:HB1	1:B:89:PRO:CD	2.43	0.48
1:H:163:ARG:NH1	1:H:163:ARG:HB2	2.27	0.48
1:J:200:ILE:HG22	1:J:208:THR:OG1	2.14	0.48
1:H:249:LYS:HD3	1:L:151:LYS:HB3	1.95	0.48
1:N:182:ARG:NH1	1:N:208:THR:HG23	2.29	0.48
1:N:193:GLU:H	2:N:802:VBP:H13	1.79	0.48
1:P:177:GLY:O	1:P:181:VAL:HG23	2.13	0.48
1:B:250:LEU:O	1:B:253:LYS:HB3	2.14	0.48
1:E:159:TRP:CE3	1:E:159:TRP:HA	2.49	0.48
1:H:162:MET:HB3	1:H:170:PHE:CZ	2.49	0.48
1:N:60:LYS:HB2	1:N:73:GLY:CA	2.44	0.48
1:P:203:ARG:HA	1:P:260:GLU:CG	2.43	0.48
1:G:237:ALA:O	1:G:241:LEU:HG	2.14	0.48
1:H:100:ILE:HD11	1:H:102:PHE:CE2	2.49	0.48
1:L:160:THR:HG22	1:L:163:ARG:HH12	1.78	0.48
1:B:199:TYR:O	1:B:203:ARG:HG2	2.14	0.48
1:B:237:ALA:O	1:B:241:LEU:HG	2.14	0.48
1:H:147:PHE:CZ	1:H:191:LEU:HD13	2.49	0.48
1:J:182:ARG:NH1	1:J:207:ASP:OD1	2.46	0.48
1:G:115:ILE:HD12	1:G:119:THR:HB	1.95	0.48
1:G:180:ARG:HD2	1:G:188:TYR:CE1	2.49	0.48
1:J:192:LEU:HD12	1:J:192:LEU:H	1.78	0.48
1:P:65:ASP:HB3	1:P:68:THR:OG1	2.14	0.48
1:J:197:ASN:ND2	1:J:210:LYS:HG3	2.29	0.48
1:P:182:ARG:HH12	1:P:205:PRO:HB2	1.79	0.48
1:B:68:THR:OG1	1:B:70:ILE:HB	2.13	0.47
1:E:234:VAL:O	1:E:237:ALA:HB3	2.14	0.47
1:E:247:LEU:HB2	3:E:286:HOH:O	2.14	0.47
1:H:181:VAL:CG1	1:H:181:VAL:O	2.62	0.47
1:H:196:MET:O	1:H:200:ILE:HG12	2.13	0.47
1:J:138:LEU:O	1:J:144:LYS:HB2	2.14	0.47
1:L:15:PRO:HD3	1:L:199:TYR:CD1	2.49	0.47
1:L:164:SER:O	1:L:165:ALA:CB	2.60	0.47
1:P:247:LEU:HB2	3:P:273:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:MET:CE	1:B:178:VAL:HA	2.44	0.47
1:E:127:LEU:HD22	1:E:135:TYR:CD2	2.49	0.47
1:L:147:PHE:CE2	1:L:191:LEU:HD13	2.49	0.47
1:P:133:ILE:HG23	1:P:187:LYS:C	2.34	0.47
1:P:113:ILE:HG12	1:P:191:LEU:CD2	2.44	0.47
1:H:192:LEU:CD1	1:H:197:ASN:HB2	2.45	0.47
1:H:249:LYS:HD3	1:L:151:LYS:CB	2.43	0.47
1:L:166:GLU:HA	1:L:167:PRO:O	2.13	0.47
1:N:144:LYS:HD3	3:N:262:HOH:O	2.15	0.47
1:B:62:GLY:HA3	1:B:75:VAL:CG2	2.43	0.47
1:H:115:ILE:HD13	1:H:119:THR:HB	1.95	0.47
1:E:13:GLU:HB3	1:E:16:TYR:HD2	1.79	0.47
1:G:182:ARG:NH1	1:G:205:PRO:HB2	2.29	0.47
1:J:145:GLU:OE1	1:J:148:ARG:HD2	2.14	0.47
1:J:16:TYR:HA	1:J:35:TYR:HB3	1.95	0.47
1:L:251:LYS:O	1:L:255:TRP:HB2	2.14	0.47
1:N:130:GLN:NE2	1:N:133:ILE:HG13	2.28	0.47
1:P:192:LEU:HD12	1:P:192:LEU:H	1.80	0.47
1:P:203:ARG:HA	1:P:260:GLU:HG3	1.96	0.47
1:B:11:ILE:O	1:B:17:VAL:CG1	2.62	0.47
1:B:97:GLU:HG3	1:B:97:GLU:O	2.13	0.47
1:E:7:VAL:HB	1:E:84:ASP:OD2	2.14	0.47
1:G:77:GLU:HG2	1:G:82:LYS:HB2	1.97	0.47
1:P:204:LYS:O	1:P:205:PRO:C	2.49	0.47
1:P:205:PRO:O	1:P:207:ASP:N	2.48	0.47
1:E:11:ILE:HG21	1:E:61:TYR:CE1	2.49	0.47
1:G:117:LYS:HE2	1:G:209:MET:CE	2.34	0.47
1:G:130:GLN:HA	1:G:130:GLN:NE2	2.25	0.47
1:G:114:MET:CE	1:G:178:VAL:HA	2.44	0.47
1:J:105:PRO:HA	1:J:220:TYR:O	2.15	0.47
1:J:114:MET:HE3	1:J:178:VAL:HG13	1.96	0.47
1:E:88:ALA:HB1	1:E:89:PRO:CD	2.39	0.47
1:J:171:VAL:HB	1:J:176:GLU:HB3	1.96	0.47
1:J:5:THR:O	1:J:5:THR:HG23	2.15	0.47
1:P:240:LYS:O	1:P:244:GLN:HG3	2.14	0.47
1:B:42:GLU:CD	1:B:246:LEU:HD21	2.35	0.47
1:E:147:PHE:CZ	1:E:191:LEU:HD13	2.49	0.47
1:E:63:ALA:N	1:E:72:ASN:OD1	2.43	0.47
1:J:113:ILE:HG22	1:J:115:ILE:HG23	1.97	0.47
1:J:137:THR:HG22	1:J:191:LEU:HB2	1.96	0.47
1:L:115:ILE:HG21	1:L:121:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:GLU:H	2:L:801:VBP:H13	1.80	0.47
1:N:11:ILE:O	1:N:17:VAL:HG13	2.15	0.47
1:N:130:GLN:HG2	1:N:133:ILE:HB	1.96	0.47
1:P:100:ILE:HD12	1:P:100:ILE:O	2.15	0.47
1:P:130:GLN:HE21	1:P:132:GLU:HB3	1.80	0.47
1:P:65:ASP:O	1:P:69:LYS:N	2.47	0.47
1:P:65:ASP:O	1:P:69:LYS:HA	2.15	0.47
1:B:172:ARG:CB	1:B:172:ARG:NH1	2.78	0.47
1:P:203:ARG:HA	1:P:203:ARG:HD3	1.70	0.47
1:J:99:VAL:HG23	1:J:100:ILE:HG23	1.96	0.47
1:J:62:GLY:HA3	1:J:75:VAL:HG23	1.97	0.47
1:G:115:ILE:HG22	1:G:121:ILE:HD11	1.98	0.46
1:G:182:ARG:HH12	1:G:205:PRO:HB2	1.80	0.46
1:N:113:ILE:HG22	1:N:115:ILE:HG23	1.96	0.46
1:N:182:ARG:NH1	1:N:207:ASP:OD1	2.48	0.46
1:P:75:VAL:O	1:P:79:VAL:HG23	2.14	0.46
1:B:172:ARG:CB	1:B:172:ARG:HH11	2.28	0.46
1:J:185:LYS:HD2	1:J:185:LYS:H	1.77	0.46
1:P:180:ARG:O	1:P:184:SER:HB3	2.15	0.46
1:B:155:PHE:CZ	1:B:215:LEU:HD22	2.50	0.46
1:E:22:ASN:N	1:E:22:ASN:HD22	1.96	0.46
1:E:241:LEU:HD22	1:E:246:LEU:HD22	1.98	0.46
1:N:51:TYR:N	1:N:51:TYR:CD2	2.83	0.46
1:B:133:ILE:HG23	1:B:187:LYS:HA	1.97	0.46
1:J:97:GLU:HA	1:J:97:GLU:OE2	2.16	0.46
1:N:42:GLU:HG3	1:N:246:LEU:CD2	2.45	0.46
1:P:130:GLN:HE21	1:P:130:GLN:HB3	1.57	0.46
1:N:61:TYR:CE1	2:N:802:VBP:H03A	2.50	0.46
1:G:68:THR:C	1:G:70:ILE:H	2.17	0.46
1:N:180:ARG:HG2	1:N:180:ARG:O	2.16	0.46
1:B:115:ILE:O	1:B:115:ILE:HD12	2.16	0.46
1:E:148:ARG:HA	1:E:159:TRP:CD1	2.51	0.46
1:E:169:VAL:CA	1:E:180:ARG:HH12	2.29	0.46
1:G:148:ARG:HB2	1:G:148:ARG:HH11	1.80	0.46
1:G:192:LEU:HD13	1:G:197:ASN:HB2	1.98	0.46
1:J:147:PHE:CE2	1:J:191:LEU:HD13	2.51	0.46
1:J:182:ARG:NH1	1:J:205:PRO:CB	2.78	0.46
1:P:96:ARG:C	1:P:98:GLU:H	2.19	0.46
1:H:118:GLY:HA2	1:N:30:GLU:HG3	1.96	0.46
1:P:184:SER:O	1:P:186:GLY:N	2.48	0.46
1:P:36:CYS:SG	1:P:88:ALA:HA	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:ASP:O	1:G:69:LYS:HD3	2.16	0.46
1:J:64:ARG:HG3	1:J:64:ARG:NH1	2.30	0.46
1:L:136:GLY:HA3	1:L:169:VAL:O	2.16	0.46
1:L:144:LYS:NZ	1:L:148:ARG:NH2	2.64	0.46
1:N:144:LYS:HB3	1:N:144:LYS:HZ3	1.80	0.46
1:N:92:ILE:HG12	1:N:102:PHE:CD1	2.51	0.46
1:P:138:LEU:HD12	1:P:139:ASP:H	1.81	0.46
1:G:111:ILE:HD12	1:G:146:PHE:CD2	2.51	0.46
1:H:14:SER:CB	1:H:18:MET:HE3	2.46	0.46
1:N:60:LYS:HB2	1:N:73:GLY:HA2	1.97	0.46
1:P:100:ILE:HD12	1:P:100:ILE:C	2.36	0.46
1:H:121:ILE:HD12	1:H:122:GLU:N	2.31	0.45
1:N:137:THR:HB	3:N:266:HOH:O	2.16	0.45
1:P:137:THR:HG22	1:P:191:LEU:HB2	1.97	0.45
1:P:62:GLY:HA3	1:P:75:VAL:CG2	2.46	0.45
1:B:211:VAL:HG13	1:B:211:VAL:O	2.16	0.45
1:E:111:ILE:O	1:E:214:ASN:HA	2.16	0.45
1:G:5:THR:N	3:G:262:HOH:O	2.49	0.45
1:H:11:ILE:O	1:H:17:VAL:HG13	2.15	0.45
1:L:121:ILE:HA	1:L:126:ASP:HB3	1.98	0.45
1:B:125:GLU:N	1:B:125:GLU:OE1	2.39	0.45
1:B:173:THR:O	1:B:176:GLU:HB3	2.16	0.45
1:H:155:PHE:CE1	1:H:215:LEU:HD13	2.51	0.45
1:J:21:LYS:CE	1:J:21:LYS:H	2.26	0.45
1:L:172:ARG:CB	1:L:172:ARG:NH1	2.80	0.45
1:N:171:VAL:CG2	1:N:176:GLU:HB3	2.46	0.45
1:N:180:ARG:O	1:N:188:TYR:CD2	2.66	0.45
1:P:180:ARG:O	1:P:184:SER:CB	2.64	0.45
1:P:197:ASN:ND2	1:P:210:LYS:HA	2.31	0.45
1:B:99:VAL:HG23	1:B:100:ILE:HG23	1.98	0.45
1:B:106:PHE:C	1:B:106:PHE:CD1	2.90	0.45
1:G:229:SER:HB2	3:G:282:HOH:O	2.17	0.45
1:L:90:LEU:O	1:L:220:TYR:HA	2.15	0.45
1:P:8:VAL:HG22	1:P:85:ILE:CG2	2.47	0.45
1:B:196:MET:HA	1:B:196:MET:HE3	1.98	0.45
1:B:205:PRO:HG2	1:B:207:ASP:OD1	2.16	0.45
1:E:11:ILE:O	1:E:17:VAL:HG13	2.15	0.45
1:H:121:ILE:CG2	1:H:133:ILE:HD12	2.46	0.45
1:J:222:ILE:HD13	1:J:238:VAL:CG2	2.46	0.45
1:L:205:PRO:O	1:L:207:ASP:OD1	2.34	0.45
1:N:172:ARG:HB3	1:N:176:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:207:ASP:OD1	1:N:208:THR:HG23	2.17	0.45
1:E:147:PHE:C	1:E:149:ARG:H	2.20	0.45
1:E:171:VAL:HB	1:E:176:GLU:HB2	1.99	0.45
1:J:182:ARG:NH1	1:J:205:PRO:HB2	2.24	0.45
1:J:51:TYR:CD2	1:J:51:TYR:N	2.84	0.45
1:P:64:ARG:HG3	1:P:64:ARG:HH11	1.82	0.45
1:B:155:PHE:HE1	1:B:215:LEU:HD13	1.82	0.45
1:J:84:ASP:O	1:J:225:PRO:HD3	2.17	0.45
1:L:64:ARG:HB2	1:L:71:TRP:CE2	2.51	0.45
1:N:109:LEU:N	1:N:109:LEU:HD23	2.31	0.45
1:N:10:THR:O	1:N:55:ILE:HA	2.17	0.45
1:P:121:ILE:CB	1:P:126:ASP:HB3	2.47	0.45
1:G:159:TRP:O	1:G:163:ARG:CB	2.63	0.45
1:H:115:ILE:HB	1:H:119:THR:HB	1.98	0.45
1:J:117:LYS:HG2	1:J:209:MET:HE2	1.98	0.45
1:L:16:TYR:HA	1:L:35:TYR:HB3	1.99	0.45
1:P:64:ARG:HG3	1:P:64:ARG:NH1	2.30	0.45
1:B:159:TRP:HE1	1:B:163:ARG:HH12	1.64	0.45
1:E:251:LYS:HD3	1:E:255:TRP:CE3	2.52	0.45
1:G:19:MET:HG3	3:N:272:HOH:O	2.17	0.45
1:J:100:ILE:C	1:J:100:ILE:HD12	2.37	0.45
1:L:187:LYS:HZ2	1:L:188:TYR:CB	2.29	0.45
1:B:201:GLU:OE1	1:B:209:MET:HB2	2.16	0.44
1:B:42:GLU:OE2	1:B:246:LEU:HD21	2.18	0.44
1:E:124:ALA:O	1:E:127:LEU:N	2.50	0.44
1:H:180:ARG:C	1:H:182:ARG:H	2.20	0.44
1:L:116:LYS:HE3	1:L:207:ASP:HB2	1.98	0.44
1:L:122:GLU:HA	1:L:211:VAL:HG21	2.00	0.44
1:P:161:TYR:CD2	1:P:162:MET:N	2.86	0.44
1:P:195:THR:HG21	1:P:220:TYR:CE2	2.50	0.44
1:E:109:LEU:HD12	1:E:193:GLU:OE1	2.18	0.44
1:E:114:MET:CE	1:E:192:LEU:HD21	2.47	0.44
1:E:197:ASN:ND2	1:E:210:LYS:HA	2.32	0.44
1:G:85:ILE:HG13	1:G:224:THR:HG22	1.99	0.44
1:G:20:LYS:HZ2	1:G:30:GLU:HG2	1.81	0.44
1:J:11:ILE:HD11	1:J:59:GLY:O	2.17	0.44
1:J:121:ILE:CD1	1:J:133:ILE:HD12	2.47	0.44
1:J:150:SER:HA	3:J:276:HOH:O	2.17	0.44
1:J:34:GLY:HA2	1:J:254:TRP:CZ3	2.52	0.44
1:N:201:GLU:OE1	1:N:210:LYS:N	2.48	0.44
1:N:28:GLY:O	1:N:31:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:65:ASP:O	1:N:69:LYS:N	2.50	0.44
1:E:14:SER:HA	3:E:278:HOH:O	2.17	0.44
1:J:137:THR:HB	1:J:143:THR:HG22	1.98	0.44
1:J:24:GLU:H	1:J:24:GLU:CD	2.20	0.44
1:N:129:LYS:O	1:N:130:GLN:C	2.54	0.44
1:B:155:PHE:CZ	1:B:215:LEU:HB3	2.53	0.44
1:E:241:LEU:CD2	1:E:246:LEU:HD22	2.48	0.44
1:H:96:ARG:O	1:H:100:ILE:HG13	2.17	0.44
1:H:106:PHE:CD1	1:H:106:PHE:C	2.91	0.44
1:J:115:ILE:CD1	1:J:121:ILE:O	2.64	0.44
1:J:178:VAL:CG1	1:J:182:ARG:HE	2.28	0.44
1:P:113:ILE:HD13	1:P:127:LEU:CD1	2.47	0.44
1:P:169:VAL:HA	1:P:180:ARG:NH1	2.31	0.44
1:B:104:LYS:HG2	1:B:235:ASN:OD1	2.18	0.44
1:E:234:VAL:O	1:E:238:VAL:HG23	2.17	0.44
1:H:68:THR:O	1:H:70:ILE:HG13	2.18	0.44
1:J:121:ILE:HG12	1:J:127:LEU:HD23	1.98	0.44
1:J:179:ALA:HA	1:J:182:ARG:HD2	1.99	0.44
1:J:69:LYS:HB2	1:J:69:LYS:HZ3	1.80	0.44
1:J:73:GLY:O	1:J:77:GLU:HG2	2.17	0.44
1:L:161:TYR:HD2	1:L:162:MET:HG3	1.83	0.44
1:P:109:LEU:N	1:P:109:LEU:HD23	2.32	0.44
1:P:130:GLN:NE2	1:P:132:GLU:HB3	2.32	0.44
1:P:204:LYS:CB	1:P:205:PRO:CD	2.87	0.44
1:E:162:MET:HB3	1:E:170:PHE:CZ	2.53	0.44
1:E:197:ASN:ND2	1:E:210:LYS:HG3	2.33	0.44
1:H:122:GLU:HB3	1:H:211:VAL:HG21	1.99	0.44
1:J:152:ILE:N	1:J:152:ILE:HD12	2.32	0.44
1:J:74:MET:O	1:J:77:GLU:HB2	2.18	0.44
1:N:183:LYS:O	1:N:185:LYS:HD2	2.18	0.44
1:P:38:ASP:HB3	1:P:250:LEU:HD11	1.99	0.44
1:H:20:LYS:CE	1:H:30:GLU:O	2.66	0.44
1:H:107:MET:HE1	1:H:251:LYS:HG2	2.00	0.44
1:L:196:MET:HE2	1:L:200:ILE:HG12	1.99	0.44
1:P:136:GLY:HA2	1:P:162:MET:SD	2.58	0.44
1:B:165:ALA:HB2	3:B:290:HOH:O	2.17	0.43
1:E:185:LYS:HB3	1:E:186:GLY:H	1.68	0.43
1:E:193:GLU:H	2:E:808:VBP:H13	1.82	0.43
1:G:179:ALA:O	1:G:183:LYS:CD	2.66	0.43
1:N:9:THR:O	1:N:86:ALA:HA	2.18	0.43
1:B:136:GLY:HA3	1:B:169:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:PHE:CZ	1:G:215:LEU:HD22	2.52	0.43
1:G:68:THR:C	1:G:70:ILE:N	2.72	0.43
1:N:114:MET:CE	1:N:192:LEU:HD21	2.48	0.43
1:P:260:GLU:O	1:P:261:CYS:SG	2.76	0.43
1:P:60:LYS:HD3	1:P:72:ASN:ND2	2.33	0.43
1:B:115:ILE:HG22	1:B:121:ILE:HD11	2.00	0.43
1:B:14:SER:HB2	3:B:279:HOH:O	2.17	0.43
1:B:56:VAL:HG13	1:B:59:GLY:HA2	2.01	0.43
1:E:12:LEU:HD13	1:E:55:ILE:CD1	2.48	0.43
1:G:11:ILE:HG12	1:G:12:LEU:N	2.33	0.43
1:H:201:GLU:CG	1:H:209:MET:HA	2.48	0.43
1:H:94:LEU:O	1:H:98:GLU:HG3	2.17	0.43
1:J:143:THR:HB	3:J:288:HOH:O	2.19	0.43
1:P:137:THR:HB	1:P:143:THR:HG22	2.00	0.43
1:L:125:GLU:C	1:L:127:LEU:N	2.70	0.43
1:B:67:ASP:OD2	1:B:68:THR:HG23	2.18	0.43
1:G:121:ILE:HD13	1:G:127:LEU:HD21	1.99	0.43
1:H:121:ILE:HG23	1:H:133:ILE:CD1	2.46	0.43
1:H:153:ALA:O	1:H:154:VAL:C	2.57	0.43
1:J:113:ILE:N	3:J:287:HOH:O	2.48	0.43
1:E:47:CYS:SG	1:E:233:ALA:HB1	2.58	0.43
1:G:16:TYR:CG	1:G:89:PRO:HG3	2.53	0.43
1:G:193:GLU:CD	1:G:218:LYS:HZ2	2.18	0.43
1:H:11:ILE:HG12	1:H:12:LEU:N	2.33	0.43
1:H:100:ILE:HD13	1:H:223:ALA:HB1	1.99	0.43
1:J:119:THR:HA	1:J:120:PRO:HD3	1.84	0.43
1:L:159:TRP:HA	1:L:159:TRP:CE3	2.54	0.43
1:B:143:THR:HG21	1:B:191:LEU:O	2.19	0.43
1:B:94:LEU:O	1:B:98:GLU:HG3	2.17	0.43
1:E:115:ILE:CG2	1:E:121:ILE:HD11	2.49	0.43
1:E:183:LYS:HB2	1:E:183:LYS:HZ2	1.83	0.43
1:G:11:ILE:CG1	1:G:12:LEU:N	2.82	0.43
1:J:20:LYS:HB2	1:J:31:ARG:C	2.39	0.43
1:L:184:SER:HB2	1:L:187:LYS:NZ	2.33	0.43
1:N:143:THR:O	1:N:146:PHE:HB3	2.18	0.43
1:N:253:LYS:HE2	1:N:258:LYS:HZ3	1.84	0.43
1:E:159:TRP:HA	1:E:159:TRP:HE3	1.82	0.43
1:E:116:LYS:NZ	1:E:185:LYS:HA	2.32	0.43
1:G:236:LEU:HD22	1:J:94:LEU:CD1	2.49	0.43
1:H:144:LYS:NZ	1:H:148:ARG:NH2	2.67	0.43
1:H:20:LYS:HZ2	1:H:30:GLU:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:THR:N	3:J:291:HOH:O	2.51	0.43
1:N:130:GLN:HE21	1:N:132:GLU:CB	2.25	0.43
1:P:193:GLU:HG2	2:P:805:VBP:C13	2.48	0.43
1:B:10:THR:OG1	1:B:11:ILE:N	2.48	0.43
1:B:84:ASP:O	1:B:85:ILE:HB	2.18	0.43
1:G:122:GLU:HA	1:G:211:VAL:CG2	2.41	0.43
1:G:64:ARG:HG3	1:G:71:TRP:CE2	2.54	0.43
1:L:37:VAL:HG13	1:L:53:LEU:HD11	2.00	0.43
1:N:130:GLN:HE21	1:N:133:ILE:N	2.16	0.43
1:P:197:ASN:HD21	1:P:210:LYS:HA	1.84	0.43
1:B:92:ILE:HG12	1:B:102:PHE:CG	2.54	0.42
1:E:115:ILE:HG22	1:E:121:ILE:HD11	2.00	0.42
1:E:161:TYR:O	1:E:165:ALA:HB2	2.18	0.42
1:E:180:ARG:HD3	1:E:188:TYR:CE2	2.54	0.42
1:H:172:ARG:HG2	1:H:173:THR:N	2.34	0.42
1:H:250:LEU:O	1:H:253:LYS:HB3	2.19	0.42
1:H:40:ALA:HA	1:H:87:ILE:HD13	2.01	0.42
1:L:55:ILE:O	1:L:56:VAL:C	2.58	0.42
1:N:100:ILE:HD12	1:N:100:ILE:C	2.40	0.42
1:N:65:ASP:HB3	1:N:68:THR:OG1	2.18	0.42
1:P:12:LEU:HD22	1:P:18:MET:HA	2.00	0.42
1:B:171:VAL:HB	1:B:176:GLU:CG	2.48	0.42
1:H:118:GLY:HA2	1:N:30:GLU:HG2	2.01	0.42
1:H:184:SER:O	1:H:186:GLY:N	2.53	0.42
1:P:250:LEU:HA	1:P:250:LEU:HD23	1.78	0.42
1:J:12:LEU:HD12	1:J:17:VAL:O	2.20	0.42
1:J:116:LYS:HG3	1:J:207:ASP:O	2.19	0.42
1:J:16:TYR:CE1	1:J:255:TRP:HH2	2.37	0.42
1:P:181:VAL:HG22	1:P:188:TYR:O	2.18	0.42
1:P:16:TYR:CE1	1:P:89:PRO:HG3	2.54	0.42
1:P:96:ARG:C	1:P:98:GLU:N	2.73	0.42
1:E:145:GLU:O	1:E:146:PHE:C	2.58	0.42
1:J:60:LYS:HB2	1:J:73:GLY:CA	2.50	0.42
1:L:21:LYS:HG2	1:L:22:ASN:N	2.33	0.42
1:P:114:MET:HE2	1:P:208:THR:HG21	2.01	0.42
1:P:88:ALA:HB1	1:P:89:PRO:CD	2.49	0.42
1:B:203:ARG:NH1	1:B:258:LYS:O	2.52	0.42
1:G:130:GLN:HG3	1:G:131:THR:H	1.84	0.42
1:L:11:ILE:HG21	1:L:61:TYR:CE1	2.54	0.42
1:E:100:ILE:HD13	1:E:223:ALA:CB	2.50	0.42
1:H:100:ILE:HD12	1:H:100:ILE:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:ILE:HG21	1:H:61:TYR:CE1	2.55	0.42
1:J:68:THR:CB	1:J:70:ILE:HG12	2.49	0.42
1:N:122:GLU:HA	1:N:211:VAL:CG2	2.49	0.42
1:P:125:GLU:OE2	1:P:125:GLU:N	2.52	0.42
1:P:159:TRP:O	1:P:160:THR:C	2.57	0.42
1:P:216:ASP:OD2	1:P:218:LYS:HD2	2.20	0.42
1:B:24:GLU:N	1:B:24:GLU:OE1	2.43	0.42
1:E:172:ARG:N	1:E:176:GLU:OE2	2.42	0.42
1:E:210:LYS:HB3	1:E:210:LYS:NZ	2.34	0.42
1:B:116:LYS:O	1:B:117:LYS:C	2.58	0.42
1:G:196:MET:CE	1:G:196:MET:HA	2.50	0.42
1:L:8:VAL:HG13	1:L:85:ILE:HG23	2.02	0.42
1:E:192:LEU:CD1	1:E:197:ASN:HB2	2.48	0.42
1:H:11:ILE:O	1:H:17:VAL:CG1	2.68	0.42
1:G:104:LYS:NZ	1:J:102:PHE:O	2.36	0.42
1:J:64:ARG:HG3	1:J:64:ARG:HH11	1.83	0.42
1:L:119:THR:HA	1:L:120:PRO:HD3	1.86	0.42
1:L:144:LYS:NZ	1:L:148:ARG:HH21	2.18	0.42
1:N:90:LEU:O	1:N:220:TYR:HA	2.19	0.42
1:P:79:VAL:HG22	1:P:99:VAL:CG1	2.50	0.42
1:P:16:TYR:CG	1:P:89:PRO:HG3	2.55	0.42
1:B:119:THR:HG22	1:B:121:ILE:H	1.85	0.42
1:E:110:GLY:O	1:E:194:SER:N	2.38	0.42
1:G:246:LEU:O	1:G:249:LYS:HB3	2.19	0.42
1:G:94:LEU:O	1:G:98:GLU:HG3	2.19	0.42
1:H:116:LYS:HG3	1:H:185:LYS:O	2.18	0.42
1:H:201:GLU:O	1:H:201:GLU:HG2	2.20	0.42
1:H:20:LYS:C	1:H:22:ASN:H	2.22	0.42
1:J:193:GLU:H	2:J:804:VBP:H13	1.84	0.42
1:B:246:LEU:O	1:B:249:LYS:HB3	2.21	0.41
1:E:116:LYS:O	1:E:117:LYS:C	2.58	0.41
1:G:10:THR:O	1:G:56:VAL:HG12	2.20	0.41
1:H:171:VAL:HB	1:H:176:GLU:OE2	2.20	0.41
1:H:46:HIS:CE1	1:H:241:LEU:HD21	2.54	0.41
1:H:88:ALA:O	1:H:90:LEU:N	2.52	0.41
1:L:234:VAL:O	1:L:237:ALA:HB3	2.20	0.41
1:B:19:MET:HA	1:B:19:MET:HE3	2.02	0.41
1:E:20:LYS:HB3	1:E:22:ASN:ND2	2.35	0.41
1:G:116:LYS:O	1:G:117:LYS:C	2.58	0.41
1:G:141:GLY:O	1:G:142:SER:C	2.58	0.41
1:G:11:ILE:O	1:G:17:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:ALA:O	1:G:188:TYR:HA	2.20	0.41
1:H:121:ILE:C	1:H:122:GLU:HG3	2.41	0.41
1:H:214:ASN:N	1:H:214:ASN:HD22	2.17	0.41
1:J:93:THR:OG1	1:J:96:ARG:HD2	2.20	0.41
1:N:119:THR:HA	1:N:120:PRO:HD3	1.82	0.41
1:N:127:LEU:O	1:N:128:SER:C	2.58	0.41
1:N:167:PRO:O	1:N:168:SER:C	2.58	0.41
1:B:166:GLU:N	1:B:166:GLU:CD	2.73	0.41
1:B:92:ILE:HG12	1:B:102:PHE:CD1	2.56	0.41
1:E:190:TYR:CD2	1:E:192:LEU:HG	2.55	0.41
1:L:21:LYS:N	1:L:21:LYS:CD	2.82	0.41
1:N:97:GLU:O	1:N:97:GLU:HG3	2.19	0.41
1:G:121:ILE:CD1	1:G:127:LEU:HD21	2.50	0.41
1:G:127:LEU:O	1:G:130:GLN:HB3	2.21	0.41
1:G:193:GLU:H	2:G:803:VBP:H13	1.84	0.41
1:N:122:GLU:HA	1:N:211:VAL:HG21	2.02	0.41
1:P:137:THR:HB	1:P:143:THR:CG2	2.50	0.41
1:B:113:ILE:C	1:B:197:ASN:HD21	2.23	0.41
1:B:15:PRO:HB3	1:B:199:TYR:CE1	2.55	0.41
1:L:121:ILE:HG22	1:L:126:ASP:C	2.41	0.41
1:N:62:GLY:HA3	1:N:75:VAL:CG2	2.51	0.41
1:P:20:LYS:NZ	1:P:30:GLU:O	2.45	0.41
1:B:109:LEU:HB2	1:B:194:SER:OG	2.20	0.41
1:E:143:THR:O	1:E:146:PHE:HB3	2.20	0.41
1:E:60:LYS:HD2	1:E:72:ASN:ND2	2.36	0.41
1:H:125:GLU:OE1	1:H:125:GLU:N	2.38	0.41
1:H:15:PRO:HA	1:H:18:MET:CE	2.43	0.41
1:L:204:LYS:HG2	1:L:260:GLU:OE1	2.21	0.41
1:N:138:LEU:HA	1:N:138:LEU:HD12	1.95	0.41
1:B:65:ASP:HB3	1:B:68:THR:OG1	2.20	0.41
1:E:148:ARG:HG3	1:E:148:ARG:O	2.21	0.41
1:B:95:VAL:HG12	1:E:69:LYS:HB3	2.03	0.41
1:G:119:THR:CG2	1:G:121:ILE:HG12	2.50	0.41
1:G:15:PRO:HA	1:G:18:MET:SD	2.60	0.41
1:G:209:MET:HE3	1:G:209:MET:HB3	1.93	0.41
1:G:65:ASP:HB3	1:G:68:THR:HG23	2.03	0.41
1:H:169:VAL:HA	1:H:180:ARG:HH22	1.85	0.41
1:H:85:ILE:HD11	1:H:222:ILE:HG21	2.02	0.41
1:P:171:VAL:HB	1:P:176:GLU:CB	2.46	0.41
1:P:55:ILE:O	1:P:56:VAL:C	2.59	0.41
1:B:95:VAL:CG1	1:E:69:LYS:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:109:LEU:HD23	1:J:109:LEU:N	2.35	0.41
1:L:62:GLY:HA3	1:L:75:VAL:HG23	2.03	0.41
1:N:136:GLY:HA2	1:N:162:MET:HE2	2.03	0.41
1:N:177:GLY:O	1:N:181:VAL:HG23	2.21	0.41
1:B:256:TYR:O	1:B:257:ASP:C	2.59	0.41
1:E:148:ARG:HB2	1:E:159:TRP:CE2	2.55	0.41
1:G:205:PRO:O	1:G:207:ASP:OD1	2.39	0.41
1:H:211:VAL:HG13	1:H:211:VAL:O	2.20	0.41
1:H:88:ALA:HB1	1:H:89:PRO:CD	2.45	0.41
1:J:155:PHE:O	1:J:158:MET:HB2	2.21	0.41
1:L:130:GLN:NE2	1:L:132:GLU:HB3	2.19	0.41
1:N:96:ARG:O	1:N:100:ILE:HG13	2.20	0.41
1:E:192:LEU:N	1:E:192:LEU:HD12	2.36	0.41
1:E:16:TYR:HB3	1:E:36:CYS:SG	2.61	0.41
1:G:130:GLN:CG	1:G:131:THR:N	2.83	0.41
1:G:204:LYS:O	1:G:205:PRO:C	2.56	0.41
1:J:21:LYS:CD	1:J:21:LYS:N	2.63	0.41
1:L:161:TYR:O	1:L:164:SER:O	2.38	0.41
1:L:187:LYS:C	1:L:187:LYS:HE3	2.39	0.41
1:P:115:ILE:HD12	1:P:119:THR:HB	2.03	0.41
1:E:110:GLY:HA3	1:E:214:ASN:HB3	2.03	0.41
1:E:199:TYR:CE1	1:E:203:ARG:NE	2.89	0.41
1:G:148:ARG:HB3	1:G:159:TRP:CZ2	2.55	0.41
1:J:201:GLU:HG3	1:J:209:MET:HA	2.02	0.41
1:J:68:THR:O	1:J:69:LYS:HB3	2.20	0.41
1:L:159:TRP:O	1:L:160:THR:C	2.60	0.41
1:N:204:LYS:CB	1:N:205:PRO:CD	2.77	0.41
1:N:34:GLY:HA2	1:N:254:TRP:CZ3	2.56	0.41
1:P:144:LYS:HZ2	1:P:159:TRP:HH2	1.69	0.41
1:E:164:SER:O	1:E:165:ALA:HB2	2.21	0.40
1:E:85:ILE:HD11	1:E:222:ILE:CG2	2.51	0.40
1:G:250:LEU:O	1:G:253:LYS:HB3	2.22	0.40
1:H:198:GLU:O	1:H:199:TYR:C	2.59	0.40
1:H:203:ARG:HB3	1:H:204:LYS:H	1.65	0.40
1:L:119:THR:HG22	1:L:121:ILE:HG13	2.03	0.40
1:L:131:THR:O	1:L:132:GLU:C	2.59	0.40
1:L:79:VAL:HG12	1:L:80:TYR:CE1	2.56	0.40
1:L:8:VAL:HG23	1:L:51:TYR:HB2	2.02	0.40
1:P:119:THR:HG22	1:P:121:ILE:CG1	2.51	0.40
1:P:192:LEU:CD1	1:P:197:ASN:HB2	2.50	0.40
1:P:201:GLU:CG	1:P:209:MET:HA	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:90:LEU:O	1:P:220:TYR:HA	2.21	0.40
1:B:67:ASP:N	1:B:67:ASP:OD2	2.53	0.40
1:J:89:PRO:HB2	2:J:804:VBP:C05	2.44	0.40
1:P:180:ARG:HD2	1:P:188:TYR:CE2	2.55	0.40
1:B:201:GLU:HG2	1:B:202:GLN:NE2	2.36	0.40
1:B:5:THR:N	3:B:262:HOH:O	2.54	0.40
1:G:146:PHE:O	1:G:150:SER:HB2	2.22	0.40
1:J:201:GLU:OE1	1:J:210:LYS:N	2.48	0.40
1:L:253:LYS:HA	1:L:257:ASP:HB2	2.02	0.40
1:P:133:ILE:HG23	1:P:187:LYS:O	2.21	0.40
1:B:64:ARG:HG3	1:B:71:TRP:CZ2	2.56	0.40
1:J:204:LYS:O	1:J:205:PRO:C	2.60	0.40
1:J:20:LYS:HG2	1:J:26:LEU:HD12	2.04	0.40
1:H:244:GLN:O	1:L:149:ARG:HG2	2.20	0.40
1:L:166:GLU:HB2	1:L:167:PRO:CA	2.52	0.40
1:N:11:ILE:O	1:N:17:VAL:CG1	2.69	0.40
1:N:228:SER:OG	1:N:230:LEU:HD12	2.21	0.40
1:E:89:PRO:HB2	2:E:808:VBP:H05	2.04	0.40
1:G:107:MET:HG2	1:G:108:SER:N	2.36	0.40
1:G:193:GLU:HG2	2:G:803:VBP:C13	2.51	0.40
1:H:130:GLN:HE22	1:H:133:ILE:N	2.17	0.40
1:N:127:LEU:O	1:N:129:LYS:N	2.55	0.40
1:N:136:GLY:HA2	1:N:162:MET:CE	2.51	0.40
1:N:39:LEU:O	1:N:43:ILE:HG12	2.20	0.40
1:N:49:PHE:CD1	1:N:49:PHE:C	2.95	0.40
1:P:5:THR:N	3:P:283:HOH:O	2.54	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	B	255/258 (99%)	227 (89%)	23 (9%)	5 (2%)	7	24
1	E	255/258 (99%)	222 (87%)	20 (8%)	13 (5%)	2	6
1	G	255/258 (99%)	223 (88%)	27 (11%)	5 (2%)	7	24
1	H	255/258 (99%)	211 (83%)	35 (14%)	9 (4%)	3	12
1	J	255/258 (99%)	228 (89%)	19 (8%)	8 (3%)	4	14
1	L	255/258 (99%)	212 (83%)	32 (12%)	11 (4%)	2	8
1	N	255/258 (99%)	220 (86%)	23 (9%)	12 (5%)	2	7
1	P	255/258 (99%)	206 (81%)	37 (14%)	12 (5%)	2	7
All	All	2040/2064 (99%)	1749 (86%)	216 (11%)	75 (4%)	3	11

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	205	PRO
1	G	206	CYS
1	B	163	ARG
1	E	14	SER
1	E	185	LYS
1	E	204	LYS
1	E	205	PRO
1	E	206	CYS
1	H	22	ASN
1	H	122	GLU
1	H	153	ALA
1	J	130	GLN
1	J	204	LYS
1	L	184	SER
1	L	204	LYS
1	L	205	PRO
1	L	206	CYS
1	N	130	GLN
1	N	204	LYS
1	N	205	PRO
1	N	206	CYS
1	P	153	ALA
1	P	165	ALA
1	P	204	LYS
1	P	205	PRO
1	G	204	LYS
1	B	66	ALA

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Mol	Chain	Res	Type
1	E	148	ARG
1	E	184	SER
1	J	120	PRO
1	J	128	SER
1	L	153	ALA
1	N	153	ALA
1	N	168	SER
1	P	206	CYS
1	G	153	ALA
1	B	153	ALA
1	E	15	PRO
1	H	172	ARG
1	H	185	LYS
1	J	21	LYS
1	N	128	SER
1	P	132	GLU
1	B	134	ALA
1	E	46	HIS
1	E	122	GLU
1	E	168	SER
1	H	132	GLU
1	H	168	SER
1	L	117	LYS
1	L	167	PRO
1	L	185	LYS
1	P	120	PRO
1	P	185	LYS
1	P	209	MET
1	G	131	THR
1	L	122	GLU
1	L	231	GLY
1	N	209	MET
1	P	126	ASP
1	B	188	TYR
1	J	172	ARG
1	L	56	VAL
1	N	120	PRO
1	H	181	VAL
1	J	17	VAL
1	J	62	GLY
1	P	56	VAL
1	E	154	VAL

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Mol	Chain	Res	Type
1	P	231	GLY
1	N	48	GLY
1	N	56	VAL
1	N	62	GLY
1	H	95	VAL
1	E	167	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	B	216/217 (100%)	206 (95%)	10 (5%)	27	60
1	E	216/217 (100%)	207 (96%)	9 (4%)	30	63
1	G	216/217 (100%)	201 (93%)	15 (7%)	15	41
1	H	216/217 (100%)	199 (92%)	17 (8%)	12	34
1	J	216/217 (100%)	203 (94%)	13 (6%)	19	48
1	L	216/217 (100%)	200 (93%)	16 (7%)	13	37
1	N	216/217 (100%)	198 (92%)	18 (8%)	11	32
1	P	216/217 (100%)	204 (94%)	12 (6%)	21	51
All	All	1728/1736 (100%)	1618 (94%)	110 (6%)	17	45

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	17	VAL
1	G	45	LYS
1	G	60	LYS
1	G	67	ASP
1	G	68	THR
1	G	78	LEU
1	G	130	GLN
1	G	132	GLU
1	G	145	GLU

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Mol	Chain	Res	Type
1	G	148	ARG
1	G	174	THR
1	G	192	LEU
1	G	205	PRO
1	G	209	MET
1	G	246	LEU
1	B	17	VAL
1	B	18	MET
1	B	22	ASN
1	B	27	GLU
1	B	90	LEU
1	B	166	GLU
1	B	192	LEU
1	B	196	MET
1	B	209	MET
1	B	255	TRP
1	E	17	VAL
1	E	22	ASN
1	E	90	LEU
1	E	109	LEU
1	E	126	ASP
1	E	145	GLU
1	E	161	TYR
1	E	192	LEU
1	E	246	LEU
1	H	17	VAL
1	H	18	MET
1	H	24	GLU
1	H	67	ASP
1	H	95	VAL
1	H	122	GLU
1	H	126	ASP
1	H	130	GLN
1	H	144	LYS
1	H	163	ARG
1	H	173	THR
1	H	174	THR
1	H	192	LEU
1	H	204	LYS
1	H	226	LYS
1	H	246	LEU
1	H	252	ASN

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Mol	Chain	Res	Type
1	J	12	LEU
1	J	17	VAL
1	J	21	LYS
1	J	64	ARG
1	J	69	LYS
1	J	78	LEU
1	J	125	GLU
1	J	144	LYS
1	J	148	ARG
1	J	156	ASP
1	J	192	LEU
1	J	250	LEU
1	J	255	TRP
1	L	15	PRO
1	L	17	VAL
1	L	21	LYS
1	L	25	MET
1	L	104	LYS
1	L	109	LEU
1	L	129	LYS
1	L	144	LYS
1	L	169	VAL
1	L	187	LYS
1	L	192	LEU
1	L	205	PRO
1	L	235	ASN
1	L	244	GLN
1	L	248	ASP
1	L	255	TRP
1	N	17	VAL
1	N	23	HIS
1	N	67	ASP
1	N	78	LEU
1	N	109	LEU
1	N	126	ASP
1	N	131	THR
1	N	144	LYS
1	N	149	ARG
1	N	150	SER
1	N	161	TYR
1	N	171	VAL
1	N	174	THR

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Mol	Chain	Res	Type
1	N	192	LEU
1	N	205	PRO
1	N	224	THR
1	N	230	LEU
1	N	255	TRP
1	P	17	VAL
1	P	18	MET
1	P	64	ARG
1	P	82	LYS
1	P	90	LEU
1	P	95	VAL
1	P	109	LEU
1	P	174	THR
1	P	187	LYS
1	P	192	LEU
1	P	218	LYS
1	P	232	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	46	HIS
1	B	46	HIS
1	B	130	GLN
1	B	244	GLN
1	E	22	ASN
1	E	46	HIS
1	E	197	ASN
1	E	244	GLN
1	H	130	GLN
1	H	197	ASN
1	H	214	ASN
1	H	244	GLN
1	H	252	ASN
1	J	130	GLN
1	J	244	GLN
1	L	46	HIS
1	L	130	GLN
1	L	197	ASN
1	L	252	ASN
1	N	46	HIS
1	N	130	GLN

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Mol	Chain	Res	Type
1	N	197	ASN
1	N	244	GLN
1	P	46	HIS
1	P	130	GLN
1	P	197	ASN
1	P	232	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	VBP	E	808	-	15,25,25	6.41	12 (80%)	16,35,35	1.60	1 (6%)
2	VBP	H	806	-	15,25,25	6.11	12 (80%)	16,35,35	1.77	2 (12%)
2	VBP	B	807	-	15,25,25	6.35	13 (86%)	16,35,35	1.50	1 (6%)
2	VBP	N	802	-	15,25,25	6.29	13 (86%)	16,35,35	1.43	1 (6%)
2	VBP	P	805	-	15,25,25	6.75	12 (80%)	16,35,35	1.37	1 (6%)
2	VBP	J	804	-	15,25,25	6.28	13 (86%)	16,35,35	1.55	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	VBP	G	803	-	15,25,25	6.48	13 (86%)	16,35,35	1.67	1 (6%)
2	VBP	L	801	-	15,25,25	6.42	13 (86%)	16,35,35	1.52	1 (6%)

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	VBP	E	808	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	H	806	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	B	807	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	N	802	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	P	805	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	J	804	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	G	803	-	1/1/3/3	0/8/16/16	0/2/2/2
2	VBP	L	801	-	1/1/3/3	0/8/16/16	0/2/2/2

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	805	VBP	C16-C15	9.91	1.56	1.38
2	P	805	VBP	C07-N09	9.40	1.51	1.38
2	G	803	VBP	C13-C12	9.22	1.55	1.38
2	E	808	VBP	C16-C15	9.18	1.55	1.38
2	J	804	VBP	C16-C15	9.15	1.55	1.38
2	P	805	VBP	C13-C12	9.13	1.55	1.38
2	L	801	VBP	C13-C12	9.08	1.55	1.38
2	N	802	VBP	C16-C15	9.04	1.55	1.38
2	G	803	VBP	C16-C15	9.02	1.55	1.38
2	B	807	VBP	C16-C15	8.98	1.55	1.38
2	L	801	VBP	C16-C15	8.93	1.55	1.38
2	H	806	VBP	C16-C15	8.74	1.54	1.38
2	L	801	VBP	C07-N09	8.68	1.50	1.38
2	J	804	VBP	C13-C12	8.67	1.54	1.38
2	B	807	VBP	C13-C12	8.65	1.54	1.38
2	E	808	VBP	C13-C12	8.60	1.54	1.38
2	G	803	VBP	C07-N09	8.48	1.50	1.38
2	B	807	VBP	C07-N09	8.44	1.50	1.38
2	H	806	VBP	C13-C12	8.38	1.54	1.38
2	N	802	VBP	C13-C12	8.38	1.54	1.38
2	N	802	VBP	C05-N04	8.20	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	808	VBP	C07-N09	8.16	1.50	1.38
2	P	805	VBP	C05-N04	8.15	1.49	1.35
2	J	804	VBP	C07-N09	8.13	1.50	1.38
2	G	803	VBP	C05-N04	8.01	1.49	1.35
2	J	804	VBP	C05-N04	7.87	1.49	1.35
2	N	802	VBP	C07-N09	7.87	1.49	1.38
2	P	805	VBP	C15-C14	7.83	1.56	1.39
2	L	801	VBP	C05-N04	7.83	1.49	1.35
2	E	808	VBP	C15-C14	7.77	1.55	1.39
2	B	807	VBP	C05-N04	7.59	1.49	1.35
2	G	803	VBP	C15-C14	7.54	1.55	1.39
2	H	806	VBP	C15-C14	7.51	1.55	1.39
2	B	807	VBP	C15-C14	7.46	1.55	1.39
2	J	804	VBP	C15-C14	7.43	1.55	1.39
2	H	806	VBP	C05-N04	7.43	1.48	1.35
2	E	808	VBP	C16-C11	7.38	1.54	1.38
2	P	805	VBP	C16-C11	7.33	1.54	1.38
2	L	801	VBP	C15-C14	7.19	1.54	1.39
2	H	806	VBP	C07-N09	7.14	1.48	1.38
2	G	803	VBP	C16-C11	7.12	1.54	1.38
2	H	806	VBP	C16-C11	7.10	1.54	1.38
2	E	808	VBP	C13-C14	7.09	1.54	1.39
2	E	808	VBP	C05-N04	7.06	1.48	1.35
2	B	807	VBP	C16-C11	7.05	1.54	1.38
2	P	805	VBP	C14-C17	7.03	1.54	1.47
2	N	802	VBP	C15-C14	7.02	1.54	1.39
2	N	802	VBP	C16-C11	6.95	1.53	1.38
2	G	803	VBP	C12-C11	6.88	1.53	1.38
2	J	804	VBP	C16-C11	6.88	1.53	1.38
2	E	808	VBP	C12-C11	6.86	1.53	1.38
2	B	807	VBP	C13-C14	6.82	1.53	1.39
2	L	801	VBP	C13-C14	6.80	1.53	1.39
2	L	801	VBP	C16-C11	6.73	1.53	1.38
2	P	805	VBP	C12-C11	6.72	1.53	1.38
2	P	805	VBP	C13-C14	6.72	1.53	1.39
2	L	801	VBP	O08-C07	6.70	1.41	1.24
2	N	802	VBP	C13-C14	6.64	1.53	1.39
2	G	803	VBP	C13-C14	6.64	1.53	1.39
2	L	801	VBP	C12-C11	6.63	1.53	1.38
2	H	806	VBP	C13-C14	6.59	1.53	1.39
2	J	804	VBP	C13-C14	6.58	1.53	1.39
2	J	804	VBP	C12-C11	6.57	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	807	VBP	C12-C11	6.55	1.53	1.38
2	E	808	VBP	O08-C07	6.51	1.40	1.24
2	P	805	VBP	O08-C07	6.48	1.40	1.24
2	J	804	VBP	O08-C07	6.45	1.40	1.24
2	G	803	VBP	O08-C07	6.41	1.40	1.24
2	H	806	VBP	C12-C11	6.37	1.52	1.38
2	N	802	VBP	C12-C11	6.37	1.52	1.38
2	N	802	VBP	O08-C07	6.14	1.39	1.24
2	B	807	VBP	O08-C07	6.05	1.39	1.24
2	H	806	VBP	O08-C07	6.04	1.39	1.24
2	H	806	VBP	C03-N04	-5.87	1.42	1.48
2	N	802	VBP	C03-N04	-5.76	1.42	1.48
2	E	808	VBP	C05-C06	5.61	1.50	1.38
2	L	801	VBP	C05-C06	5.60	1.50	1.38
2	B	807	VBP	C05-C06	5.52	1.50	1.38
2	G	803	VBP	C05-C06	5.39	1.50	1.38
2	G	803	VBP	C03-N04	-5.39	1.42	1.48
2	P	805	VBP	C05-C06	5.38	1.49	1.38
2	H	806	VBP	C05-C06	5.38	1.49	1.38
2	L	801	VBP	C14-C17	5.35	1.52	1.47
2	J	804	VBP	C05-C06	5.34	1.49	1.38
2	B	807	VBP	C14-C17	5.28	1.52	1.47
2	E	808	VBP	C14-C17	5.27	1.52	1.47
2	N	802	VBP	C05-C06	5.25	1.49	1.38
2	B	807	VBP	C03-N04	-5.13	1.42	1.48
2	G	803	VBP	C14-C17	5.09	1.52	1.47
2	E	808	VBP	C03-N04	-5.04	1.43	1.48
2	N	802	VBP	C14-C17	5.03	1.52	1.47
2	J	804	VBP	C03-N04	-4.65	1.43	1.48
2	L	801	VBP	C03-N04	-4.55	1.43	1.48
2	P	805	VBP	C03-N04	-4.40	1.43	1.48
2	J	804	VBP	C14-C17	4.37	1.51	1.47
2	H	806	VBP	C14-C17	3.48	1.50	1.47
2	L	801	VBP	C10-N09	-2.41	1.44	1.48
2	N	802	VBP	C10-N09	-2.34	1.44	1.48
2	J	804	VBP	C10-N09	-2.22	1.44	1.48
2	B	807	VBP	C10-N09	-2.02	1.44	1.48
2	G	803	VBP	C10-N09	-2.02	1.44	1.48

All (9) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	806	VBP	C10-N09-C20	5.62	124.50	117.92
2	G	803	VBP	C10-N09-C20	5.24	124.05	117.92
2	E	808	VBP	C10-N09-C20	5.08	123.87	117.92
2	B	807	VBP	C10-N09-C20	4.87	123.63	117.92
2	L	801	VBP	C10-N09-C20	4.85	123.59	117.92
2	J	804	VBP	C10-N09-C20	4.64	123.35	117.92
2	N	802	VBP	C10-N09-C20	4.23	122.88	117.92
2	P	805	VBP	C10-N09-C20	4.02	122.63	117.92
2	H	806	VBP	C16-C11-C12	2.18	121.59	118.17

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	806	VBP	C02
2	E	808	VBP	C02
2	N	802	VBP	C02
2	B	807	VBP	C02
2	P	805	VBP	C02
2	J	804	VBP	C02
2	G	803	VBP	C02
2	L	801	VBP	C02

There are no torsion outliers.

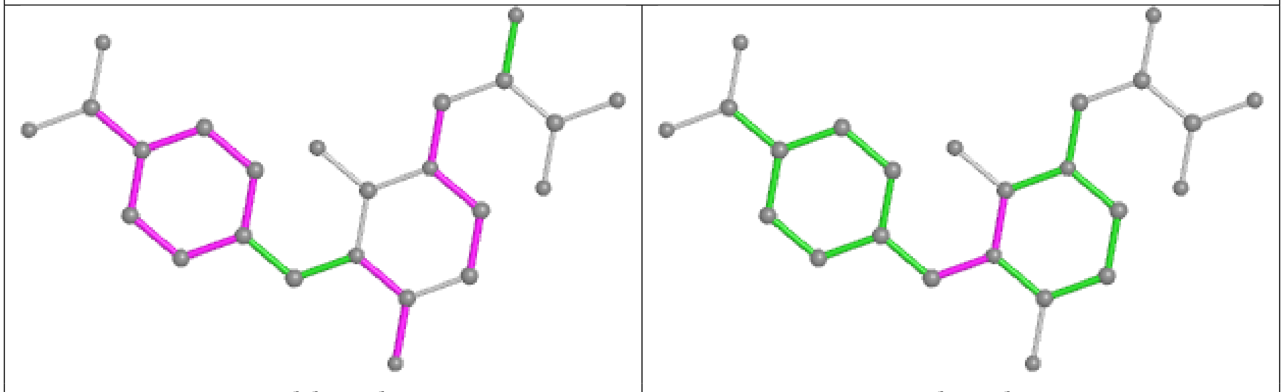
There are no ring outliers.

8 monomers are involved in 29 short contacts:

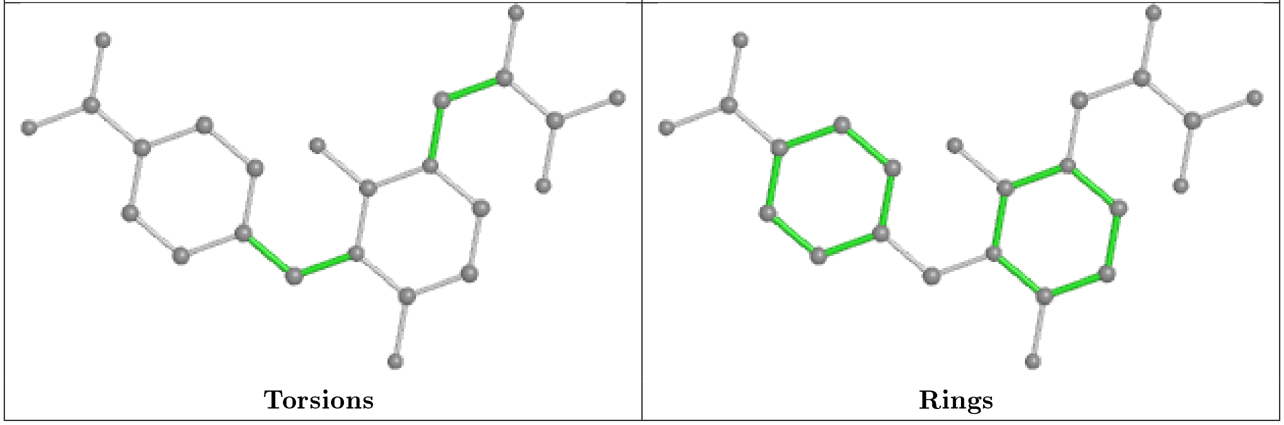
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	808	VBP	4	0
2	H	806	VBP	3	0
2	B	807	VBP	3	0
2	N	802	VBP	3	0
2	P	805	VBP	5	0
2	J	804	VBP	4	0
2	G	803	VBP	5	0
2	L	801	VBP	2	0

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 then 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 VBP E 808

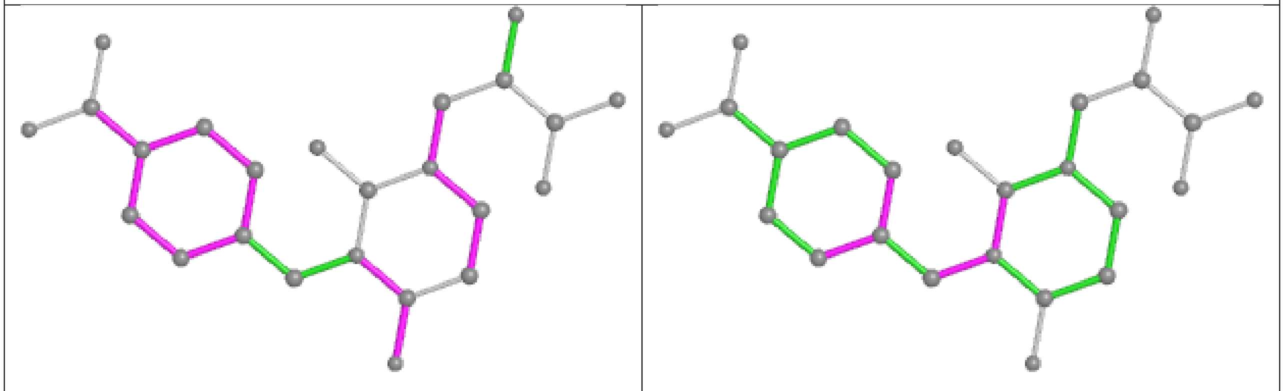


Bond lengths **Bond angles**



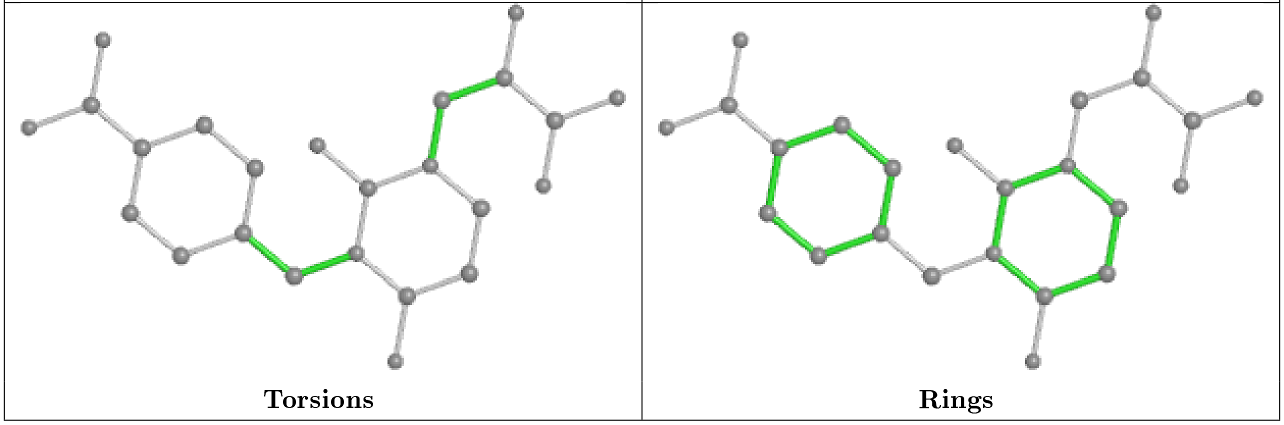
Torsions **Rings**

Ligand VBP H 806



Bond lengths

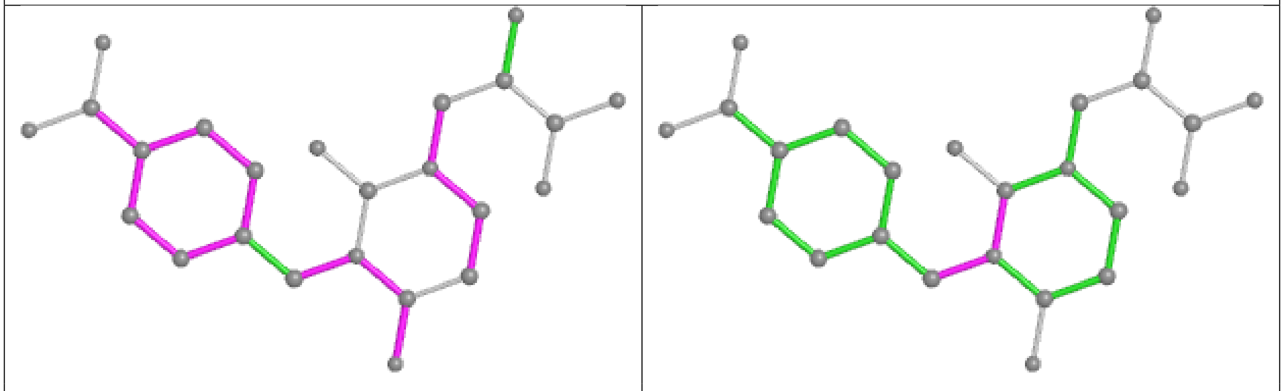
Bond angles



Torsions

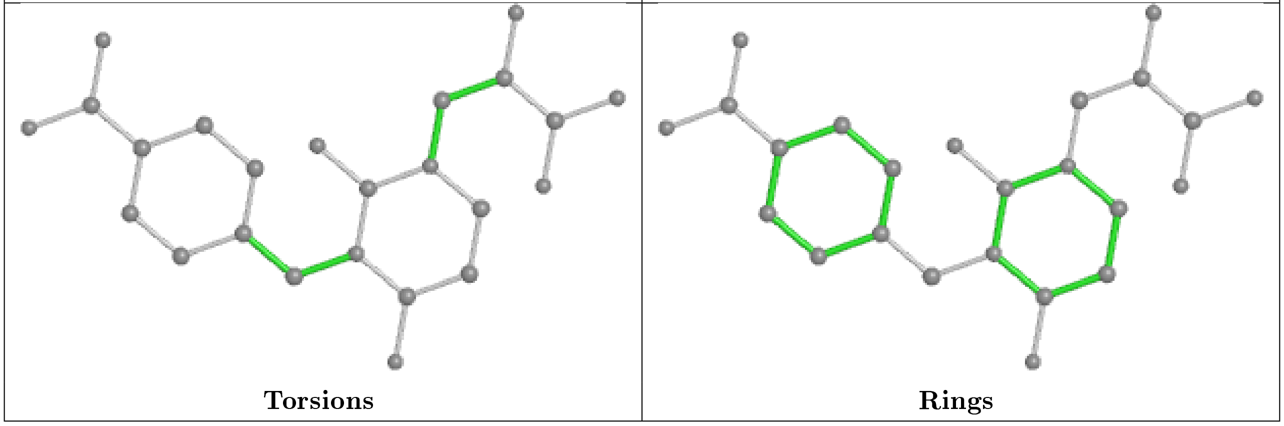
Rings

Ligand VBP B 807



Bond lengths

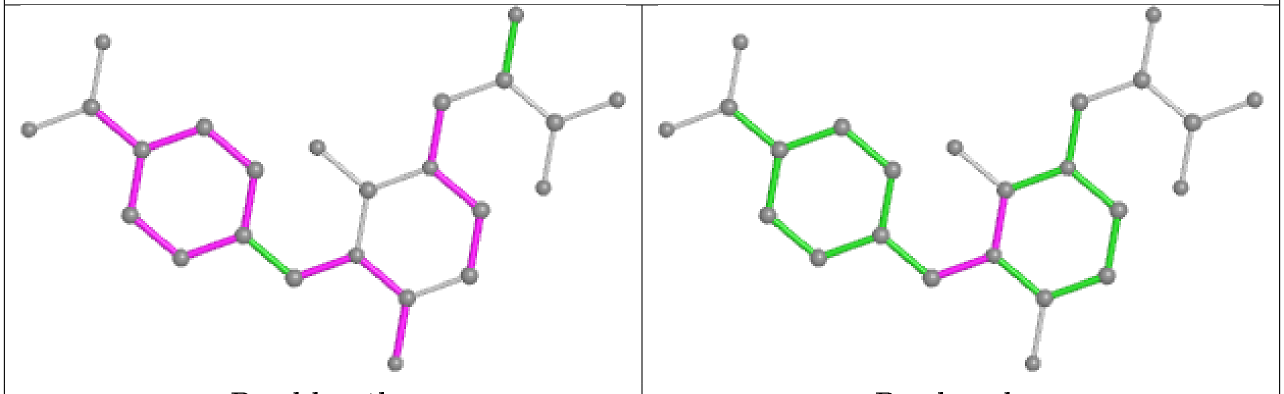
Bond angles



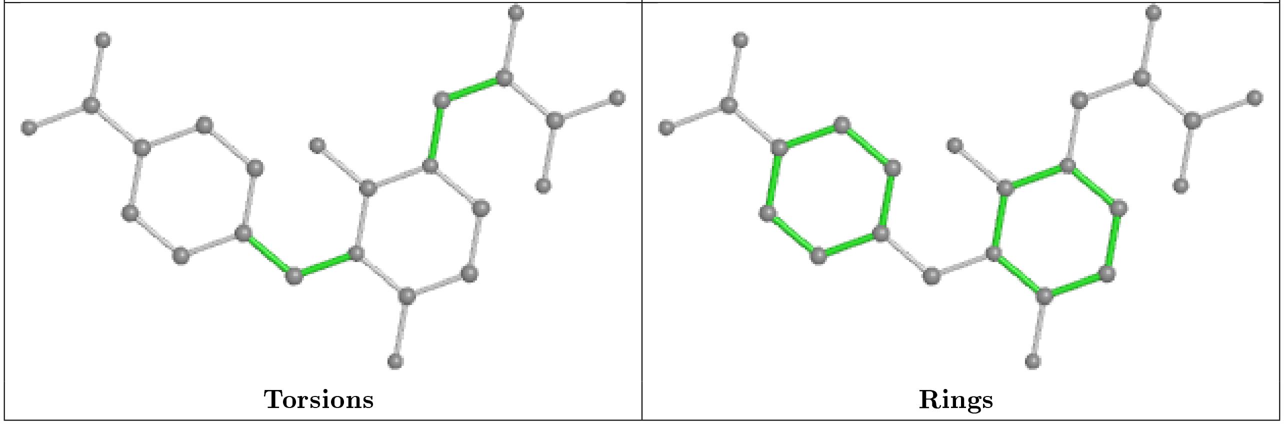
Torsions

Rings

Ligand VBP N 802

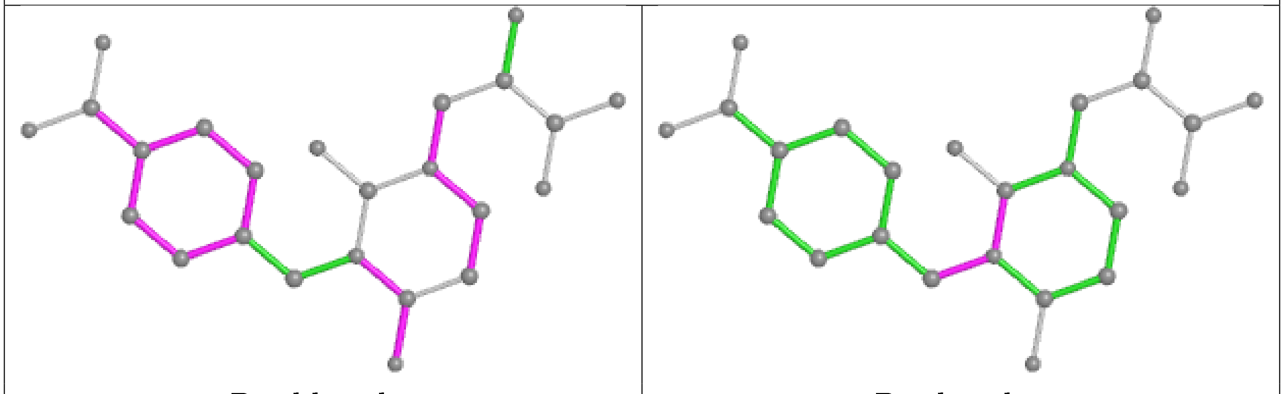


Bond lengths **Bond angles**

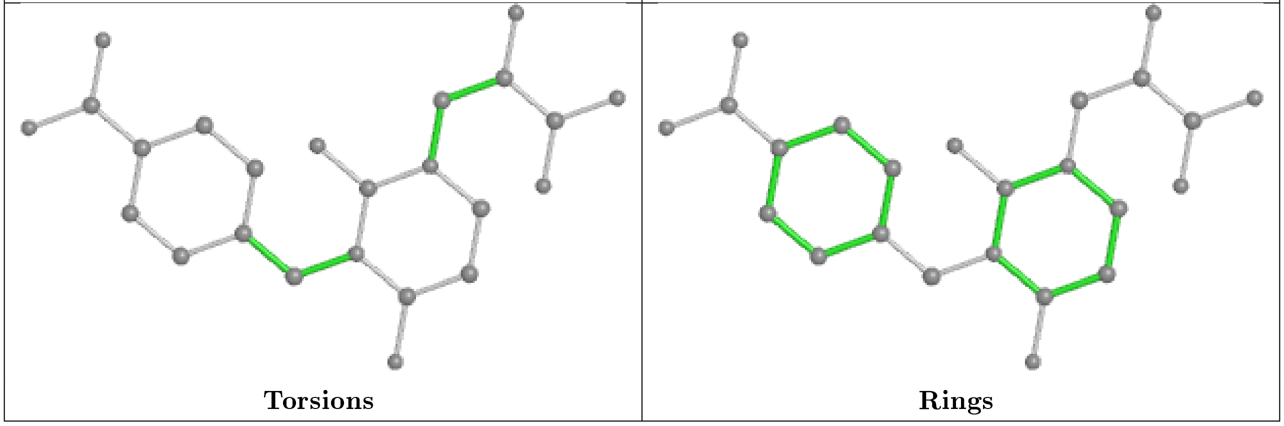


Torsions **Rings**

Ligand VBP P 805

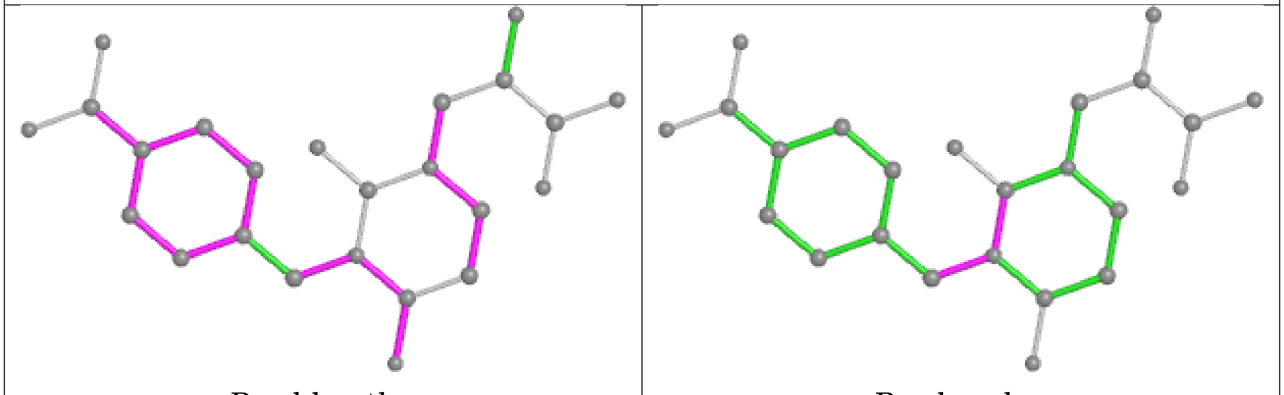


Bond lengths **Bond angles**



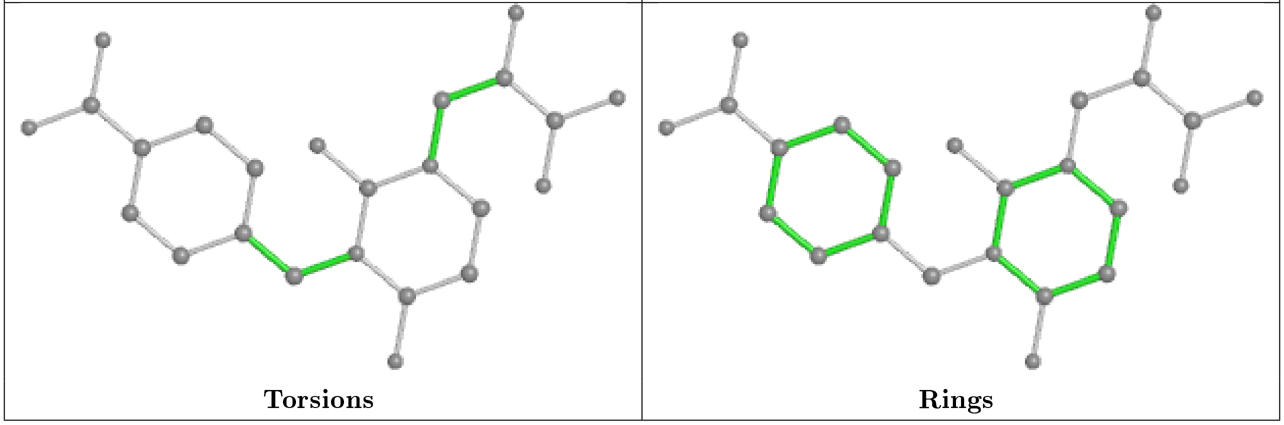
Torsions **Rings**

Ligand VBP J 804



Bond lengths

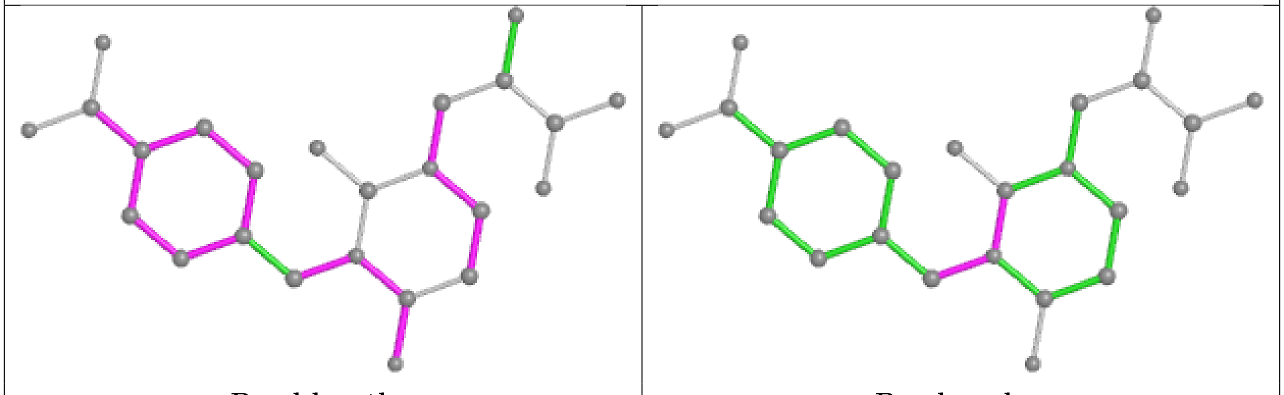
Bond angles



Torsions

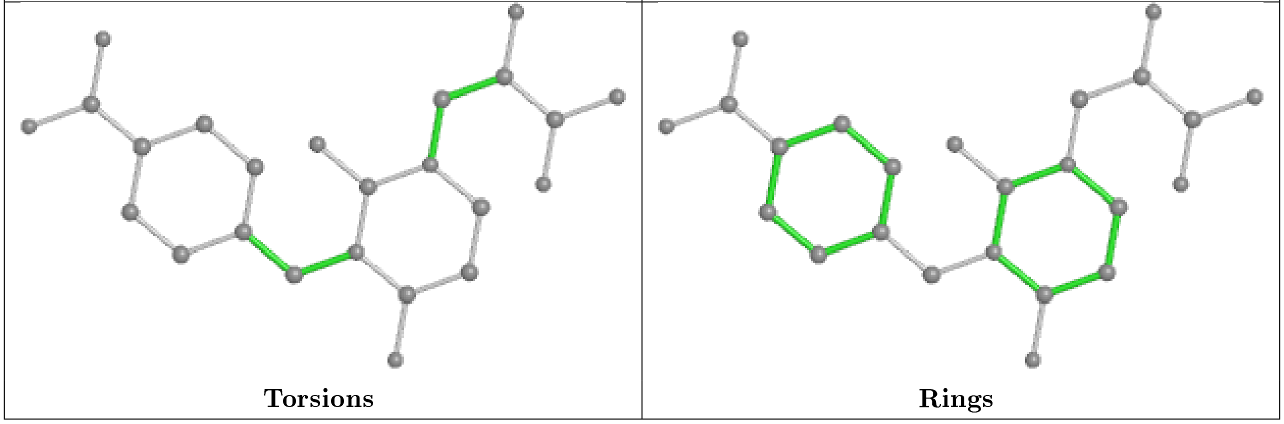
Rings

Ligand VBP G 803



Bond lengths

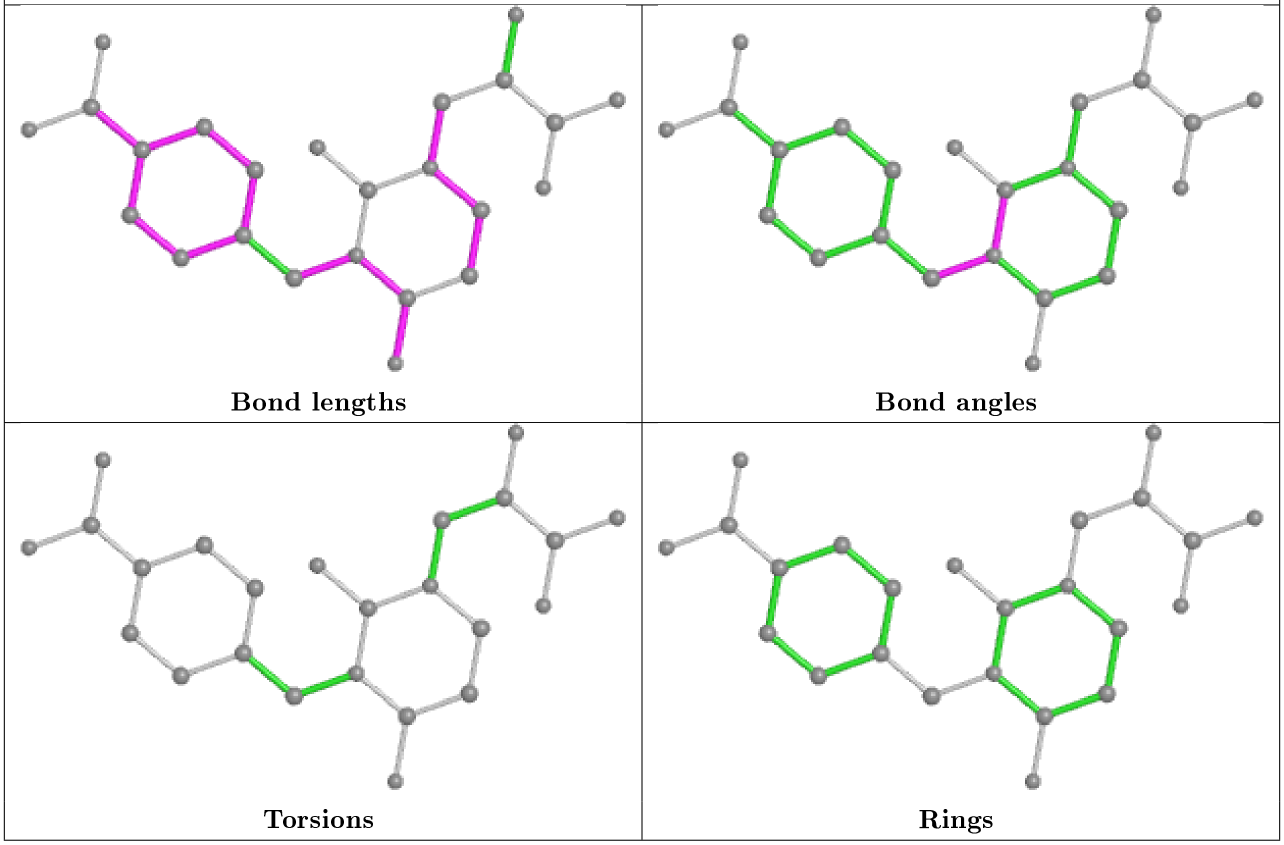
Bond angles



Torsions

Rings

Ligand VBP L 801



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

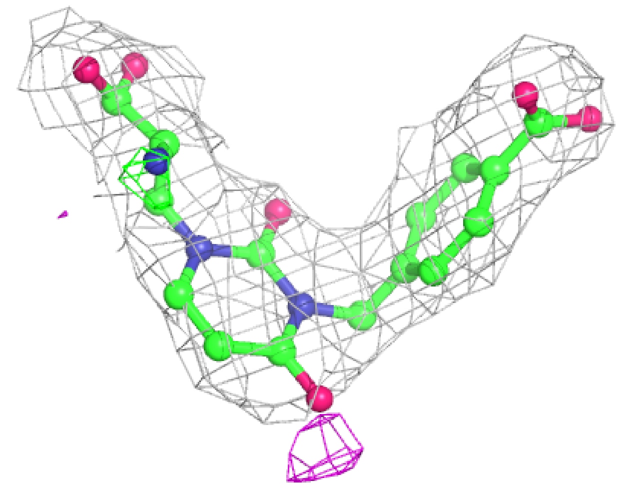
6.4 Ligands

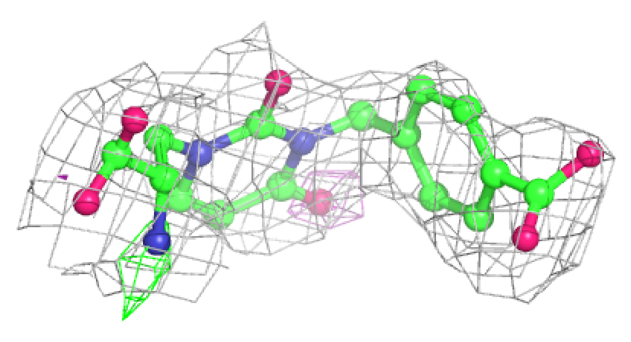
Unable to reproduce the depositors R factor - this section is therefore empty.

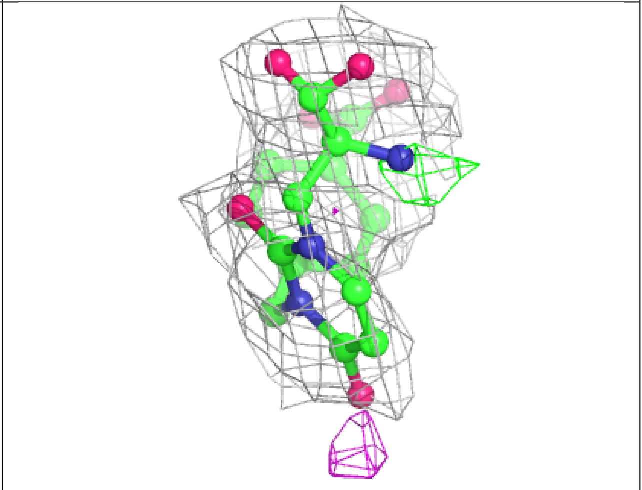
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

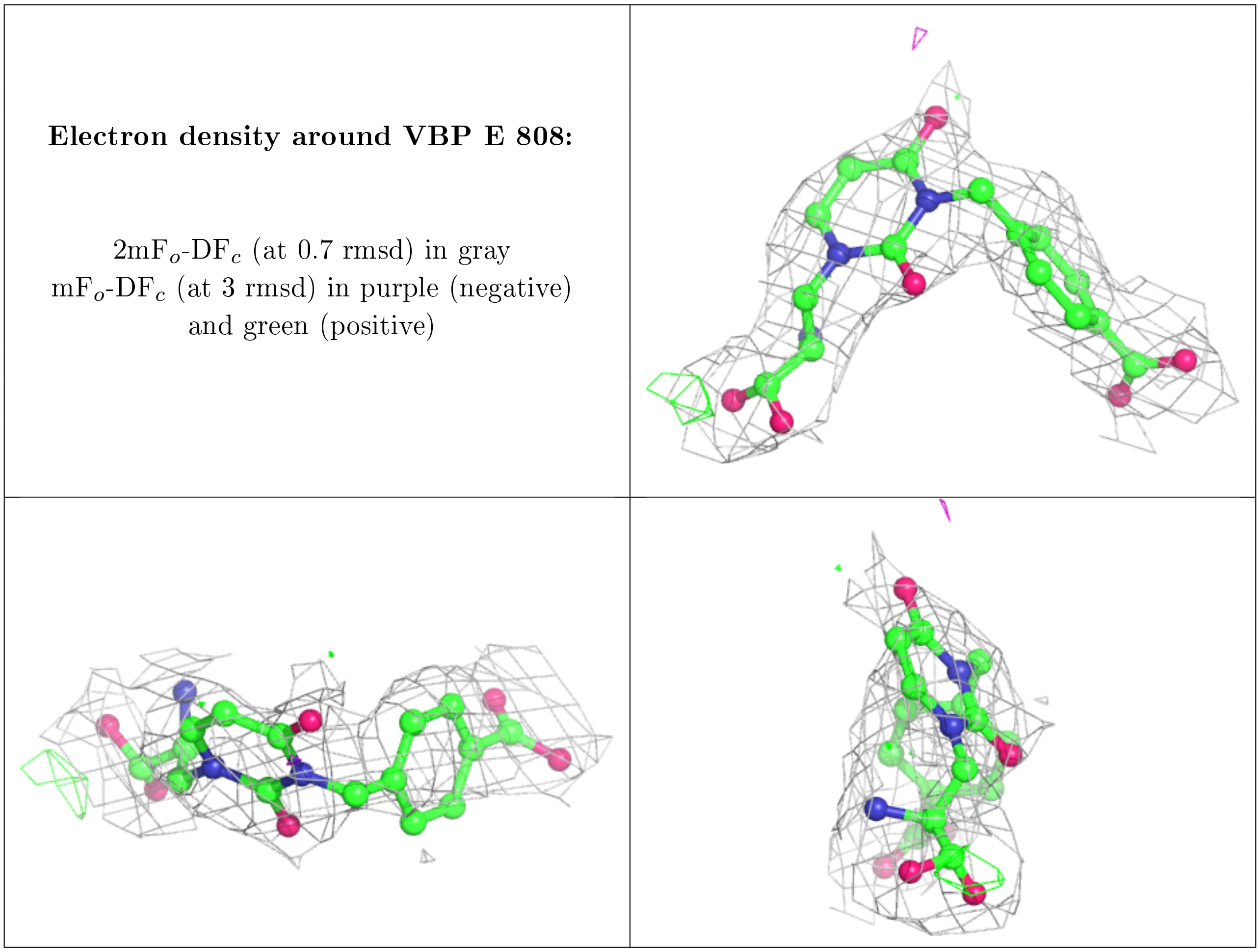
Electron density around VBP H 806:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







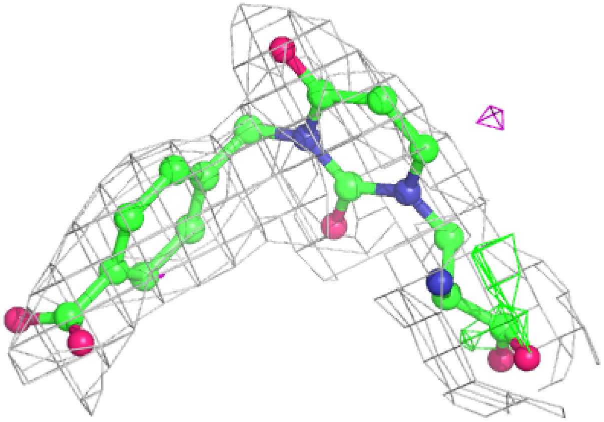


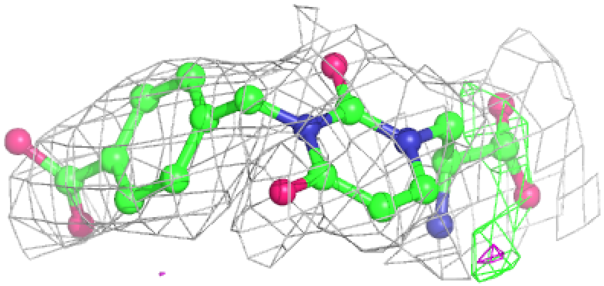
Electron density around VBP E 808:

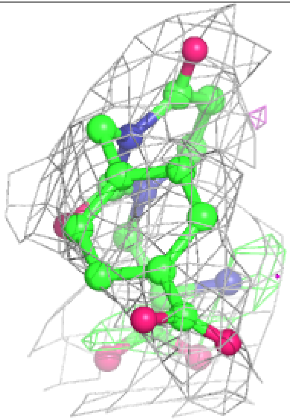
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around VBP N 802:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

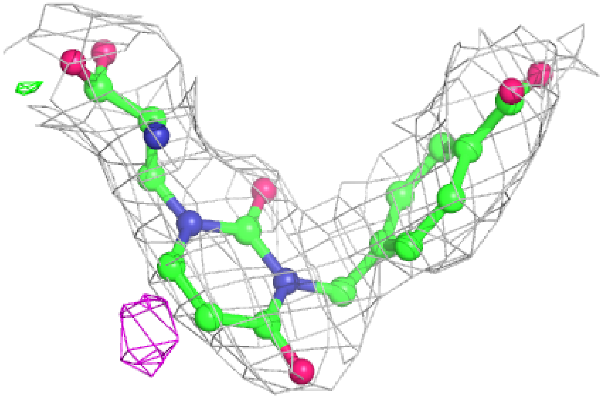


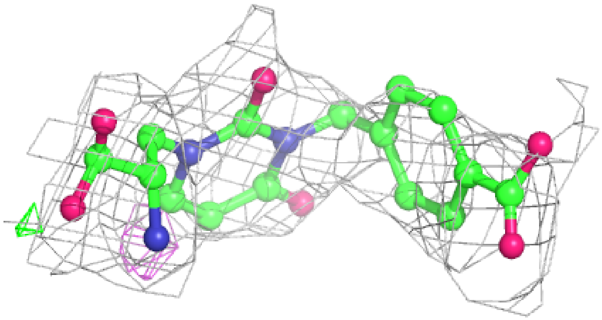


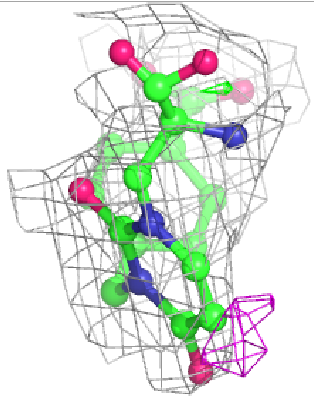


Electron density around VBP B 807:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

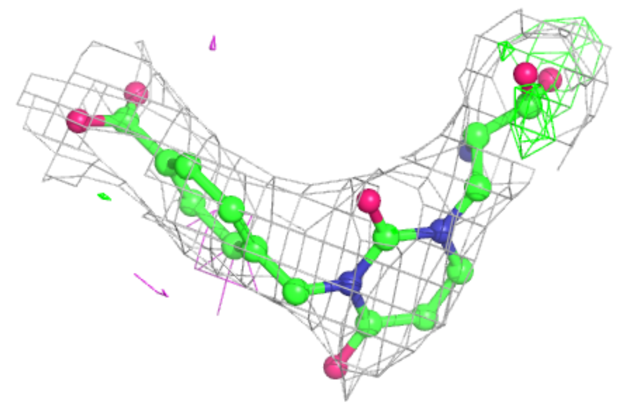


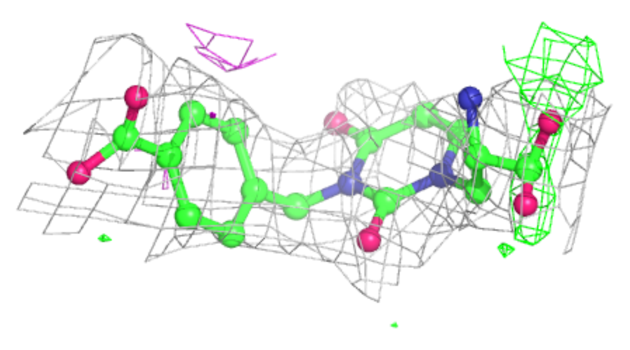


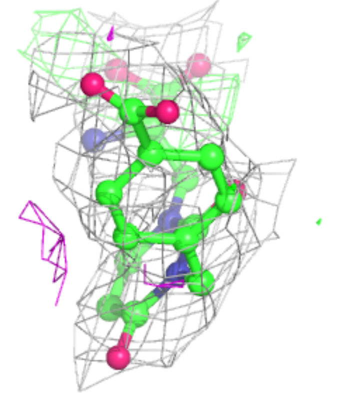


Electron density around VBP P 805:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

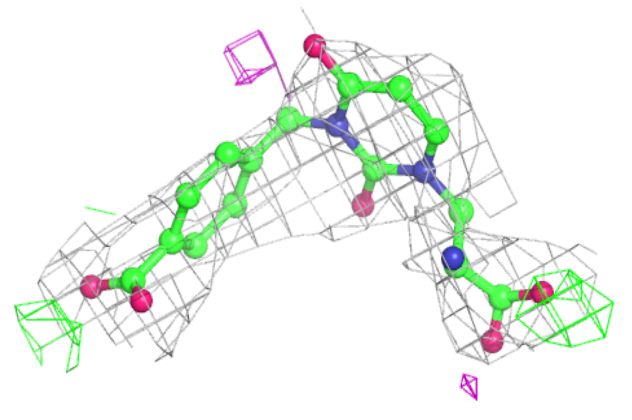


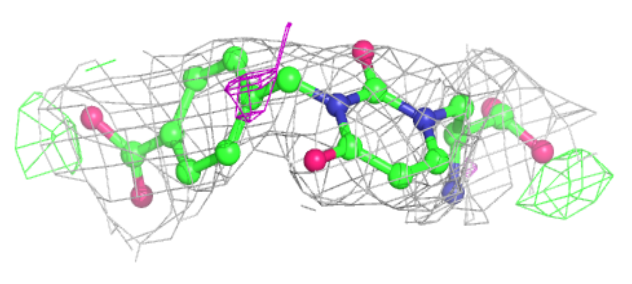


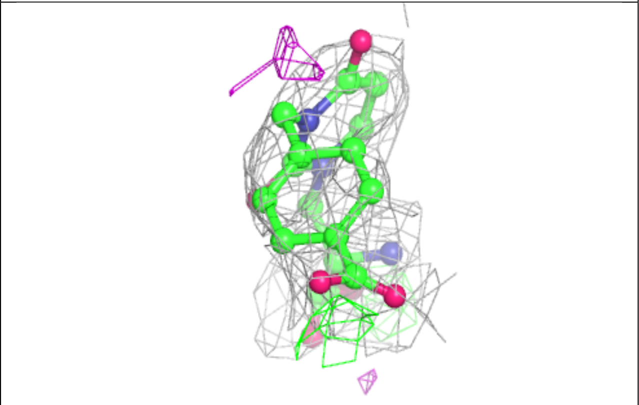


Electron density around VBP J 804:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

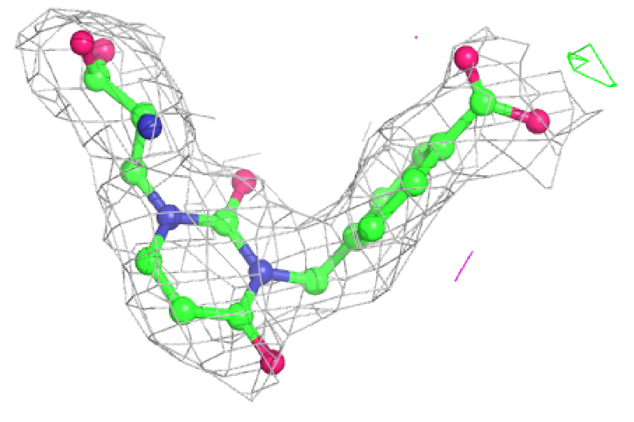


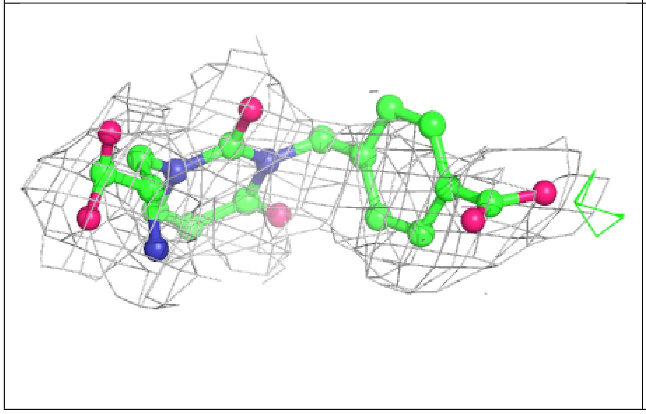


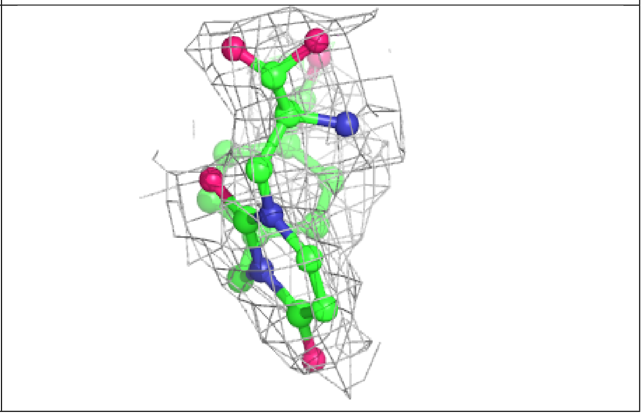


Electron density around VBP G 803:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

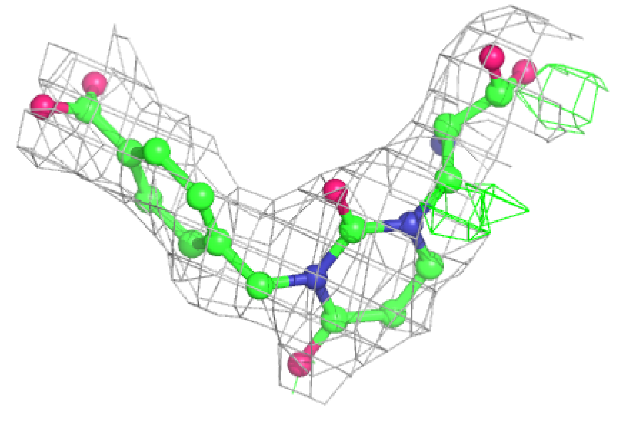


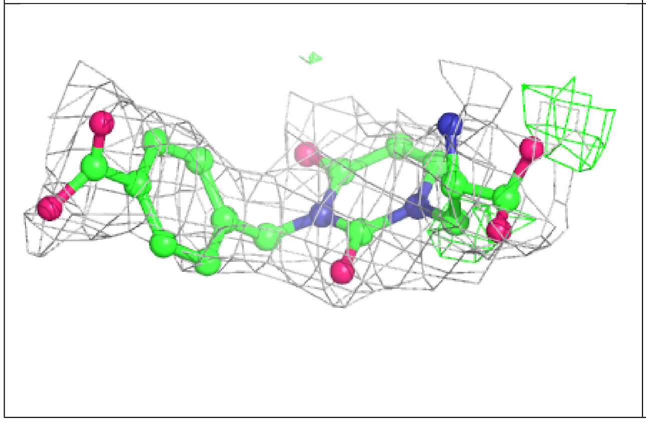


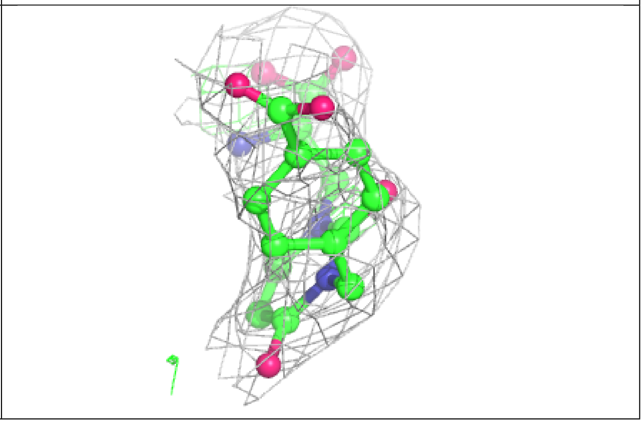


Electron density around VBP L 801:

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.