Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 06:03 AM EDT

PDB ID	:	3ILT
Title	:	Crystal structure of the AMPA subunit GluR2 bound to the allosteric modulator, trichlormethiazide
Authors	:	Ahmed, A.H.; Ptak, C.P.; Oswald, R.E.
Deposited on	:	2009-08-07
Resolution	:	2.11 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

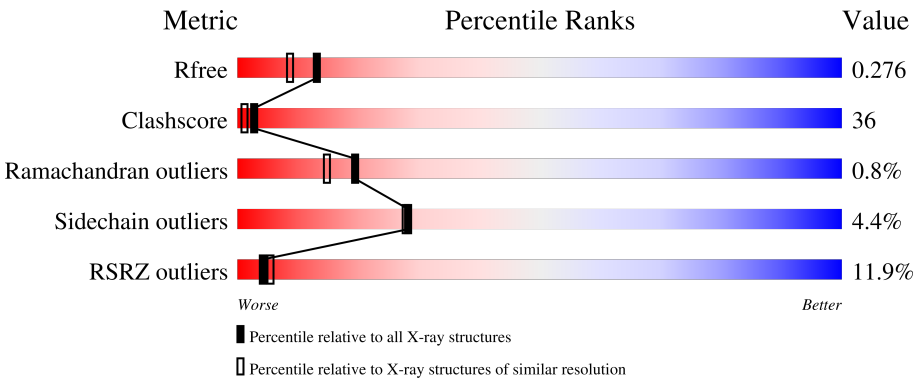
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.11 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of 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% 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	B	258	11% 47% 48% ·
1	E	258	12% 48% 47% 5%
1	H	258	12% 48% 49% ·

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRU	B	800	-	-	X	-
4	TRU	E	800	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6132 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.

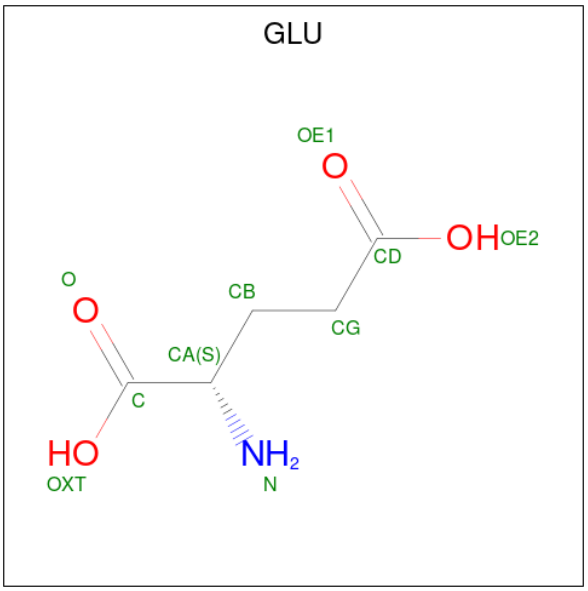
- Molecule 1 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	258	1953	1248	324	367	14	0	0	0
1	E	258	1962	1254	325	369	14	0	0	0
1	H	258	1969	1258	326	371	14	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	118	GLY	-	linker	UNP P19491
B	119	THR	-	linker	UNP P19491
B	242	SER	ASN	engineered mutation	UNP P19491
E	118	GLY	-	linker	UNP P19491
E	119	THR	-	linker	UNP P19491
E	242	SER	ASN	engineered mutation	UNP P19491
H	118	GLY	-	linker	UNP P19491
H	119	THR	-	linker	UNP P19491
H	242	SER	ASN	engineered mutation	UNP P19491

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).

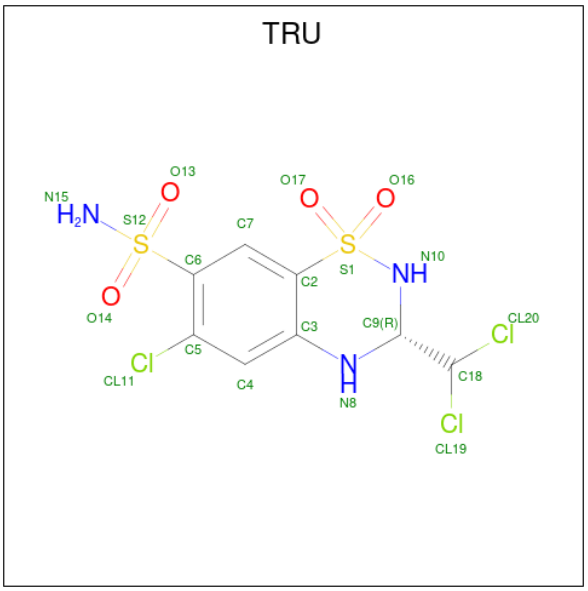


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	10	5	1	4	0	0
			Total	C	N	O		
2	E	1	10	5	1	4	0	0
			Total	C	N	O		
2	H	1	10	5	1	4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	2	2	2	0	0
			Total	Zn		
3	E	1	1	1	0	0
			Total	Zn		
3	H	2	2	2	0	0

- Molecule 4 is 6-CHLORO-3-(DICHLOROMETHYL)-3,4-DIHYDRO-2H-1,2,4-BENZOTHIADIAZINE-7-SULFONAMIDE 1,1-DIOXIDE (three-letter code: TRU) (formula: $C_8H_8Cl_3N_3O_4S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
4	B	1	20	8	3	3	4	2	0	0
			Total	C	Cl	N	O	S		
4	E	1	20	8	3	3	4	2	0	0
			Total	C	Cl	N	O	S		
4	H	1	20	8	3	3	4	2	0	0

- Molecule 5 is water.

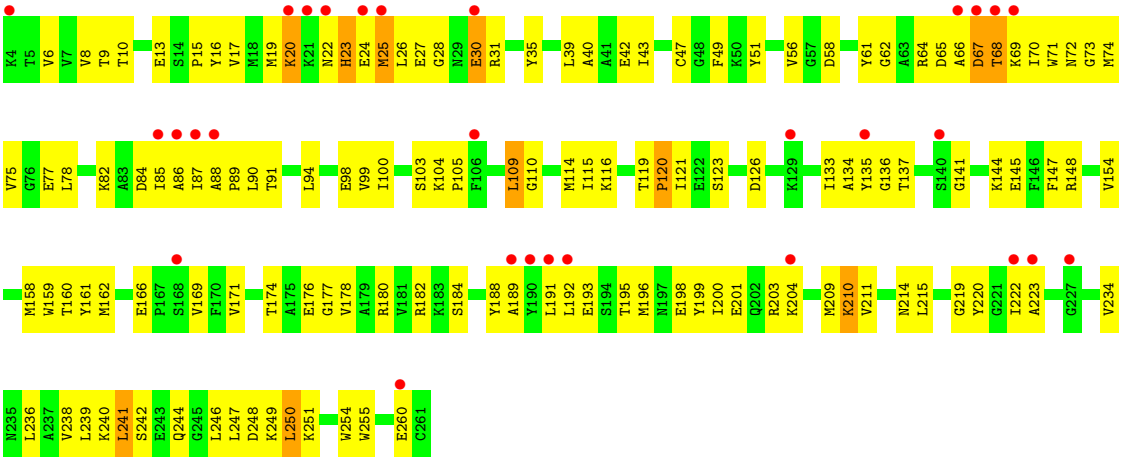
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	41	41	41	0	0
			Total	O		
5	E	50	50	50	0	0
			Total	O		
5	H	62	62	62	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

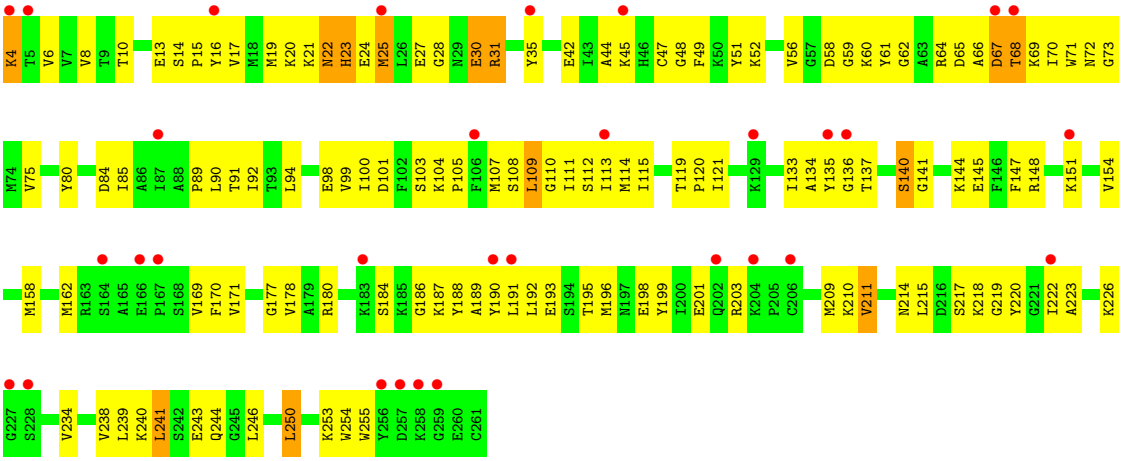
• Molecule 1: Glutamate receptor 2

Chain B: 11% 47% 48%



• Molecule 1: Glutamate receptor 2

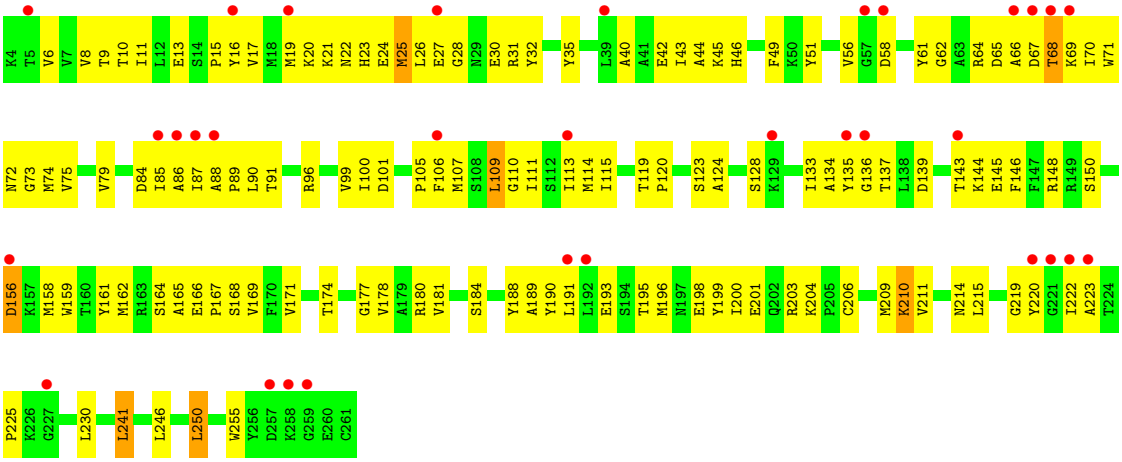
Chain E: 12% 48% 47% 5%



• Molecule 1: Glutamate receptor 2

Chain H:

12%
48%
49%


K4 T5 V6 V7 V8 T9 T10 I11 L12 E13 S14 P15 Y16 V17 M18 M19 K20 K21 N22 H23 E24 M25 L26 E27 G28 N29 E30 R31 Y32 Y35 L39 A40 A41 E42 I43 A44 K45 H46 F49 K50 Y51 V56 G57 D58 Y61 G62 A63 R64 D65 A66 D67 T68 K69 I70 W71
N72 G73 M74 V75 V79 D84 I85 A86 I87 A88 P89 L90 T91 R96 V99 I100 D101 P105 F106 M107 S108 L109 G110 I111 S112 I113 M114 I115 T119 P120 S123 A124 S128 K129 I133 A134 Y135 G136 T137 L138 D139 T143 K144 E145 F146 F147 R148 R149 S150
D156 K157 M158 W159 T160 Y161 M162 R163 S164 A165 E166 P167 S168 V169 F170 V171 T174 G177 V178 A179 R180 V181 S184 Y188 A189 Y190 L191 L192 E193 S194 T195 M196 N197 E198 Y199 I200 E201 Q202 R203 K204 P205 C206 M209 K210 V211 N214 L215 G219 Y220 G221 I222 A223 T224
P225 K226 G227 L230 L241 L246 L250 W255 Y256 D257 K258 G259 E260 C261

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.18Å 107.82Å 157.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.23 – 2.11 21.23 – 2.11	Depositor EDS
% Data completeness (in resolution range)	81.2 (21.23-2.11) 81.2 (21.23-2.11)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	8.31 (at 2.11Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.261 0.237 , 0.276	Depositor DCC
R_{free} test set	2000 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6132	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.57	1/1989 (0.1%)	0.67	0/2684
1	E	0.56	0/1998	0.68	0/2694
1	H	0.59	0/2005	0.69	0/2702
All	All	0.58	1/5992 (0.0%)	0.68	0/8080

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	42	GLU	CB-CG	5.41	1.62	1.52

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	1953	0	1933	151	3
1	E	1962	0	1950	130	1
1	H	1969	0	1963	146	3
2	B	10	0	5	1	0
2	E	10	0	5	0	0
2	H	10	0	5	1	0
3	B	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	H	2	0	0	0	1
4	B	20	0	8	8	0
4	E	20	0	8	7	0
4	H	20	0	8	1	0
5	B	41	0	0	2	0
5	E	50	0	0	1	0
5	H	62	0	0	8	0
All	All	6132	0	5885	424	4

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 36.

All (424) 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:239:LEU:HD23	4:E:800:TRU:CL20	1.70	1.28
1:H:42:GLU:HG3	1:H:246:LEU:CD2	1.77	1.15
1:E:42:GLU:OE2	1:E:45:LYS:HD3	1.49	1.11
1:E:239:LEU:CD2	4:E:800:TRU:CL20	2.36	1.09
1:H:42:GLU:HG3	1:H:246:LEU:HD22	1.13	1.08
1:B:241:LEU:HG	1:B:246:LEU:HD23	1.39	1.03
1:E:65:ASP:HB3	1:E:68:THR:HG22	1.42	1.00
1:E:241:LEU:HG	1:E:246:LEU:HD23	1.51	0.93
1:B:65:ASP:HB3	1:B:68:THR:HG22	1.50	0.93
1:E:42:GLU:OE2	1:E:45:LYS:CD	2.18	0.91
1:H:241:LEU:HG	1:H:246:LEU:HD23	1.54	0.90
1:H:166:GLU:HA	1:H:167:PRO:C	1.92	0.89
1:E:20:LYS:HE3	1:E:30:GLU:O	1.74	0.88
1:H:19:MET:HB3	5:H:263:HOH:O	1.73	0.88
1:E:240:LYS:NZ	1:E:244:GLN:HE21	1.72	0.86
1:E:31:ARG:HG3	1:E:31:ARG:HH11	1.41	0.84
1:B:19:MET:O	1:B:20:LYS:O	1.95	0.84
1:B:68:THR:HG23	1:B:70:ILE:H	1.39	0.84
1:H:139:ASP:HA	1:H:144:LYS:HD2	1.61	0.83
1:B:105:PRO:O	4:B:800:TRU:H9	1.77	0.83
1:B:22:ASN:C	1:B:24:GLU:H	1.77	0.82
1:E:68:THR:HG23	1:E:70:ILE:H	1.43	0.81
1:E:27:GLU:O	1:E:30:GLU:HG2	1.83	0.79
1:H:19:MET:SD	5:H:263:HOH:O	2.40	0.79
4:H:800:TRU:O13	4:H:800:TRU:CL11	2.39	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:GLU:CG	1:H:246:LEU:HD22	2.05	0.77
1:B:100:ILE:HD12	1:B:223:ALA:HB1	1.66	0.76
1:H:241:LEU:HG	1:H:246:LEU:CD2	2.17	0.75
1:H:65:ASP:HB3	1:H:68:THR:HG22	1.68	0.75
4:E:800:TRU:CL11	4:E:800:TRU:O13	2.42	0.75
1:B:147:PHE:CZ	1:B:191:LEU:HD13	2.22	0.74
1:B:22:ASN:O	1:B:24:GLU:N	2.19	0.74
1:B:35:TYR:CD1	1:B:250:LEU:HB3	2.23	0.73
1:E:201:GLU:HG3	1:E:209:MET:HA	1.70	0.72
1:B:23:HIS:NE2	3:B:2:ZN:ZN	1.50	0.72
1:E:105:PRO:O	4:E:800:TRU:H9	1.89	0.72
1:E:144:LYS:HE2	1:E:148:ARG:NH2	2.06	0.71
1:B:65:ASP:HB3	1:B:68:THR:CG2	2.21	0.71
1:B:115:ILE:HD11	1:B:211:VAL:HG11	1.73	0.70
1:E:28:GLY:O	1:E:31:ARG:HG3	1.90	0.70
1:B:105:PRO:HA	1:B:220:TYR:O	1.90	0.70
1:H:61:TYR:HE1	1:H:89:PRO:HG2	1.58	0.69
1:B:25:MET:CG	1:B:25:MET:O	2.41	0.69
1:E:199:TYR:O	1:E:203:ARG:HG2	1.93	0.69
1:E:105:PRO:HA	1:E:220:TYR:O	1.92	0.68
1:B:22:ASN:OD1	1:B:26:LEU:HD11	1.93	0.68
1:B:121:ILE:HG12	1:B:133:ILE:HD13	1.75	0.67
1:B:240:LYS:NZ	1:B:244:GLN:HE21	1.92	0.67
1:H:110:GLY:HA3	1:H:214:ASN:HB3	1.77	0.67
1:H:42:GLU:CG	1:H:246:LEU:CD2	2.66	0.67
1:H:171:VAL:HG11	1:H:177:GLY:HA2	1.76	0.66
1:B:20:LYS:HE3	1:B:26:LEU:HD13	1.77	0.66
1:E:244:GLN:HA	1:E:244:GLN:OE1	1.95	0.66
1:H:28:GLY:N	1:H:31:ARG:NH1	2.44	0.66
1:B:22:ASN:C	1:B:24:GLU:N	2.45	0.66
1:H:214:ASN:OD1	5:H:282:HOH:O	2.14	0.66
1:B:10:THR:OG1	1:B:17:VAL:HG21	1.96	0.65
1:B:134:ALA:HA	1:B:161:TYR:OH	1.96	0.65
1:E:31:ARG:HG3	1:E:31:ARG:NH1	2.09	0.65
1:H:150:SER:O	1:H:156:ASP:HB2	1.97	0.65
1:B:201:GLU:HG3	1:B:209:MET:HA	1.78	0.64
1:E:22:ASN:O	1:E:24:GLU:N	2.27	0.64
1:H:166:GLU:CA	1:H:167:PRO:C	2.66	0.64
1:B:35:TYR:CE1	1:B:250:LEU:HB3	2.32	0.64
1:B:23:HIS:O	1:B:23:HIS:ND1	2.30	0.64
1:E:137:THR:HG22	1:E:191:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:LEU:HD23	1:H:193:GLU:HG2	1.79	0.63
1:H:165:ALA:HB1	1:H:169:VAL:HG13	1.79	0.63
1:B:192:LEU:HD23	1:B:192:LEU:H	1.64	0.63
1:H:42:GLU:OE2	1:H:45:LYS:NZ	2.31	0.63
1:B:199:TYR:O	1:B:203:ARG:HG2	1.99	0.63
1:E:147:PHE:CZ	1:E:191:LEU:HD13	2.34	0.62
1:H:68:THR:CG2	1:H:70:ILE:H	2.12	0.62
1:E:71:TRP:CE3	1:E:75:VAL:HG11	2.34	0.62
1:B:68:THR:CG2	1:B:70:ILE:H	2.08	0.62
1:E:68:THR:CG2	1:E:70:ILE:H	2.10	0.62
1:H:42:GLU:OE2	1:H:45:LYS:CE	2.48	0.62
1:H:35:TYR:CE1	1:H:250:LEU:HB3	2.35	0.62
1:B:147:PHE:CE2	1:B:191:LEU:HD13	2.35	0.61
1:H:137:THR:HG22	1:H:191:LEU:HB2	1.80	0.61
1:B:109:LEU:HB3	1:B:195:THR:HG23	1.82	0.61
1:H:42:GLU:HG3	1:H:246:LEU:HD21	1.77	0.61
1:E:66:ALA:O	1:E:67:ASP:CB	2.49	0.61
4:B:800:TRU:CL19	1:E:218:LYS:HA	2.38	0.61
1:H:210:LYS:HE3	5:H:282:HOH:O	2.01	0.61
1:B:136:GLY:HA3	1:B:169:VAL:O	2.01	0.60
1:E:10:THR:OG1	1:E:17:VAL:HG21	2.01	0.60
1:H:8:VAL:HG23	1:H:51:TYR:HB2	1.83	0.60
1:B:20:LYS:HE3	1:B:30:GLU:O	2.00	0.60
1:E:240:LYS:HZ3	1:E:244:GLN:HE21	1.49	0.60
1:H:8:VAL:HG22	1:H:85:ILE:CG2	2.31	0.60
1:B:85:ILE:HD11	1:B:222:ILE:HG21	1.83	0.60
1:B:28:GLY:O	1:B:31:ARG:HG3	2.02	0.60
1:B:110:GLY:HA3	1:B:214:ASN:HB3	1.84	0.59
1:B:198:GLU:HG3	1:B:210:LYS:HZ1	1.67	0.59
1:B:198:GLU:HG3	1:B:210:LYS:NZ	2.17	0.59
1:E:151:LYS:HE2	1:H:164:SER:HB3	1.85	0.59
1:H:28:GLY:N	1:H:31:ARG:HH11	2.00	0.59
1:B:91:THR:OG1	1:B:193:GLU:OE2	2.20	0.59
1:H:40:ALA:HA	1:H:87:ILE:HD13	1.85	0.59
1:B:65:ASP:CB	1:B:68:THR:HG22	2.31	0.59
1:B:85:ILE:HD12	1:B:234:VAL:HG21	1.85	0.59
1:E:100:ILE:HD12	1:E:223:ALA:HB1	1.85	0.59
1:B:148:ARG:HA	1:B:159:TRP:CE2	2.38	0.58
1:E:15:PRO:HB3	1:E:199:TYR:CE1	2.38	0.58
1:H:15:PRO:HB3	1:H:199:TYR:CE1	2.38	0.58
1:B:68:THR:HG23	1:B:70:ILE:N	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ASP:OD1	1:E:73:GLY:HA2	2.04	0.58
1:E:135:TYR:HA	1:E:189:ALA:O	2.04	0.58
1:B:180:ARG:O	1:B:184:SER:HB3	2.04	0.58
1:E:28:GLY:O	1:E:31:ARG:NH1	2.37	0.58
4:B:800:TRU:CL19	1:E:218:LYS:HB3	2.40	0.57
1:E:222:ILE:HG21	1:E:234:VAL:HG11	1.86	0.57
1:H:27:GLU:HA	1:H:31:ARG:HD3	1.86	0.57
1:H:180:ARG:O	1:H:184:SER:HB3	2.04	0.57
1:H:100:ILE:HD12	1:H:223:ALA:HB1	1.86	0.57
1:B:27:GLU:O	1:B:30:GLU:HG2	2.04	0.57
1:H:42:GLU:HB3	1:H:241:LEU:HD21	1.86	0.57
1:B:105:PRO:HB2	4:B:800:TRU:O16	2.05	0.56
1:H:84:ASP:O	1:H:225:PRO:HD3	2.04	0.56
1:B:64:ARG:HD3	1:B:69:LYS:HD2	1.87	0.56
1:E:30:GLU:HG3	5:E:305:HOH:O	2.04	0.56
1:H:28:GLY:O	1:H:31:ARG:HG3	2.05	0.56
1:H:43:ILE:HG13	1:H:222:ILE:CD1	2.35	0.56
1:E:112:SER:HB2	1:E:210:LYS:HG3	1.86	0.56
1:H:6:VAL:O	1:H:51:TYR:HA	2.05	0.56
1:H:158:MET:O	1:H:162:MET:HG3	2.05	0.56
1:H:164:SER:O	1:H:166:GLU:HG2	2.05	0.56
1:B:105:PRO:HB3	1:B:219:GLY:HA3	1.88	0.56
1:B:242:SER:HB2	1:B:247:LEU:HD12	1.87	0.56
1:B:248:ASP:N	4:B:800:TRU:CL11	2.75	0.56
1:B:244:GLN:OE1	1:B:244:GLN:HA	2.05	0.56
1:H:75:VAL:O	1:H:79:VAL:HG23	2.06	0.56
1:B:137:THR:HG22	1:B:191:LEU:HB2	1.88	0.56
1:E:8:VAL:HG22	1:E:85:ILE:CG2	2.36	0.56
1:H:199:TYR:O	1:H:203:ARG:HG2	2.06	0.56
1:E:113:ILE:HG12	1:E:191:LEU:CD2	2.36	0.55
1:B:94:LEU:O	1:B:98:GLU:HG3	2.06	0.55
1:B:61:TYR:HE1	1:B:89:PRO:HG2	1.70	0.55
1:H:198:GLU:HG3	1:H:210:LYS:NZ	2.21	0.55
1:B:196:MET:O	1:B:200:ILE:HG12	2.06	0.55
1:B:58:ASP:OD1	1:B:73:GLY:HA2	2.06	0.55
1:E:171:VAL:HG11	1:E:177:GLY:HA2	1.88	0.55
1:E:85:ILE:HD11	1:E:222:ILE:HG21	1.89	0.55
1:H:135:TYR:HA	1:H:189:ALA:O	2.07	0.54
1:H:42:GLU:OE1	1:H:241:LEU:HD11	2.08	0.54
1:E:215:LEU:N	1:E:215:LEU:HD12	2.22	0.53
1:B:171:VAL:HG11	1:B:177:GLY:HA2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:GLY:O	1:H:31:ARG:NH1	2.42	0.53
1:H:64:ARG:NH2	1:H:71:TRP:HE1	2.05	0.53
1:E:198:GLU:HG3	1:E:210:LYS:HZ1	1.72	0.53
1:H:68:THR:HG22	1:H:70:ILE:H	1.72	0.53
1:H:61:TYR:CE1	1:H:89:PRO:HG2	2.40	0.53
1:E:110:GLY:HA3	1:E:214:ASN:HB3	1.89	0.53
1:H:58:ASP:OD1	1:H:73:GLY:HA2	2.09	0.53
1:H:42:GLU:OE2	1:H:45:LYS:HD2	2.08	0.53
1:B:56:VAL:HG23	1:B:77:GLU:HG3	1.91	0.53
1:E:85:ILE:HD12	1:E:234:VAL:HG21	1.91	0.53
1:E:222:ILE:CG2	1:E:234:VAL:HG11	2.39	0.53
1:B:62:GLY:HA2	1:B:72:ASN:O	2.09	0.52
1:B:85:ILE:CD1	1:B:234:VAL:HG21	2.39	0.52
1:B:192:LEU:HD23	1:B:192:LEU:N	2.23	0.52
1:E:136:GLY:HA3	1:E:169:VAL:O	2.08	0.52
1:B:77:GLU:OE1	1:B:82:LYS:HB2	2.10	0.52
1:B:215:LEU:N	1:B:215:LEU:HD12	2.25	0.52
1:H:165:ALA:C	1:H:166:GLU:HG2	2.30	0.52
1:H:101:ASP:O	1:H:223:ALA:HA	2.10	0.52
1:E:47:CYS:HB2	1:E:49:PHE:CE2	2.44	0.52
1:B:114:MET:HE2	5:B:275:HOH:O	2.09	0.52
1:H:35:TYR:CD1	1:H:250:LEU:HB3	2.45	0.52
1:H:135:TYR:HB3	1:H:189:ALA:HB3	1.91	0.52
1:H:201:GLU:HG3	1:H:209:MET:HA	1.91	0.52
1:B:25:MET:O	1:B:25:MET:HG3	2.10	0.52
1:B:20:LYS:HG3	1:B:30:GLU:O	2.09	0.52
1:H:13:GLU:OE1	1:H:174:THR:HB	2.09	0.51
1:E:85:ILE:HD11	1:E:222:ILE:CG2	2.40	0.51
1:B:222:ILE:HD12	1:B:238:VAL:CG2	2.41	0.51
1:E:94:LEU:O	1:E:98:GLU:HG3	2.10	0.51
1:E:19:MET:HB3	1:E:23:HIS:ND1	2.26	0.51
1:H:9:THR:O	1:H:86:ALA:HA	2.11	0.51
1:H:42:GLU:O	1:H:46:HIS:HD2	1.94	0.51
1:H:196:MET:O	1:H:200:ILE:HG12	2.11	0.51
1:B:115:ILE:HD11	1:B:211:VAL:CG1	2.38	0.51
1:E:22:ASN:OD1	1:E:22:ASN:N	2.40	0.51
1:H:119:THR:CG2	1:H:133:ILE:HD13	2.40	0.51
1:H:20:LYS:O	1:H:21:LYS:C	2.48	0.51
1:B:115:ILE:HD12	1:B:119:THR:HB	1.93	0.50
5:B:295:HOH:O	1:E:94:LEU:HB3	2.11	0.50
1:E:60:LYS:HD3	1:E:140:SER:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:GLU:HG3	1:E:210:LYS:NZ	2.26	0.50
1:H:19:MET:CB	5:H:263:HOH:O	2.46	0.50
1:B:19:MET:HB3	1:B:23:HIS:CD2	2.47	0.50
1:B:103:SER:O	1:E:104:LYS:HE3	2.11	0.50
1:E:42:GLU:HG3	1:E:246:LEU:HD22	1.92	0.50
1:E:58:ASP:O	1:E:60:LYS:HG3	2.11	0.50
1:E:240:LYS:HZ2	1:E:244:GLN:HE21	1.57	0.50
1:B:66:ALA:O	1:B:67:ASP:CB	2.59	0.50
1:B:25:MET:O	1:B:25:MET:HG2	2.10	0.50
1:H:20:LYS:HB2	1:H:31:ARG:O	2.11	0.50
1:B:9:THR:O	1:B:86:ALA:HA	2.12	0.50
1:E:190:TYR:CE2	1:E:192:LEU:HB3	2.47	0.50
1:B:115:ILE:CD1	1:B:211:VAL:HG11	2.42	0.50
1:H:56:VAL:HG21	1:H:73:GLY:HA2	1.92	0.50
1:H:120:PRO:HD2	1:H:133:ILE:HD11	1.94	0.50
1:H:180:ARG:HG2	1:H:188:TYR:CD2	2.47	0.50
1:E:13:GLU:HG2	1:E:61:TYR:OH	2.12	0.50
1:B:13:GLU:OE1	1:B:174:THR:HB	2.12	0.49
1:H:156:ASP:OD1	1:H:156:ASP:O	2.30	0.49
1:H:91:THR:OG1	1:H:193:GLU:OE2	2.28	0.49
1:B:71:TRP:CE3	1:B:75:VAL:HG11	2.48	0.49
1:E:16:TYR:OH	1:E:195:THR:HB	2.12	0.49
1:E:154:VAL:O	1:E:158:MET:HG3	2.12	0.49
1:H:65:ASP:HB3	1:H:68:THR:CG2	2.38	0.49
1:B:236:LEU:HD22	1:E:94:LEU:HD12	1.95	0.49
1:E:239:LEU:HD22	4:E:800:TRU:CL20	2.43	0.49
1:B:121:ILE:CG1	1:B:133:ILE:HD13	2.43	0.49
1:B:123:SER:O	1:B:126:ASP:HB2	2.13	0.49
1:B:135:TYR:HA	1:B:189:ALA:O	2.12	0.49
1:H:107:MET:SD	1:H:195:THR:HG21	2.53	0.49
1:B:15:PRO:HB3	1:B:199:TYR:CE1	2.48	0.48
1:E:60:LYS:HD3	1:E:140:SER:OG	2.12	0.48
1:B:6:VAL:HG13	1:B:84:ASP:HB2	1.94	0.48
1:E:16:TYR:CE1	1:E:255:TRP:HH2	2.31	0.48
1:H:68:THR:HG23	1:H:70:ILE:H	1.78	0.48
1:H:99:VAL:HG23	1:H:100:ILE:HG23	1.94	0.48
1:H:168:SER:HA	5:H:274:HOH:O	2.13	0.48
1:H:105:PRO:HA	1:H:220:TYR:O	2.12	0.48
1:H:134:ALA:HA	1:H:161:TYR:OH	2.13	0.48
1:H:181:VAL:CG2	1:H:190:TYR:HB2	2.43	0.48
1:B:246:LEU:HG	1:B:250:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:MET:C	1:B:20:LYS:O	2.52	0.48
1:B:215:LEU:N	1:B:215:LEU:CD1	2.77	0.48
1:E:109:LEU:C	1:E:109:LEU:HD22	2.33	0.48
1:E:115:ILE:HB	1:E:119:THR:HB	1.94	0.48
1:H:20:LYS:O	1:H:23:HIS:ND1	2.46	0.48
1:H:44:ALA:HB1	1:H:49:PHE:O	2.13	0.48
1:B:39:LEU:O	1:B:43:ILE:HG12	2.13	0.48
1:H:128:SER:HB3	1:H:158:MET:HG3	1.96	0.48
1:E:62:GLY:HA2	1:E:72:ASN:OD1	2.13	0.48
1:E:64:ARG:HH21	1:E:71:TRP:HE1	1.61	0.48
1:H:23:HIS:HA	1:H:26:LEU:HD13	1.94	0.48
1:H:136:GLY:HA3	1:H:169:VAL:O	2.14	0.48
1:E:105:PRO:HB2	4:E:800:TRU:O16	2.14	0.48
1:B:204:LYS:HG3	1:B:260:GLU:HB3	1.96	0.48
1:E:134:ALA:N	1:E:187:LYS:O	2.42	0.48
1:H:86:ALA:HB3	1:H:223:ALA:HB3	1.94	0.48
1:B:104:LYS:HG3	1:E:92:ILE:HG21	1.95	0.47
1:E:215:LEU:N	1:E:215:LEU:CD1	2.76	0.47
1:H:106:PHE:CZ	1:H:220:TYR:HB3	2.49	0.47
1:B:141:GLY:O	1:B:145:GLU:HG2	2.14	0.47
1:E:35:TYR:CD1	1:E:250:LEU:HB3	2.49	0.47
1:H:109:LEU:N	1:H:109:LEU:HD13	2.29	0.47
1:E:91:THR:OG1	1:E:193:GLU:OE2	2.30	0.47
1:H:156:ASP:OD1	1:H:156:ASP:C	2.53	0.47
1:B:47:CYS:HB2	1:B:49:PHE:CE2	2.49	0.47
1:H:10:THR:OG1	1:H:17:VAL:HG21	2.13	0.47
1:B:22:ASN:OD1	1:B:26:LEU:CD1	2.61	0.47
1:E:64:ARG:NH2	1:E:71:TRP:HE1	2.12	0.47
1:H:193:GLU:OE1	2:H:400:GLU:N	2.48	0.47
1:E:65:ASP:HB3	1:E:68:THR:CG2	2.30	0.47
1:E:253:LYS:HE2	1:E:254:TRP:CZ2	2.50	0.47
1:H:68:THR:CG2	1:H:70:ILE:HB	2.44	0.47
1:B:109:LEU:HD22	1:B:109:LEU:C	2.36	0.47
1:E:101:ASP:O	1:E:223:ALA:HA	2.15	0.46
1:H:10:THR:HA	1:H:74:MET:SD	2.55	0.46
1:H:111:ILE:CD1	1:H:146:PHE:CG	2.98	0.46
1:B:135:TYR:HB3	1:B:189:ALA:HB3	1.96	0.46
1:E:35:TYR:CZ	1:E:107:MET:CE	2.98	0.46
1:H:88:ALA:O	1:H:90:LEU:N	2.46	0.46
1:B:6:VAL:O	1:B:51:TYR:HA	2.15	0.46
1:B:40:ALA:HA	1:B:87:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:THR:CG2	1:E:70:ILE:HB	2.45	0.46
1:E:180:ARG:O	1:E:184:SER:HB3	2.15	0.46
1:E:180:ARG:HG2	1:E:188:TYR:CD2	2.51	0.46
1:B:89:PRO:O	2:B:400:GLU:N	2.49	0.46
1:E:61:TYR:HE1	1:E:89:PRO:HG2	1.81	0.46
1:E:108:SER:OG	4:E:800:TRU:H7	2.16	0.46
1:H:65:ASP:O	1:H:69:LYS:N	2.39	0.46
1:H:113:ILE:HG22	1:H:115:ILE:HG23	1.97	0.46
1:B:178:VAL:HG21	1:B:200:ILE:HG13	1.97	0.46
1:E:16:TYR:OH	1:E:220:TYR:HE2	1.97	0.46
1:H:110:GLY:HA3	1:H:214:ASN:CB	2.44	0.46
1:B:234:VAL:O	1:B:238:VAL:HG23	2.16	0.46
1:B:85:ILE:HD11	1:B:222:ILE:CG2	2.47	0.45
1:B:134:ALA:O	1:B:188:TYR:HA	2.16	0.45
1:E:180:ARG:HG2	1:E:188:TYR:CG	2.51	0.45
1:H:61:TYR:HA	1:H:74:MET:HE3	1.99	0.45
1:H:23:HIS:HE1	5:H:323:HOH:O	1.98	0.45
1:H:20:LYS:HE3	1:H:32:TYR:O	2.17	0.45
1:E:65:ASP:OD1	1:E:66:ALA:O	2.34	0.45
1:B:56:VAL:HG23	1:B:77:GLU:CG	2.46	0.45
1:B:8:VAL:HG22	1:B:85:ILE:CG2	2.46	0.45
1:B:171:VAL:HB	1:B:176:GLU:HB3	1.99	0.45
1:B:239:LEU:HD23	1:B:239:LEU:HA	1.63	0.45
1:E:42:GLU:HG3	1:E:246:LEU:CD2	2.46	0.45
1:H:145:GLU:HA	1:H:145:GLU:OE1	2.16	0.45
1:E:42:GLU:OE2	1:E:45:LYS:HD2	2.12	0.45
1:H:25:MET:HE3	1:H:25:MET:H	1.82	0.45
1:B:62:GLY:HA3	1:B:75:VAL:CG2	2.46	0.45
1:B:247:LEU:C	4:B:800:TRU:CL11	2.92	0.45
1:E:121:ILE:HG12	1:E:133:ILE:HD13	1.98	0.45
1:H:23:HIS:O	1:H:26:LEU:HB2	2.16	0.45
1:B:64:ARG:HG2	1:B:69:LYS:HA	1.99	0.44
1:B:99:VAL:HG23	1:B:100:ILE:HG23	1.99	0.44
1:B:144:LYS:HE2	1:B:148:ARG:NH2	2.32	0.44
1:E:4:LYS:HE3	1:E:4:LYS:HB3	1.80	0.44
1:H:8:VAL:HG11	1:H:87:ILE:HD12	1.98	0.44
1:B:90:LEU:O	1:B:220:TYR:HA	2.17	0.44
1:B:119:THR:HA	1:B:120:PRO:HD3	1.84	0.44
1:E:35:TYR:HA	1:E:254:TRP:CD1	2.53	0.44
1:H:124:ALA:HB1	1:H:158:MET:SD	2.58	0.44
1:H:16:TYR:OH	1:H:195:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:GLU:C	1:H:31:ARG:HH11	2.21	0.44
1:E:101:ASP:OD1	1:E:226:LYS:HD2	2.17	0.44
1:H:65:ASP:OD1	1:H:66:ALA:O	2.36	0.44
1:H:165:ALA:CB	1:H:169:VAL:HG13	2.45	0.44
1:B:94:LEU:HB3	1:E:243:GLU:OE1	2.18	0.44
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.77	0.44
1:B:119:THR:O	1:B:121:ILE:N	2.37	0.44
1:H:96:ARG:O	1:H:100:ILE:HG12	2.18	0.44
1:H:215:LEU:HD12	1:H:215:LEU:N	2.32	0.44
1:B:154:VAL:O	1:B:158:MET:HG3	2.18	0.44
1:B:135:TYR:O	1:B:162:MET:HG2	2.17	0.44
1:E:111:ILE:O	1:E:215:LEU:HD13	2.18	0.44
1:H:143:THR:O	1:H:146:PHE:HB3	2.17	0.44
1:H:204:LYS:HA	1:H:206:CYS:SG	2.58	0.44
1:B:251:LYS:O	1:B:255:TRP:HB2	2.18	0.43
1:E:64:ARG:NH2	1:E:99:VAL:HG11	2.33	0.43
1:H:113:ILE:HD11	1:H:124:ALA:N	2.33	0.43
1:B:16:TYR:HA	1:B:35:TYR:HB3	2.00	0.43
1:H:42:GLU:OE2	1:H:45:LYS:CD	2.66	0.43
1:E:14:SER:HA	1:E:15:PRO:HA	1.82	0.43
1:E:90:LEU:HD23	1:E:223:ALA:HB2	2.01	0.43
1:B:28:GLY:O	1:B:31:ARG:NH1	2.51	0.43
1:B:56:VAL:HG21	1:B:73:GLY:C	2.37	0.43
1:B:222:ILE:HD12	1:B:238:VAL:HG22	2.00	0.43
1:H:123:SER:HB2	5:H:325:HOH:O	2.18	0.43
1:B:115:ILE:HB	1:B:119:THR:HB	2.01	0.43
1:E:162:MET:HB3	1:E:170:PHE:CZ	2.53	0.43
1:H:119:THR:HA	1:H:120:PRO:HD3	1.81	0.43
1:B:6:VAL:HG13	1:B:84:ASP:CB	2.49	0.43
1:E:6:VAL:HG13	1:E:84:ASP:HB2	2.01	0.43
1:B:109:LEU:HD13	1:B:109:LEU:N	2.34	0.43
1:E:68:THR:HG23	1:E:70:ILE:N	2.23	0.43
1:E:115:ILE:CD1	1:E:211:VAL:HG11	2.48	0.43
1:E:134:ALA:O	1:E:188:TYR:HA	2.18	0.43
1:B:159:TRP:HA	1:B:162:MET:HE2	2.01	0.43
1:B:241:LEU:CG	1:B:246:LEU:HD23	2.27	0.43
1:H:107:MET:O	1:H:219:GLY:HA2	2.19	0.43
1:B:65:ASP:O	1:B:69:LYS:N	2.51	0.43
1:E:114:MET:HE1	1:E:178:VAL:HG22	2.00	0.43
1:E:20:LYS:O	1:E:21:LYS:C	2.57	0.43
1:E:147:PHE:CE2	1:E:191:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:ARG:HG2	1:H:188:TYR:CG	2.54	0.43
1:B:15:PRO:HG2	1:B:255:TRP:CZ3	2.54	0.42
1:E:44:ALA:O	1:E:48:GLY:N	2.52	0.42
1:H:26:LEU:O	1:H:31:ARG:HD3	2.19	0.42
1:B:22:ASN:O	1:B:25:MET:N	2.51	0.42
1:B:35:TYR:HA	1:B:254:TRP:CD1	2.53	0.42
1:B:47:CYS:HB2	1:B:49:PHE:CD2	2.53	0.42
1:B:88:ALA:O	1:B:90:LEU:N	2.49	0.42
1:B:104:LYS:HB3	4:B:800:TRU:CL20	2.56	0.42
1:H:42:GLU:O	1:H:46:HIS:CD2	2.72	0.42
1:H:148:ARG:HA	1:H:159:TRP:CE2	2.54	0.42
1:H:198:GLU:HG3	1:H:210:LYS:HZ1	1.83	0.42
1:H:16:TYR:CE1	1:H:255:TRP:HH2	2.38	0.42
1:H:21:LYS:O	1:H:22:ASN:HB2	2.20	0.42
1:H:66:ALA:O	1:H:67:ASP:CB	2.68	0.42
1:B:240:LYS:O	1:B:244:GLN:HG2	2.19	0.42
1:E:20:LYS:O	1:E:23:HIS:ND1	2.50	0.42
1:E:35:TYR:CE1	1:E:250:LEU:HB3	2.55	0.42
1:E:52:LYS:HE2	1:E:52:LYS:HB3	1.70	0.42
1:E:119:THR:HA	1:E:120:PRO:HD3	1.78	0.42
1:B:61:TYR:CE1	1:B:89:PRO:HG2	2.53	0.42
1:B:62:GLY:HA3	1:B:75:VAL:HG23	2.01	0.42
1:E:113:ILE:HG12	1:E:191:LEU:HD23	2.01	0.42
1:H:6:VAL:HG21	1:H:49:PHE:CD1	2.55	0.42
1:H:64:ARG:HG3	1:H:69:LYS:O	2.19	0.42
1:B:23:HIS:O	1:B:23:HIS:CG	2.72	0.42
1:B:180:ARG:HG2	1:B:188:TYR:CD2	2.54	0.42
1:B:104:LYS:HE3	1:E:103:SER:O	2.18	0.42
1:E:105:PRO:HB3	1:E:219:GLY:HA3	2.01	0.42
1:H:89:PRO:HA	1:H:220:TYR:CG	2.55	0.42
1:H:134:ALA:O	1:H:188:TYR:HA	2.20	0.41
1:B:89:PRO:HB2	1:B:196:MET:CE	2.50	0.41
1:B:116:LYS:HD2	1:B:182:ARG:HA	2.02	0.41
1:E:70:ILE:HA	1:E:80:TYR:OH	2.20	0.41
1:E:192:LEU:HD23	1:E:192:LEU:H	1.85	0.41
1:H:88:ALA:C	1:H:90:LEU:N	2.73	0.41
1:B:56:VAL:HB	1:B:74:MET:HG2	2.02	0.41
1:E:56:VAL:HG13	1:E:59:GLY:HA2	2.03	0.41
1:E:141:GLY:O	1:E:145:GLU:HG2	2.21	0.41
1:H:115:ILE:HD11	1:H:211:VAL:HG11	2.02	0.41
1:B:162:MET:HE2	1:B:162:MET:HB2	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD12	1:B:246:LEU:O	2.21	0.41
1:E:19:MET:HB3	1:E:23:HIS:CG	2.55	0.41
1:E:133:ILE:HG12	1:E:186:GLY:O	2.20	0.41
1:H:62:GLY:HA2	1:H:72:ASN:O	2.21	0.41
1:B:114:MET:HE3	1:B:192:LEU:HD11	2.03	0.41
1:E:64:ARG:HD3	1:E:69:LYS:HD2	2.03	0.41
1:H:64:ARG:HB2	1:H:71:TRP:CE2	2.56	0.41
1:H:241:LEU:HA	1:H:241:LEU:HD12	1.82	0.41
1:E:25:MET:HE3	1:E:25:MET:HB2	1.96	0.41
1:B:110:GLY:HA3	1:B:214:ASN:CB	2.49	0.41
1:B:135:TYR:CZ	1:B:161:TYR:CD2	3.09	0.41
1:B:148:ARG:HA	1:B:159:TRP:CD2	2.54	0.41
1:B:159:TRP:O	1:B:160:THR:C	2.59	0.41
1:E:6:VAL:O	1:E:51:TYR:HA	2.21	0.41
1:E:114:MET:SD	1:E:178:VAL:HG22	2.61	0.41
1:H:24:GLU:H	1:H:24:GLU:CD	2.23	0.41
1:H:68:THR:HG23	1:H:70:ILE:HB	2.02	0.41
1:H:85:ILE:HD11	1:H:222:ILE:HG21	2.03	0.41
1:B:240:LYS:HZ2	1:B:244:GLN:HE21	1.65	0.41
1:E:13:GLU:HG2	1:E:196:MET:HE2	2.02	0.41
1:E:234:VAL:O	1:E:238:VAL:HG23	2.21	0.40
1:B:78:LEU:HD11	1:B:86:ALA:HB2	2.03	0.40
4:B:800:TRU:CL11	4:B:800:TRU:O13	2.76	0.40
1:H:148:ARG:HA	1:H:159:TRP:CD2	2.57	0.40
1:H:230:LEU:HA	1:H:230:LEU:HD23	1.76	0.40
1:H:11:ILE:HD13	1:H:61:TYR:CE2	2.55	0.40
1:H:115:ILE:HD11	1:H:211:VAL:CG1	2.51	0.40
1:H:16:TYR:OH	1:H:220:TYR:HE2	2.04	0.40
1:H:109:LEU:HD13	1:H:109:LEU:H	1.86	0.40
1:H:114:MET:SD	1:H:178:VAL:HG22	2.62	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:OE2	3:H:262:ZN:ZN[4_654]	1.46	0.74
1:B:166:GLU:OE1	1:H:46:HIS:CE1[4_654]	1.52	0.68
1:B:166:GLU:OE1	1:H:46:HIS:NE2[4_654]	1.78	0.42
1:E:23:HIS:NE2	1:H:30:GLU:OE2[3_645]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	256/258 (99%)	245 (96%)	7 (3%)	4 (2%)	9	5
1	E	256/258 (99%)	247 (96%)	7 (3%)	2 (1%)	19	15
1	H	256/258 (99%)	246 (96%)	10 (4%)	0	100	100
All	All	768/774 (99%)	738 (96%)	24 (3%)	6 (1%)	19	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	LYS
1	E	23	HIS
1	B	23	HIS
1	B	67	ASP
1	E	67	ASP
1	B	120	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	201/217 (93%)	193 (96%)	8 (4%)	31	32
1	E	203/217 (94%)	191 (94%)	12 (6%)	19	17
1	H	205/217 (94%)	198 (97%)	7 (3%)	37	39
All	All	609/651 (94%)	582 (96%)	27 (4%)	28	28

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	MET
1	B	30	GLU
1	B	68	THR
1	B	109	LEU
1	B	210	LYS
1	B	241	LEU
1	B	249	LYS
1	B	250	LEU
1	E	4	LYS
1	E	22	ASN
1	E	25	MET
1	E	30	GLU
1	E	31	ARG
1	E	68	THR
1	E	109	LEU
1	E	140	SER
1	E	211	VAL
1	E	217	SER
1	E	241	LEU
1	E	250	LEU
1	H	25	MET
1	H	68	THR
1	H	109	LEU
1	H	156	ASP
1	H	210	LYS
1	H	241	LEU
1	H	250	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	244	GLN
1	E	244	GLN
1	H	22	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLU	B	400	-	8,9,9	1.06	0	10,11,11	1.15	1 (10%)
2	GLU	E	400	-	8,9,9	1.19	1 (12%)	10,11,11	1.16	1 (10%)
4	TRU	E	800	-	21,21,21	6.13	14 (66%)	26,34,34	2.52	4 (15%)
4	TRU	H	800	-	21,21,21	6.14	15 (71%)	26,34,34	2.52	5 (19%)
4	TRU	B	800	-	21,21,21	6.13	14 (66%)	26,34,34	2.51	5 (19%)
2	GLU	H	400	-	8,9,9	1.10	1 (12%)	10,11,11	1.10	2 (20%)

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	GLU	B	400	-	-	1/9/9/9	-
2	GLU	E	400	-	-	2/9/9/9	-
4	TRU	E	800	-	-	6/6/25/25	0/2/2/2
4	TRU	H	800	-	-	6/6/25/25	0/2/2/2
4	TRU	B	800	-	-	0/6/25/25	0/2/2/2
2	GLU	H	400	-	-	1/9/9/9	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	800	TRU	C6-S12	-18.70	1.54	1.77
4	E	800	TRU	C6-S12	-18.66	1.54	1.77
4	B	800	TRU	C6-S12	-18.65	1.54	1.77
4	H	800	TRU	C2-S1	12.47	1.86	1.75
4	B	800	TRU	C2-S1	12.45	1.86	1.75
4	E	800	TRU	C2-S1	12.38	1.86	1.75
4	B	800	TRU	C9-N8	8.10	1.56	1.46
4	H	800	TRU	C9-N8	8.07	1.56	1.46
4	E	800	TRU	C9-N8	8.02	1.56	1.46
4	B	800	TRU	S12-N15	-6.90	1.46	1.60
4	E	800	TRU	S12-N15	-6.88	1.46	1.60
4	H	800	TRU	S12-N15	-6.85	1.46	1.60
4	E	800	TRU	C9-N10	6.26	1.53	1.46
4	H	800	TRU	C9-N10	6.24	1.53	1.46
4	B	800	TRU	C9-N10	6.19	1.53	1.46
4	H	800	TRU	S1-N10	-6.17	1.54	1.62
4	E	800	TRU	S1-N10	-6.14	1.54	1.62
4	B	800	TRU	S1-N10	-6.08	1.54	1.62
4	E	800	TRU	C3-N8	6.05	1.50	1.39
4	B	800	TRU	C3-N8	6.02	1.50	1.39
4	H	800	TRU	C3-N8	6.01	1.50	1.39
4	H	800	TRU	O16-S1	3.19	1.47	1.43
4	E	800	TRU	O16-S1	3.18	1.47	1.43
4	B	800	TRU	O16-S1	3.10	1.47	1.43
4	B	800	TRU	O17-S1	2.98	1.46	1.43
4	E	800	TRU	O17-S1	2.97	1.46	1.43
4	H	800	TRU	O17-S1	2.96	1.46	1.43
4	B	800	TRU	C7-C6	2.88	1.43	1.39
4	E	800	TRU	C7-C6	2.87	1.43	1.39
4	H	800	TRU	C7-C6	2.81	1.43	1.39
4	E	800	TRU	C4-C5	2.54	1.42	1.38
4	H	800	TRU	C4-C5	2.52	1.42	1.38
4	B	800	TRU	C4-C5	2.51	1.42	1.38
2	E	400	GLU	OXT-C	-2.48	1.22	1.30
4	B	800	TRU	C4-C3	2.34	1.43	1.39
4	E	800	TRU	C5-CL11	2.34	1.79	1.73
4	H	800	TRU	C5-CL11	2.33	1.79	1.73
4	B	800	TRU	C5-CL11	2.31	1.79	1.73
4	H	800	TRU	C4-C3	2.30	1.43	1.39
4	H	800	TRU	C7-C2	2.30	1.42	1.39
4	E	800	TRU	C4-C3	2.29	1.43	1.39
4	E	800	TRU	C7-C2	2.27	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	800	TRU	C7-C2	2.22	1.42	1.39
2	H	400	GLU	OXT-C	-2.18	1.23	1.30
4	H	800	TRU	C5-C6	2.01	1.43	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	800	TRU	O16-S1-O17	-8.88	109.40	118.46
4	E	800	TRU	O16-S1-O17	-8.87	109.41	118.46
4	B	800	TRU	O16-S1-O17	-8.85	109.43	118.46
4	H	800	TRU	O13-S12-O14	-5.65	109.47	118.76
4	E	800	TRU	O13-S12-O14	-5.65	109.47	118.76
4	B	800	TRU	O13-S12-O14	-5.63	109.51	118.76
4	B	800	TRU	C2-S1-N10	4.19	108.78	103.43
4	E	800	TRU	C2-S1-N10	4.19	108.78	103.43
4	H	800	TRU	C2-S1-N10	4.17	108.76	103.43
4	E	800	TRU	C5-C6-S12	-2.69	120.08	123.49
4	H	800	TRU	C5-C6-S12	-2.68	120.09	123.49
4	B	800	TRU	C5-C6-S12	-2.66	120.11	123.49
2	B	400	GLU	OXT-C-CA	2.28	121.13	113.38
2	H	400	GLU	OXT-C-CA	2.22	120.93	113.38
2	E	400	GLU	OXT-C-O	-2.10	119.33	124.09
4	H	800	TRU	C6-C5-CL11	-2.06	119.98	121.49
4	B	800	TRU	C6-C5-CL11	-2.05	119.99	121.49
2	H	400	GLU	OXT-C-O	-2.03	119.49	124.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	800	TRU	C5-C6-S12-N15
4	E	800	TRU	C5-C6-S12-O14
4	E	800	TRU	C5-C6-S12-O13
4	H	800	TRU	C5-C6-S12-N15
4	H	800	TRU	C5-C6-S12-O14
4	H	800	TRU	C5-C6-S12-O13
4	E	800	TRU	C7-C6-S12-O14
4	H	800	TRU	C7-C6-S12-O14
4	H	800	TRU	C7-C6-S12-O13
4	H	800	TRU	C7-C6-S12-N15
4	E	800	TRU	C7-C6-S12-O13
4	E	800	TRU	C7-C6-S12-N15

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Mol	Chain	Res	Type	Atoms
2	H	400	GLU	O-C-CA-N
2	E	400	GLU	OE2-CD-CG-CB
2	E	400	GLU	OE1-CD-CG-CB
2	B	400	GLU	O-C-CA-CB

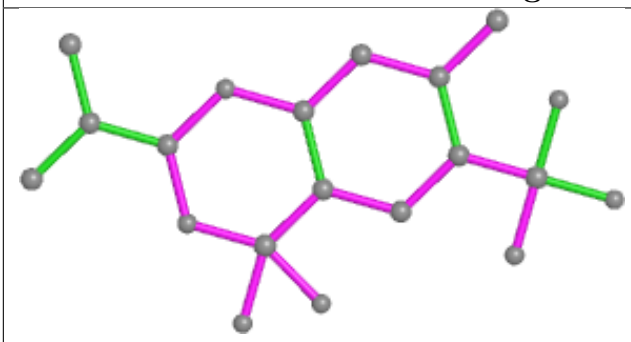
There are no ring outliers.

5 monomers are involved in 18 short contacts:

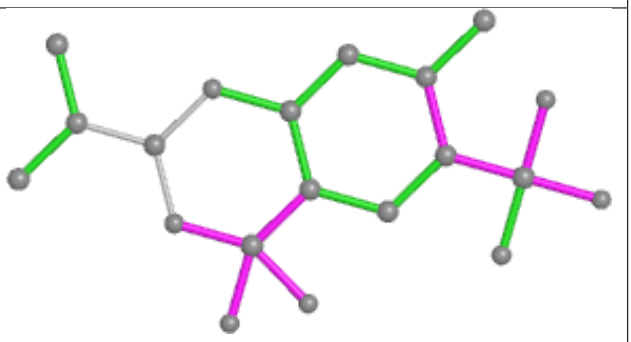
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	GLU	1	0
4	E	800	TRU	7	0
4	H	800	TRU	1	0
4	B	800	TRU	8	0
2	H	400	GLU	1	0

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.

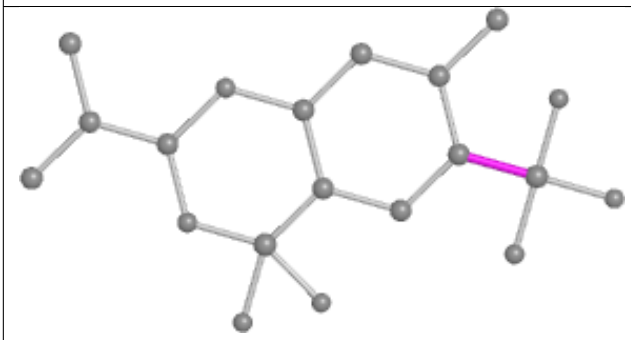
Ligand TRU E 800



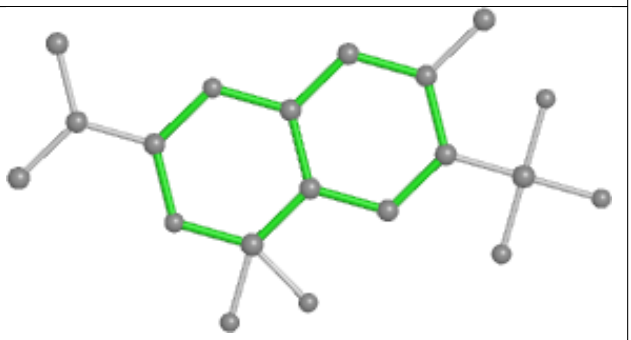
Bond lengths



Bond angles

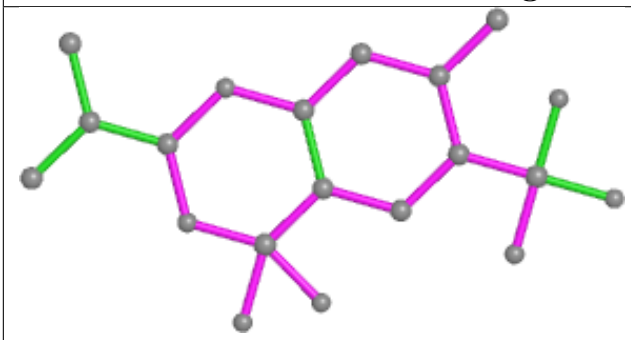


Torsions

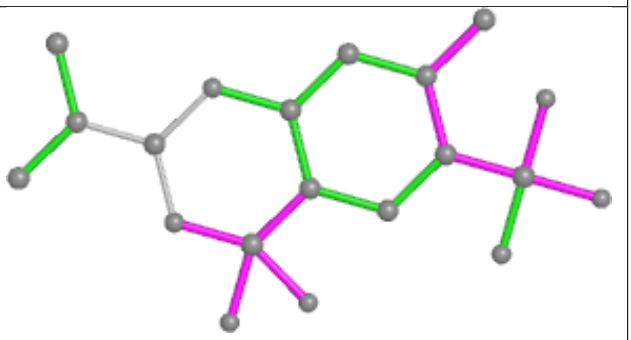


Rings

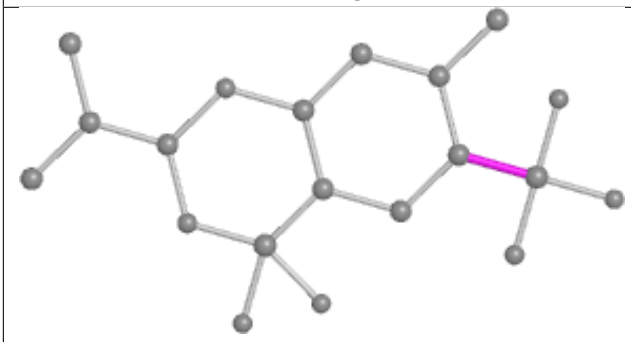
Ligand TRU H 800



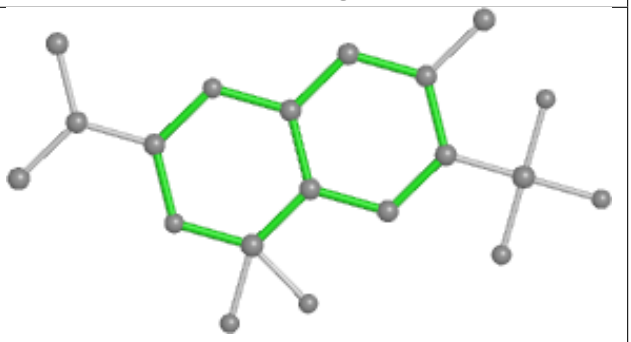
Bond lengths



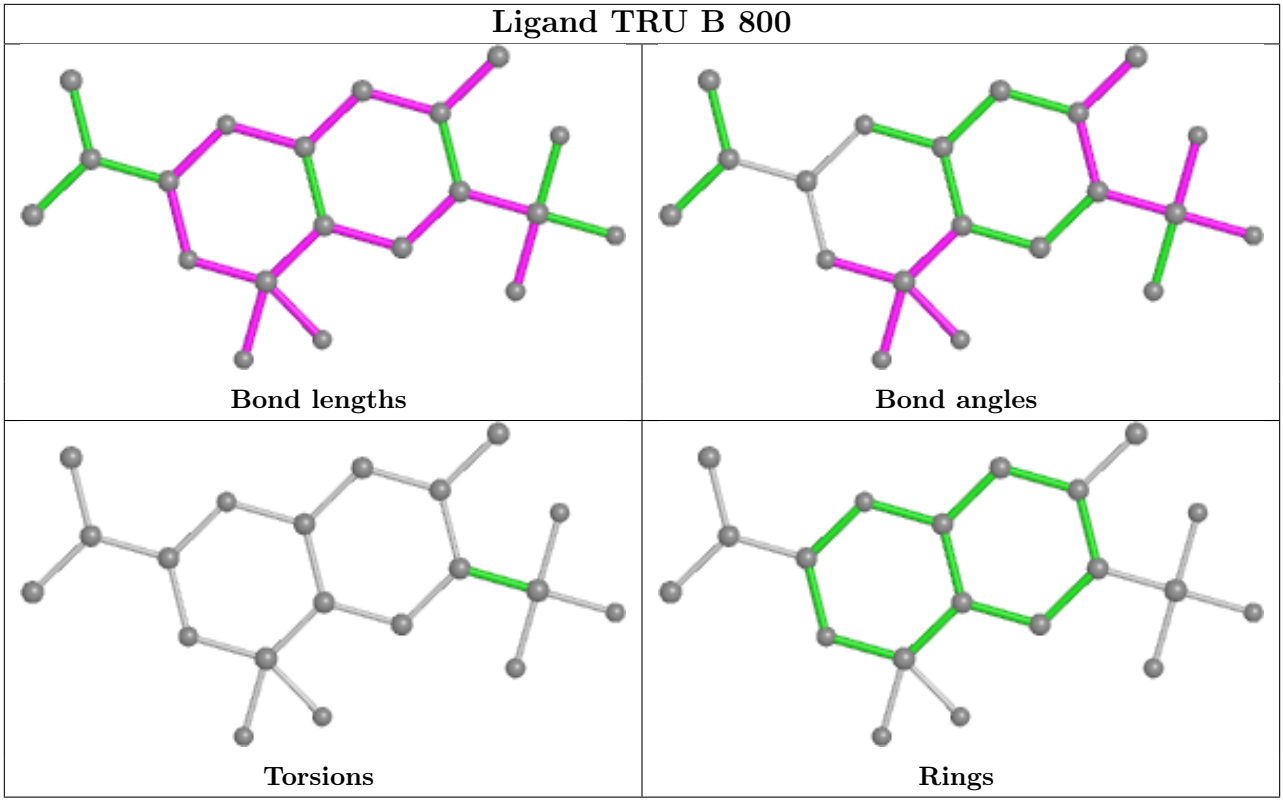
Bond angles



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	B	258/258 (100%)	0.79	29 (11%)	5	6	31, 43, 60, 75	0
1	E	258/258 (100%)	0.76	31 (12%)	4	5	32, 43, 60, 72	0
1	H	258/258 (100%)	0.77	32 (12%)	4	5	29, 39, 58, 70	0
All	All	774/774 (100%)	0.77	92 (11%)	4	5	29, 42, 60, 75	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	67	ASP	7.8
1	B	67	ASP	7.8
1	B	21	LYS	7.1
1	B	24	GLU	6.5
1	B	66	ALA	6.1
1	H	66	ALA	5.8
1	B	22	ASN	4.9
1	E	256	TYR	4.8
1	E	227	GLY	4.7
1	E	258	LYS	4.6
1	E	259	GLY	4.2
1	B	25	MET	4.0
1	E	87	ILE	3.9
1	H	69	LYS	3.8
1	E	191	LEU	3.8
1	H	227	GLY	3.7
1	E	167	PRO	3.7
1	E	257	ASP	3.6
1	B	191	LEU	3.6
1	H	129	LYS	3.5
1	E	4	LYS	3.3
1	E	129	LYS	3.3
1	B	227	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	222	ILE	3.3
1	H	259	GLY	3.2
1	H	192	LEU	3.1
1	E	113	ILE	3.0
1	H	257	ASP	3.0
1	E	151	LYS	3.0
1	B	85	ILE	3.0
1	H	16	TYR	2.9
1	B	204	LYS	2.9
1	H	191	LEU	2.9
1	E	222	ILE	2.8
1	B	190	TYR	2.8
1	B	86	ALA	2.8
1	H	19	MET	2.8
1	H	85	ILE	2.8
1	H	5	THR	2.8
1	B	192	LEU	2.8
1	H	58	ASP	2.7
1	E	166	GLU	2.7
1	H	156	ASP	2.7
1	E	190	TYR	2.7
1	B	20	LYS	2.7
1	E	16	TYR	2.6
1	H	106	PHE	2.6
1	B	135	TYR	2.6
1	H	87	ILE	2.6
1	E	25	MET	2.6
1	H	88	ALA	2.6
1	E	35	TYR	2.5
1	B	106	PHE	2.5
1	E	183	LYS	2.5
1	E	106	PHE	2.5
1	E	202	GLN	2.4
1	B	68	THR	2.4
1	H	143	THR	2.4
1	B	69	LYS	2.4
1	H	68	THR	2.4
1	B	140	SER	2.4
1	E	164	SER	2.4
1	H	220	TYR	2.4
1	H	223	ALA	2.4
1	H	57	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	223	ALA	2.3
1	E	228	SER	2.3
1	E	67	ASP	2.3
1	H	39	LEU	2.3
1	E	136	GLY	2.3
1	H	86	ALA	2.3
1	E	204	LYS	2.3
1	H	136	GLY	2.3
1	H	221	GLY	2.3
1	B	4	LYS	2.2
1	E	68	THR	2.2
1	B	30	GLU	2.2
1	E	5	THR	2.2
1	H	258	LYS	2.2
1	B	87	ILE	2.2
1	B	260	GLU	2.2
1	B	88	ALA	2.1
1	H	27	GLU	2.1
1	B	189	ALA	2.1
1	B	222	ILE	2.1
1	B	168	SER	2.1
1	E	135	TYR	2.1
1	H	135	TYR	2.1
1	B	129	LYS	2.0
1	E	206	CYS	2.0
1	E	45	LYS	2.0
1	H	113	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

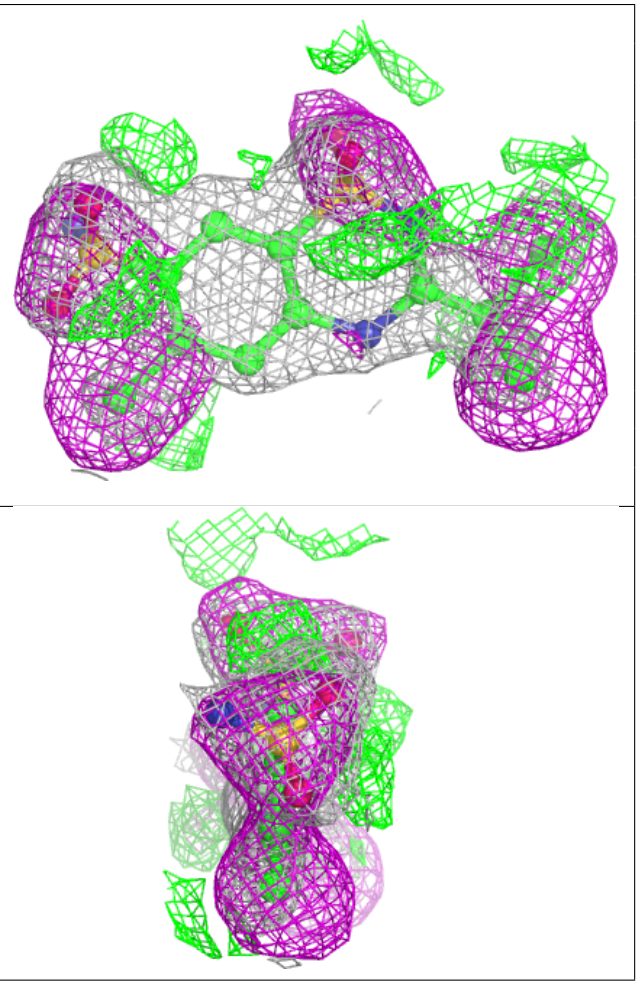
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TRU	H	800	20/20	0.76	0.36	20,20,20,20	0
4	TRU	E	800	20/20	0.77	0.29	20,20,20,20	0
4	TRU	B	800	20/20	0.80	0.39	20,20,20,20	0
3	ZN	H	3	1/1	0.88	0.11	46,46,46,46	0
3	ZN	B	2	1/1	0.91	0.06	45,45,45,45	0
2	GLU	B	400	10/10	0.93	0.16	35,38,41,42	0
2	GLU	H	400	10/10	0.94	0.14	30,34,40,41	0
3	ZN	E	262	1/1	0.94	0.40	40,40,40,40	0
3	ZN	B	1	1/1	0.94	0.11	46,46,46,46	0
3	ZN	H	262	1/1	0.95	0.18	47,47,47,47	0
2	GLU	E	400	10/10	0.95	0.13	35,37,41,42	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.

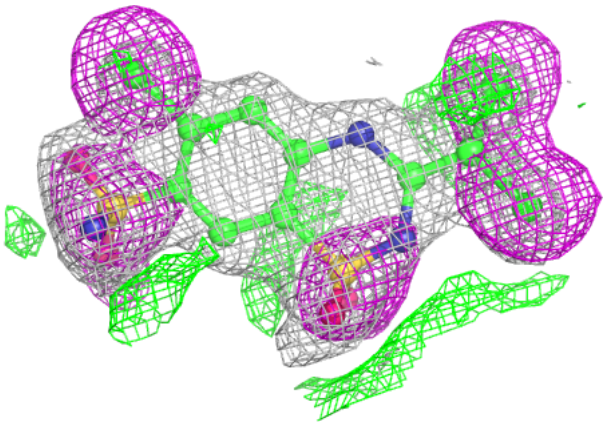
Electron density around TRU H 800:

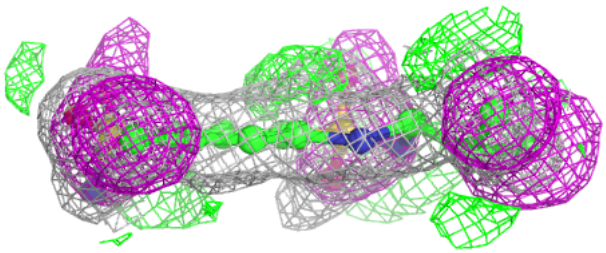
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

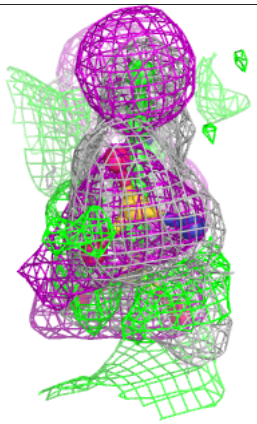


Electron density around TRU E 800:

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

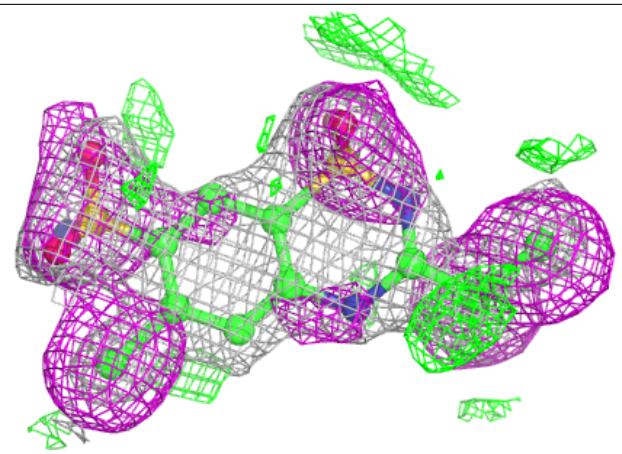


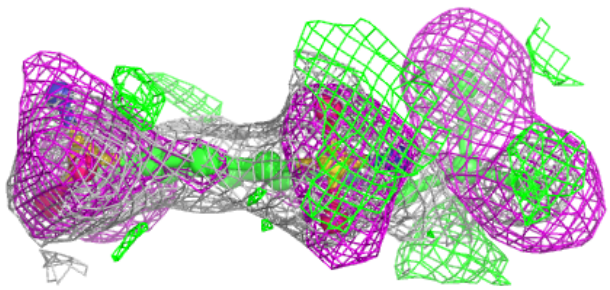


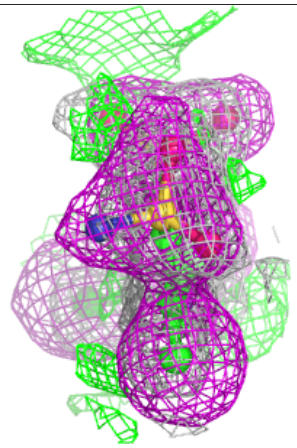


Electron density around TRU B 800:

$2mF_o$-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.