



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 06:05 PM EDT

PDB ID : 3ILT / pdb_00003ilt
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

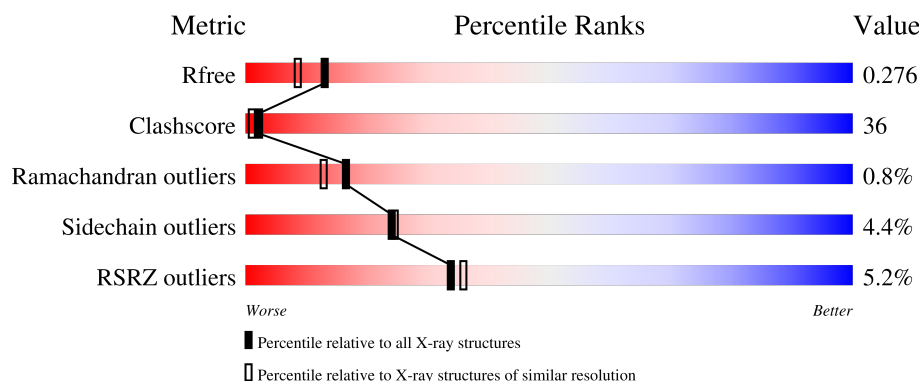
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	258	<div> <div>5%</div> <div>47%</div> <div>48%</div> <div>.</div> </div>
1	E	258	<div> <div>5%</div> <div>48%</div> <div>47%</div> <div>5%</div> </div>
1	H	258	<div> <div>5%</div> <div>48%</div> <div>49%</div> <div>.</div> </div>

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

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.

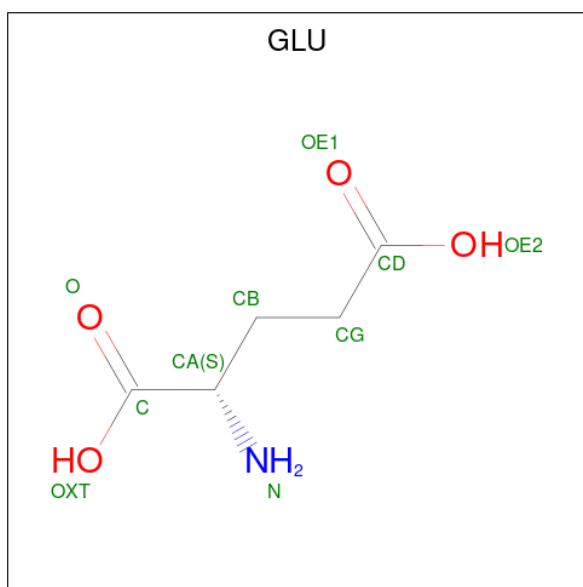
- Molecule 1 is a protein called Glutamate receptor 2.

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

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 (CCD ID: GLU) (formula: C₅H₉NO₄).

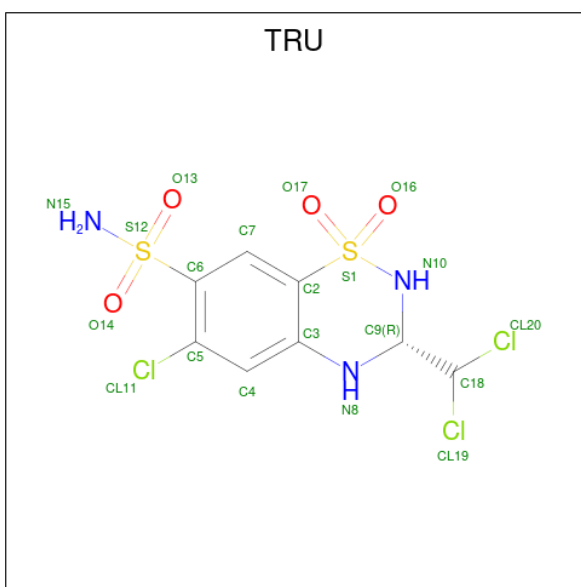


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	H	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

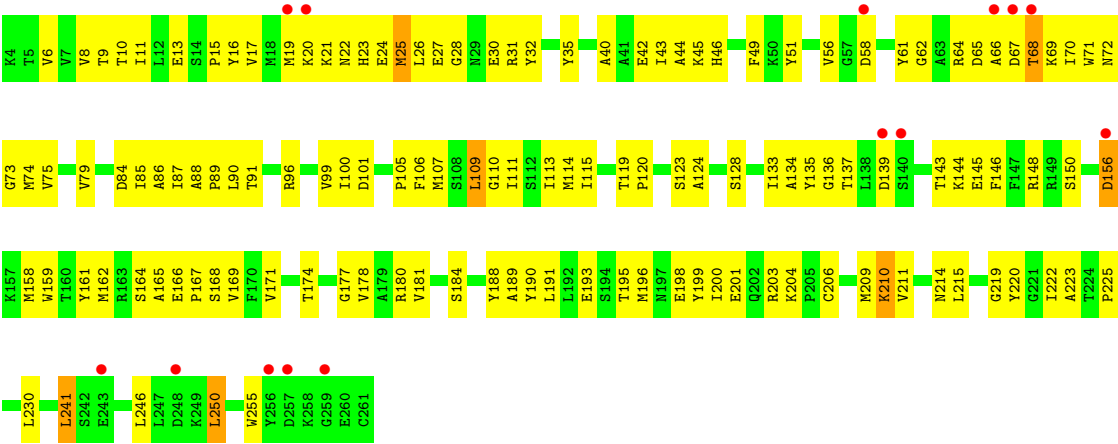
- Molecule 4 is 6-CHLORO-3-(DICHLOROMETHYL)-3,4-DIHYDRO-2H-1,2,4-BENZOTHIADIAZINE-7-SULFONAMIDE 1,1-DIOXIDE (CCD ID: TRU) (formula: C₈H₈Cl₃N₃O₄S₂).



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

- Molecule 5 is water.

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



4 Data and refinement statistics

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) 81.1 (21.23-2.11)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.261 0.238 , 0.276	Depositor DCC
R_{free} test set	2000 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 46.6	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	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: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

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	256/258 (99%)	245 (96%)	7 (3%)	4 (2%)	8	4
1	E	256/258 (99%)	247 (96%)	7 (3%)	2 (1%)	16	13
1	H	256/258 (99%)	246 (96%)	10 (4%)	0	100	100
All	All	768/774 (99%)	738 (96%)	24 (3%)	6 (1%)	16	13

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

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%)	27	28
1	E	203/217 (94%)	191 (94%)	12 (6%)	16	14
1	H	205/217 (94%)	198 (97%)	7 (3%)	32	35
All	All	609/651 (94%)	582 (96%)	27 (4%)	24	24

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 ⓘ

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 oligosaccharides 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
4	TRU	B	800	-	20,21,21	6.15	14 (70%)	27,34,34	2.54	5 (18%)
2	GLU	B	400	-	8,9,9	1.09	1 (12%)	8,11,11	0.96	0
2	GLU	H	400	-	8,9,9	1.14	1 (12%)	8,11,11	0.92	1 (12%)
4	TRU	E	800	-	20,21,21	6.14	14 (70%)	27,34,34	2.55	5 (18%)
2	GLU	E	400	-	8,9,9	1.23	1 (12%)	8,11,11	1.10	1 (12%)
4	TRU	H	800	-	20,21,21	6.16	14 (70%)	27,34,34	2.55	5 (18%)

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
4	TRU	B	800	-	-	0/6/25/25	0/2/2/2
2	GLU	B	400	-	-	1/9/9/9	-
2	GLU	H	400	-	-	1/9/9/9	-
4	TRU	E	800	-	-	6/6/25/25	0/2/2/2
2	GLU	E	400	-	-	3/9/9/9	-
4	TRU	H	800	-	-	6/6/25/25	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	800	TRU	C6-S12	-18.87	1.54	1.77
4	E	800	TRU	C6-S12	-18.83	1.54	1.77
4	B	800	TRU	C6-S12	-18.82	1.54	1.77
4	H	800	TRU	C2-S1	12.31	1.86	1.75
4	B	800	TRU	C2-S1	12.29	1.86	1.75
4	E	800	TRU	C2-S1	12.23	1.86	1.75
4	B	800	TRU	C9-N8	8.35	1.56	1.46
4	H	800	TRU	C9-N8	8.32	1.56	1.46
4	E	800	TRU	C9-N8	8.27	1.56	1.46
4	B	800	TRU	S12-N15	-7.03	1.46	1.60
4	E	800	TRU	S12-N15	-7.00	1.46	1.60
4	H	800	TRU	S12-N15	-6.97	1.46	1.60
4	E	800	TRU	C3-N8	6.12	1.50	1.39
4	B	800	TRU	C3-N8	6.08	1.50	1.39
4	H	800	TRU	C3-N8	6.08	1.50	1.39
4	H	800	TRU	S1-N10	-6.07	1.54	1.62
4	E	800	TRU	S1-N10	-6.04	1.54	1.62
4	B	800	TRU	S1-N10	-5.99	1.54	1.62
4	H	800	TRU	O16-S1	3.11	1.47	1.43
4	E	800	TRU	O16-S1	3.10	1.47	1.43
4	B	800	TRU	O16-S1	3.02	1.47	1.43
4	B	800	TRU	O17-S1	2.91	1.46	1.43
4	E	800	TRU	O17-S1	2.89	1.46	1.43
4	H	800	TRU	O17-S1	2.89	1.46	1.43
4	B	800	TRU	C7-C6	2.66	1.43	1.39
4	E	800	TRU	C7-C6	2.65	1.43	1.39
4	H	800	TRU	C7-C6	2.60	1.43	1.39
2	E	400	GLU	OXT-C	-2.58	1.22	1.30
4	E	800	TRU	C4-C5	2.52	1.42	1.38
4	H	800	TRU	C4-C5	2.50	1.42	1.38
4	B	800	TRU	C4-C5	2.49	1.42	1.38
4	E	800	TRU	C5-CL11	2.35	1.79	1.73
4	H	800	TRU	C5-CL11	2.34	1.79	1.73
4	B	800	TRU	C5-CL11	2.33	1.79	1.73
4	B	800	TRU	C4-C3	2.31	1.43	1.39
2	H	400	GLU	OXT-C	-2.27	1.23	1.30
4	H	800	TRU	C4-C3	2.27	1.43	1.39
4	E	800	TRU	C4-C3	2.27	1.43	1.39
4	H	800	TRU	C7-C2	2.12	1.42	1.39
4	E	800	TRU	C7-C2	2.10	1.42	1.39
4	H	800	TRU	C5-C6	2.10	1.43	1.40
4	B	800	TRU	C5-C6	2.07	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	800	TRU	C7-C2	2.05	1.42	1.39
2	B	400	GLU	OXT-C	-2.05	1.24	1.30
4	E	800	TRU	C5-C6	2.02	1.42	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	800	TRU	O16-S1-O17	-8.88	109.40	118.44
4	E	800	TRU	O16-S1-O17	-8.87	109.41	118.44
4	B	800	TRU	O16-S1-O17	-8.85	109.43	118.44
4	H	800	TRU	O13-S12-O14	-6.07	109.47	118.80
4	E	800	TRU	O13-S12-O14	-6.06	109.47	118.80
4	B	800	TRU	O13-S12-O14	-6.04	109.51	118.80
4	B	800	TRU	C2-S1-N10	4.41	108.78	103.42
4	E	800	TRU	C2-S1-N10	4.41	108.78	103.42
4	H	800	TRU	C2-S1-N10	4.39	108.76	103.42
4	E	800	TRU	C5-C6-S12	-2.83	120.08	123.47
4	H	800	TRU	C5-C6-S12	-2.81	120.09	123.47
4	B	800	TRU	C5-C6-S12	-2.80	120.11	123.47
4	H	800	TRU	C6-C5-CL11	-2.12	119.98	121.52
4	B	800	TRU	C6-C5-CL11	-2.11	119.99	121.52
2	E	400	GLU	OXT-C-O	-2.09	119.33	124.08
4	E	800	TRU	C6-C5-CL11	-2.06	120.03	121.52
2	H	400	GLU	OXT-C-O	-2.02	119.49	124.08

There are no chirality outliers.

All (17) 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
2	H	400	GLU	O-C-CA-N

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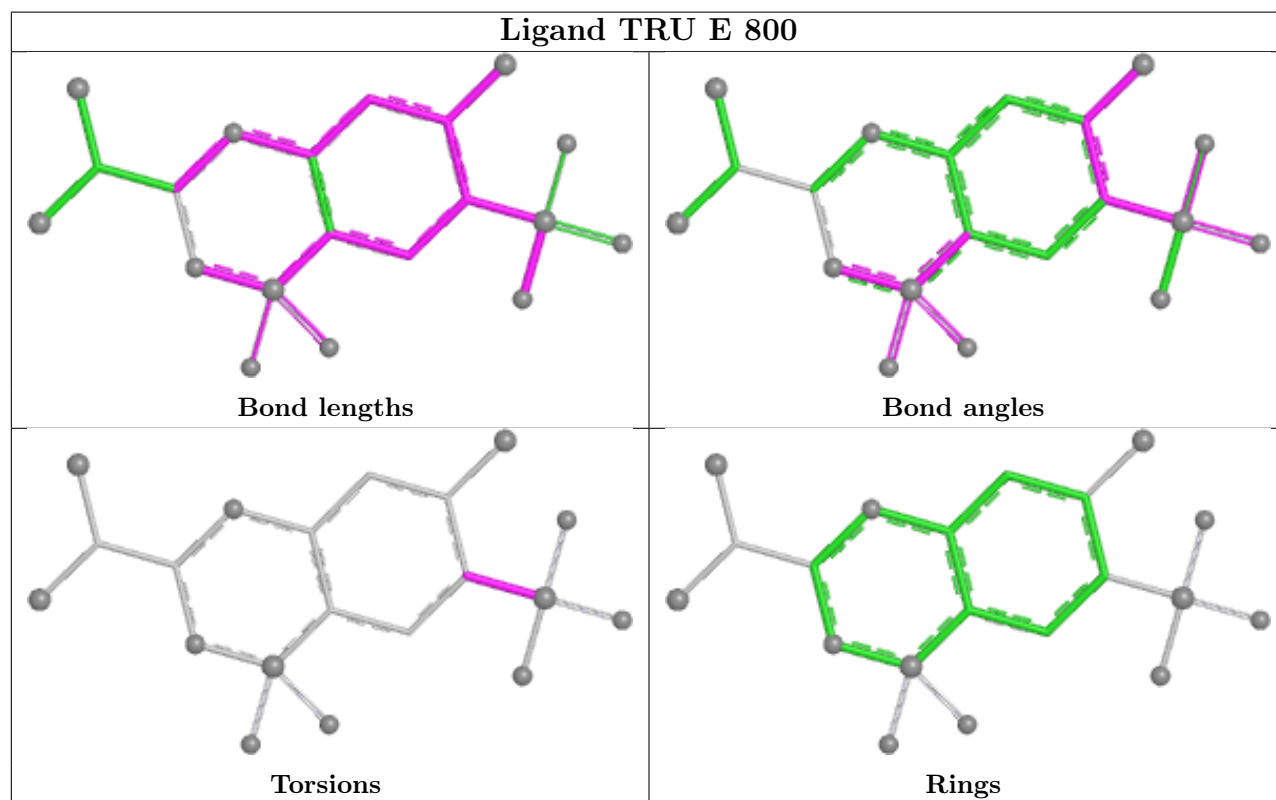
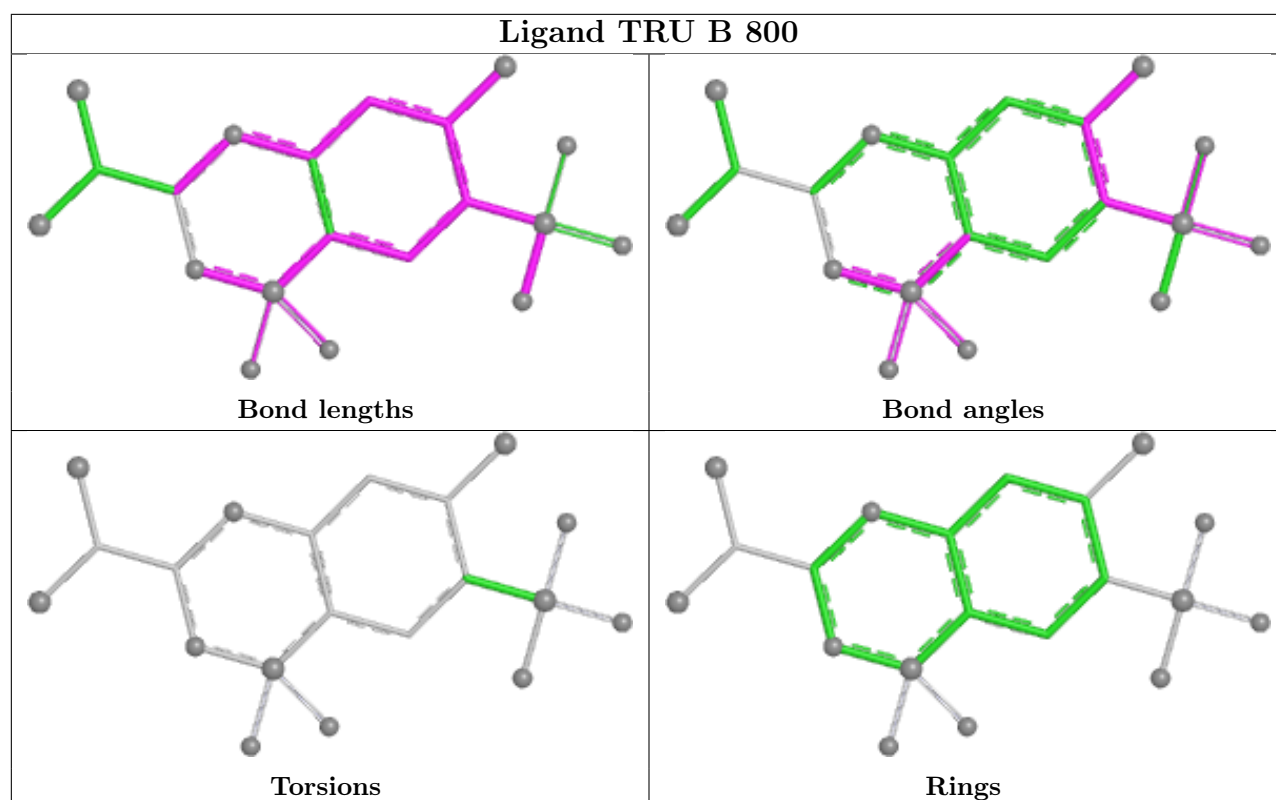
Mol	Chain	Res	Type	Atoms
2	E	400	GLU	OE2-CD-CG-CB
2	E	400	GLU	OE1-CD-CG-CB
2	B	400	GLU	O-C-CA-CB
2	E	400	GLU	O-C-CA-CB

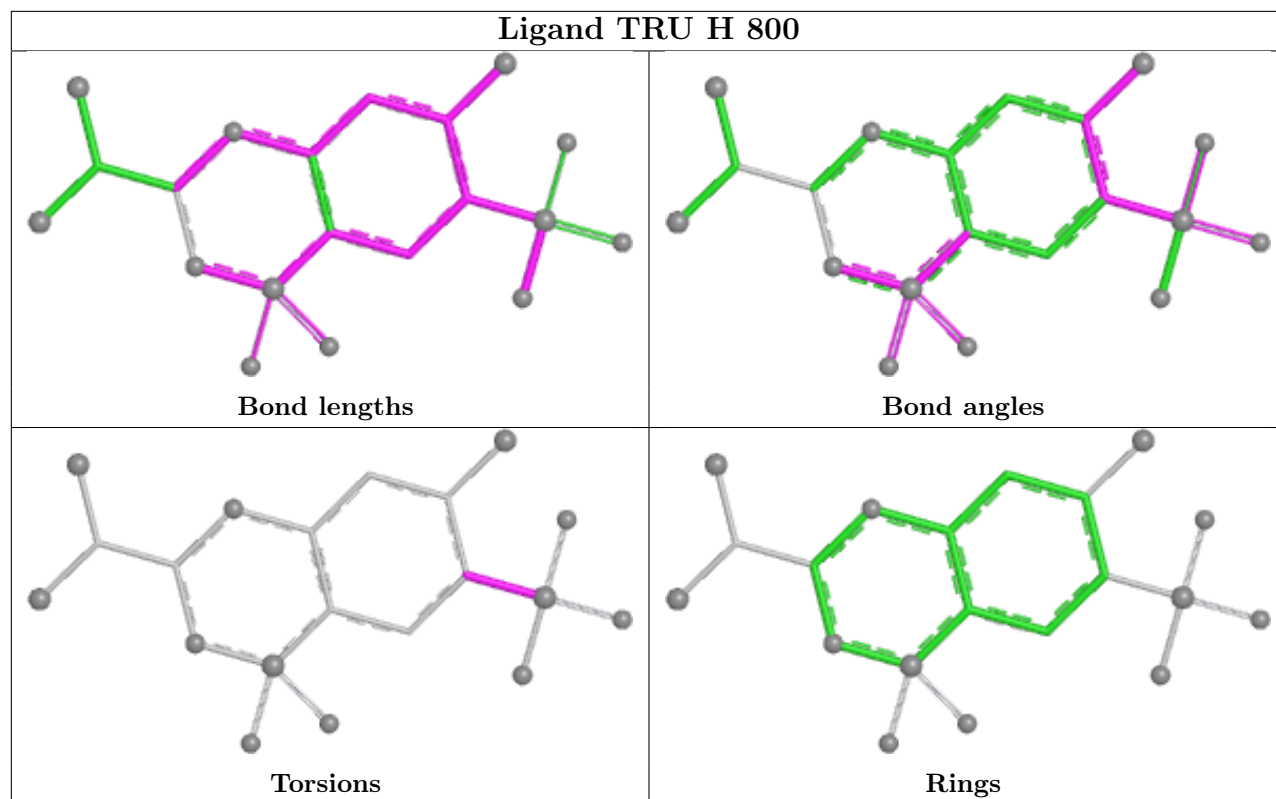
There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800	TRU	8	0
2	B	400	GLU	1	0
2	H	400	GLU	1	0
4	E	800	TRU	7	0
4	H	800	TRU	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	258/258 (100%)	0.61	13 (5%) 35 37	31, 43, 60, 75	0
1	E	258/258 (100%)	0.61	13 (5%) 35 37	32, 43, 60, 72	0
1	H	258/258 (100%)	0.55	14 (5%) 32 35	29, 39, 58, 70	0
All	All	774/774 (100%)	0.59	40 (5%) 34 36	29, 42, 60, 75	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	GLU	7.6
1	B	67	ASP	5.8
1	H	67	ASP	4.8
1	H	156	ASP	4.3
1	E	256	TYR	4.0
1	B	25	MET	3.8
1	E	227	GLY	3.8
1	B	21	LYS	3.7
1	H	66	ALA	3.4
1	E	259	GLY	3.4
1	H	20	LYS	3.2
1	E	206	CYS	3.0
1	B	66	ALA	3.0
1	H	19	MET	2.8
1	B	20	LYS	2.7
1	E	139	ASP	2.7
1	B	22	ASN	2.7
1	E	67	ASP	2.6
1	E	258	LYS	2.6
1	E	66	ALA	2.6
1	H	243	GLU	2.6
1	H	140	SER	2.6
1	B	140	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	23	HIS	2.6
1	H	139	ASP	2.5
1	E	25	MET	2.4
1	B	68	THR	2.4
1	B	211	VAL	2.4
1	H	68	THR	2.3
1	H	257	ASP	2.3
1	E	131	THR	2.3
1	H	256	TYR	2.3
1	H	58	ASP	2.2
1	E	261	CYS	2.1
1	B	156	ASP	2.1
1	B	160	THR	2.1
1	H	259	GLY	2.1
1	E	4	LYS	2.0
1	E	68	THR	2.0
1	H	248	ASP	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.

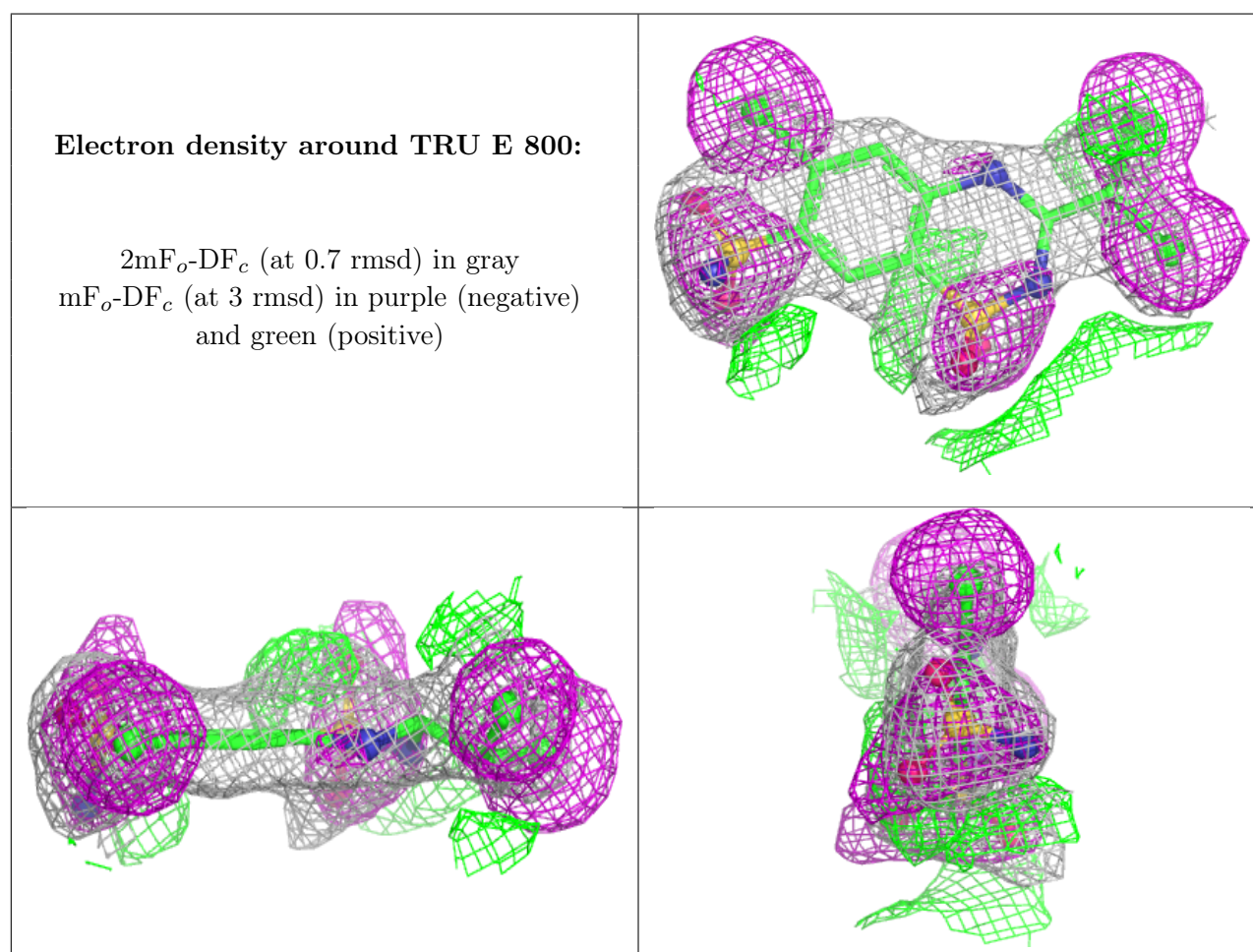
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	TRU	E	800	20/20	0.69	0.20	20,20,20,20	0
4	TRU	H	800	20/20	0.69	0.19	20,20,20,20	0
4	TRU	B	800	20/20	0.70	0.19	20,20,20,20	0
3	ZN	H	3	1/1	0.86	0.10	46,46,46,46	0
3	ZN	E	262	1/1	0.87	0.35	40,40,40,40	0
3	ZN	B	1	1/1	0.88	0.10	46,46,46,46	0

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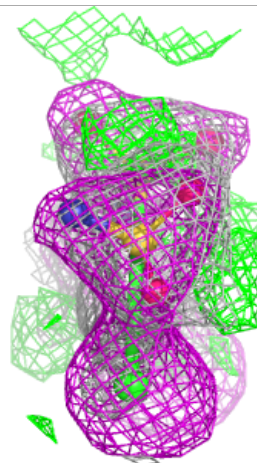
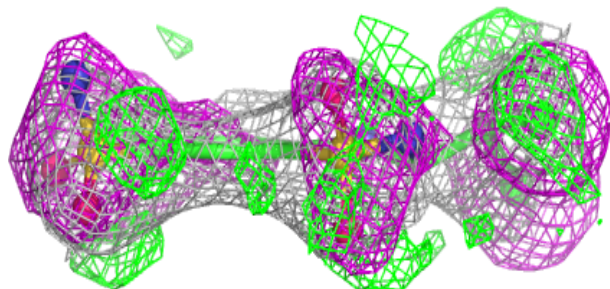
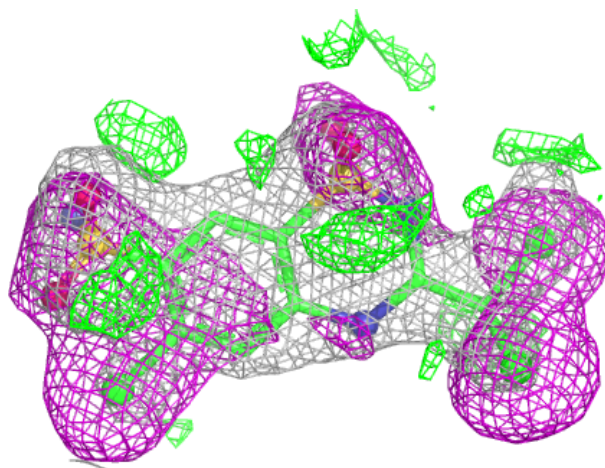
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	H	262	1/1	0.91	0.15	47,47,47,47	0
2	GLU	H	400	10/10	0.92	0.09	30,34,40,41	0
2	GLU	B	400	10/10	0.92	0.08	35,38,41,42	0
3	ZN	B	2	1/1	0.92	0.08	45,45,45,45	0
2	GLU	E	400	10/10	0.94	0.07	35,37,41,42	0

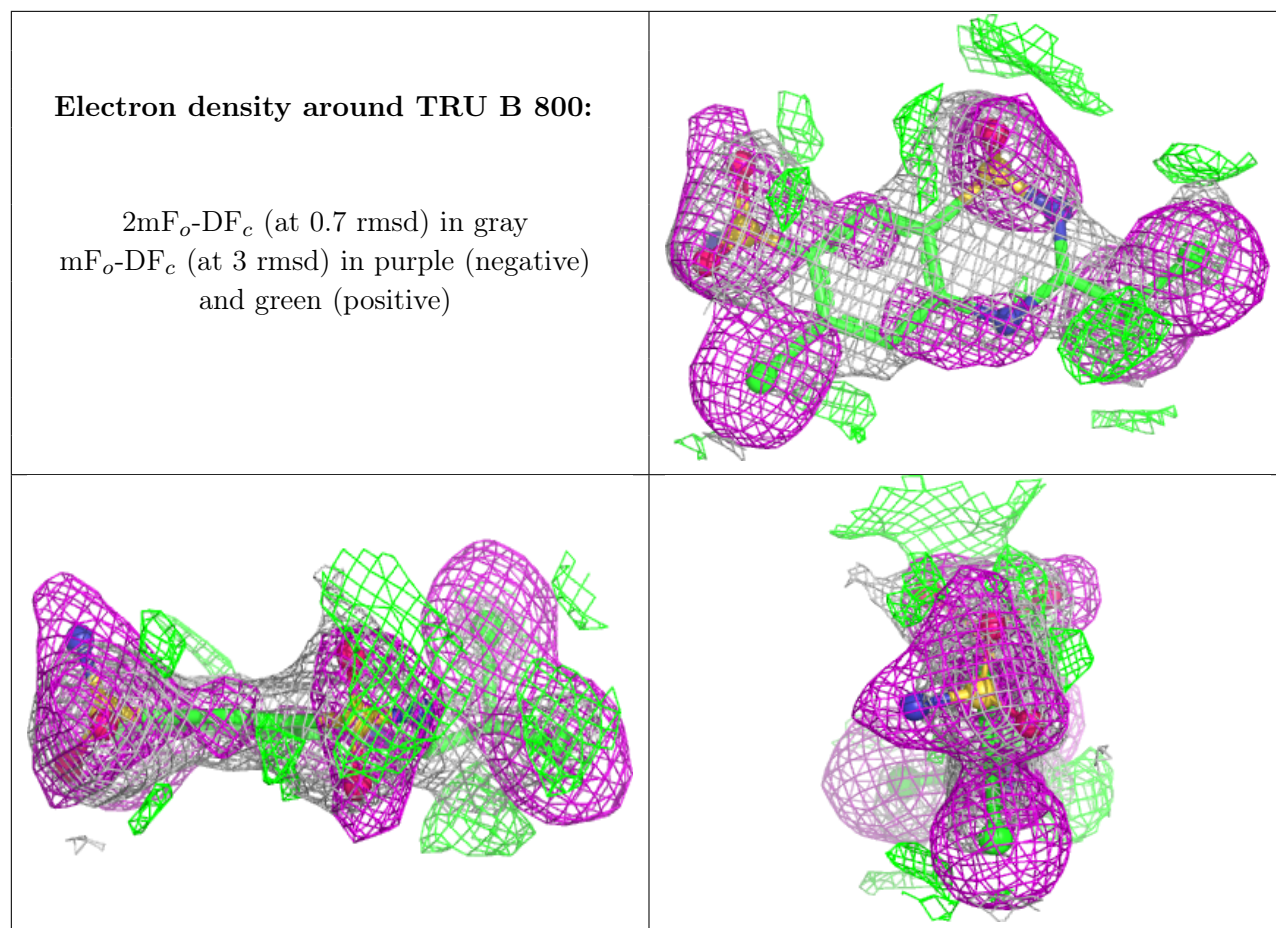
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





6.5 Other polymers ⓘ

There are no such residues in this entry.