WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2023 – 06:03 PM EDT

PDB ID	:	1N94
Title	:	Aryl Tetrahydropyridine Inhbitors of Farnesyltransferase: Glycine, Phenylala- nine and Histidine Derivates
Authors	:	Gwaltney II, S.L.; O'Connor, S.J.; Nelson, L.T.; Sullivan, G.M.; Imade, H.; Wang, W.; Hasvold, L.; Li, Q.; Cohen, J.; Gu, W.Z.
Deposited on	:	2002-11-22
Resolution	:	3.50 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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

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 3.50 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	Percentile Ranks	Value
Rfree		0.198
Clashscore		48
Ramachandran outliers		6.1%
Sidechain outliers		3.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
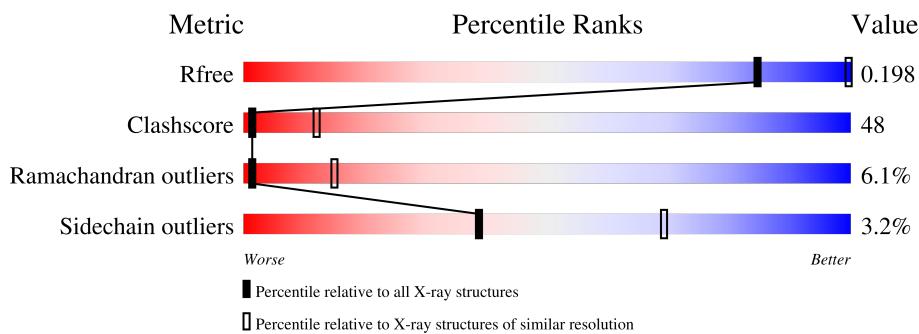
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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%

Mol	Chain	Length	Quality of chain
1	A	315	33% 60% 7%
2	B	397	39% 54% 6% ·
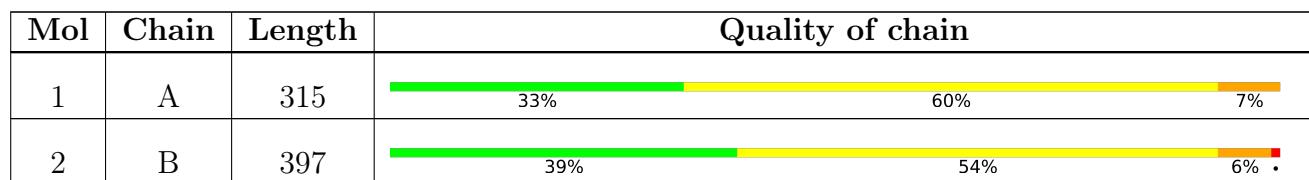
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HFP	A	501	X	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5873 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 Protein farnesyltransferase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total 2689	C 1712	N 473	O 499	S 5	0	0	0

- Molecule 2 is a protein called Protein farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	397	Total 3125	C 1995	N 539	O 568	S 23	0	0	0

- Molecule 3 is ALPHA-HYDROXYFARNESYLPHOSPHONIC ACID (three-letter code: HFP) (formula: $C_{15}H_{33}O_4P$).
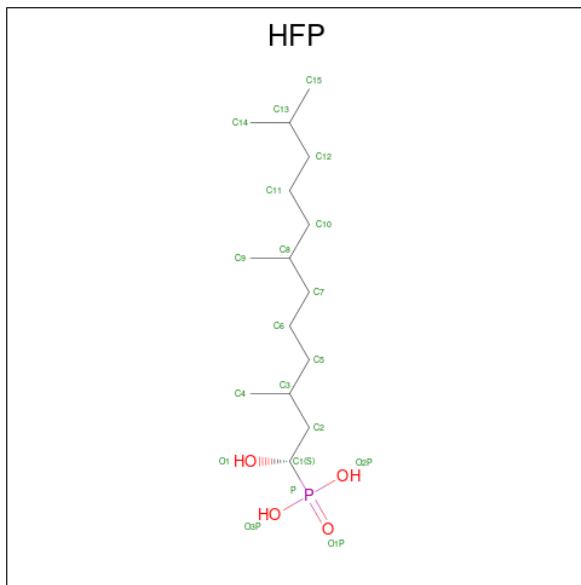
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 20	C 15	O 4	P 1	0	0

- Molecule 4 is 2-{(5-{[BUTYL-(2-CYCLOHEXYL-ETHYL)-AMINO]-METHYL}-2'-ME

THYL-BIPHENYL-2-CARBONYL)-AMINO]-4-METHYLSULFANYL-BUTYRIC ACID
(three-letter code: TIN) (formula: $C_{32}H_{46}N_2O_3S$).
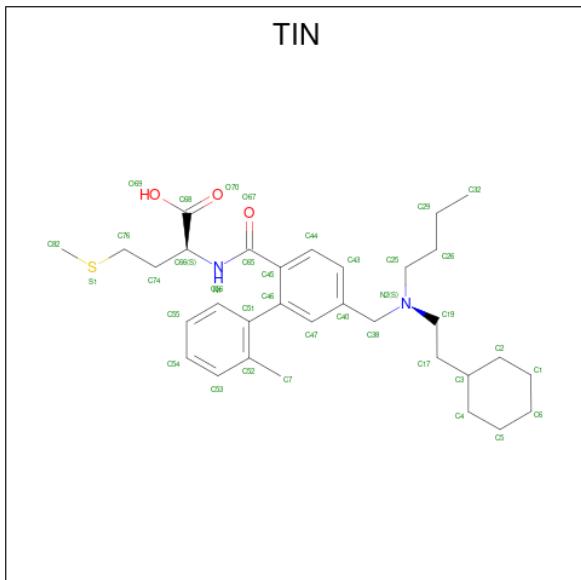
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	38	32	2	3	1	0	0

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	B	1	1	1	0	0

3 Residue-property plots ⓘ

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. 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: Protein farnesyltransferase alpha subunit

Chain A:

• Molecule 2: Protein farnesyltransferase beta subunit

Chain B:

M381 L382 V385 V386 M387 G388 V389 P390 E391 N392 V393 L394 Q395 P396 T397 H398 P399 V400 Y401 N402 I403 G404 P405 D406 K407 V408 A411 T412 T413 H414 F415 K418
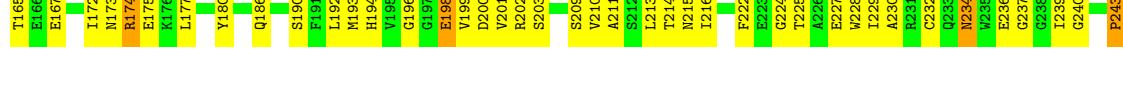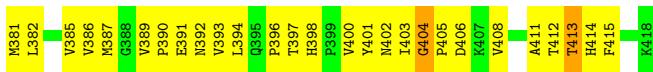
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	172.11Å 172.11Å 69.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.94 – 3.50 40.40 – 3.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (33.94-3.50) 84.6 (40.40-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 3.18Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.295 , 0.296 0.197 , 0.198	Depositor DCC
R_{free} test set	1811 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å^2)	59.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 54.5	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5873	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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 ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.40	0/2755	0.65	0/3738
2	B	0.42	0/3208	0.70	0/4353
All	All	0.41	0/5963	0.68	0/8091

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	93	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2689	0	2614	282	0
2	B	3125	0	3058	287	0
3	A	20	0	28	20	0
4	A	38	0	45	10	0
5	B	1	0	0	0	0
All	All	5873	0	5745	552	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 48.

All (552) 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:A:164:LYS:HD3	3:A:501:HFP:O1P	1.18	1.30
1:A:200:TYR:CB	3:A:501:HFP:H43	1.86	1.04
1:A:200:TYR:CG	3:A:501:HFP:H43	1.93	1.03
2:B:280:ARG:HH12	2:B:292:CYS:HA	1.21	1.00
1:A:165:ASN:ND2	1:A:168:VAL:H	1.61	0.99
2:B:158:ASN:HD21	2:B:403:ILE:HG21	1.30	0.96
2:B:74:GLN:HB3	2:B:77:LYS:HB2	1.48	0.95
2:B:308:LEU:HD12	2:B:330:PHE:HD1	1.29	0.94
1:A:239:GLN:HE21	1:A:239:GLN:HA	1.34	0.92
2:B:386:VAL:HG21	2:B:393:VAL:HG22	1.52	0.92
1:A:200:TYR:CG	3:A:501:HFP:C4	2.54	0.90
2:B:291:ARG:HH21	2:B:294:LYS:HE2	1.36	0.90
2:B:336:GLN:NE2	2:B:374:GLN:HG2	1.85	0.90
2:B:336:GLN:HE21	2:B:374:GLN:HG2	1.38	0.89
1:A:164:LYS:NZ	4:A:1:TIN:H321	1.88	0.88
2:B:158:ASN:ND2	2:B:403:ILE:HG21	1.89	0.87
2:B:280:ARG:HH12	2:B:292:CYS:CA	1.88	0.86
1:A:270:VAL:HG22	2:B:40:VAL:HG21	1.58	0.85
2:B:158:ASN:HD21	2:B:403:ILE:CG2	1.90	0.84
2:B:87:ARG:NH1	2:B:122:VAL:HG12	1.93	0.83
2:B:281:GLN:HE22	2:B:331:HIS:HB3	1.42	0.82
2:B:73:LEU:HA	2:B:344:GLN:HE22	1.44	0.82
2:B:119:PRO:O	2:B:122:VAL:HG22	1.80	0.81
2:B:59:PHE:HA	2:B:341:MET:HE1	1.62	0.80
2:B:64:PHE:HD1	2:B:65:ASN:H	1.30	0.80
1:A:253:ARG:HE	1:A:253:ARG:HA	1.47	0.80
1:A:164:LYS:HD2	3:A:501:HFP:O1P	1.82	0.80
2:B:234:ASN:ND2	2:B:236:GLU:H	1.81	0.79
1:A:286:ASP:HB2	1:A:287:ARG:HH21	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:ARG:NH1	2:B:292:CYS:HA	1.97	0.78
2:B:134:GLN:HE22	2:B:173:ASN:H	1.31	0.78
2:B:86:LEU:HB2	2:B:107:ILE:HG21	1.66	0.77
2:B:308:LEU:HD12	2:B:330:PHE:CD1	2.18	0.77
2:B:200:ASP:OD1	2:B:202:ARG:HB3	1.85	0.77
1:A:165:ASN:HD21	1:A:167:GLN:HG2	1.50	0.76
2:B:386:VAL:CG2	2:B:393:VAL:HG22	2.15	0.76
2:B:386:VAL:HG21	2:B:393:VAL:CG2	2.15	0.76
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.51	0.75
1:A:96:PHE:HA	1:A:126:LEU:HD13	1.68	0.75
1:A:208:TRP:NE1	1:A:212:GLU:HG3	2.02	0.75
1:A:289:LEU:HD13	1:A:318:ILE:HG12	1.68	0.75
1:A:167:GLN:H	1:A:167:GLN:NE2	1.85	0.74
2:B:186:GLN:HB2	2:B:190:SER:O	1.87	0.74
2:B:59:PHE:HD1	2:B:341:MET:HE2	1.51	0.74
1:A:156:ILE:HG23	1:A:188:PHE:CE1	2.23	0.74
1:A:165:ASN:HD22	1:A:168:VAL:HG12	1.51	0.74
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.52	0.73
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.71	0.72
1:A:263:THR:HG21	1:A:280:LEU:HB2	1.71	0.72
1:A:200:TYR:CD2	3:A:501:HFP:H43	2.24	0.72
1:A:268:LYS:HE3	1:A:302:LEU:HD21	1.71	0.72
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.25	0.72
2:B:109:HIS:O	2:B:112:GLU:HG2	1.88	0.72
1:A:151:GLU:HG3	1:A:175:LEU:HD11	1.70	0.72
2:B:38:ASP:O	2:B:40:VAL:HG23	1.89	0.72
1:A:164:LYS:HZ3	4:A:1:TIN:H321	1.55	0.71
2:B:306:GLY:O	2:B:309:PRO:HD2	1.91	0.71
1:A:92:TYR:HB2	1:A:97:ARG:HB2	1.72	0.71
2:B:79:PHE:CZ	2:B:83:LYS:HD2	2.26	0.70
1:A:167:GLN:H	1:A:167:GLN:CD	1.94	0.70
2:B:174:ARG:HD2	2:B:415:PHE:CD1	2.26	0.70
1:A:323:LEU:HB3	1:A:367:HIS:NE2	2.07	0.70
2:B:321:PRO:HG2	2:B:322:ALA:H	1.57	0.69
1:A:256:LEU:HD23	1:A:256:LEU:O	1.92	0.69
2:B:396:PRO:HB2	2:B:405:PRO:HG2	1.74	0.69
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.26	0.69
2:B:175:GLU:CD	2:B:175:GLU:H	1.94	0.69
1:A:96:PHE:HA	1:A:126:LEU:CD1	2.21	0.69
1:A:329:ASN:C	1:A:331:GLU:H	1.96	0.69
3:A:501:HFP:H62	2:B:248:HIS:NE2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:ARG:NH1	2:B:292:CYS:CA	2.55	0.69
1:A:121:ARG:NH1	1:A:121:ARG:HB3	2.07	0.68
1:A:159:ILE:HG13	1:A:168:VAL:HG22	1.74	0.68
1:A:240:ARG:HD3	1:A:259:GLU:OE2	1.94	0.68
2:B:101:PRO:HD3	2:B:142:GLY:O	1.93	0.68
1:A:175:LEU:O	1:A:179:LEU:HD23	1.93	0.68
2:B:192:LEU:HA	2:B:199:VAL:HG12	1.76	0.67
1:A:165:ASN:HD22	1:A:168:VAL:CG1	2.07	0.67
1:A:200:TYR:CD2	3:A:501:HFP:C4	2.77	0.67
1:A:166:TYR:OH	4:A:1:TIN:HC44	1.95	0.67
2:B:33:GLU:HB3	2:B:283:ARG:O	1.94	0.67
1:A:317:ASP:HA	1:A:320:GLU:OE1	1.94	0.66
1:A:334:LEU:HD21	1:A:367:HIS:O	1.95	0.66
1:A:200:TYR:HB2	3:A:501:HFP:H43	1.78	0.66
3:A:501:HFP:H153	2:B:254:CYS:SG	2.36	0.66
2:B:404:GLY:O	2:B:408:VAL:HG23	1.96	0.65
1:A:200:TYR:HB3	3:A:501:HFP:H43	1.78	0.65
1:A:328:ASP:O	1:A:329:ASN:HB2	1.95	0.65
2:B:315:LEU:HB2	2:B:323:LEU:HD11	1.78	0.65
2:B:412:THR:C	2:B:414:HIS:H	1.99	0.65
2:B:73:LEU:HD12	2:B:344:GLN:NE2	2.11	0.65
2:B:345:CYS:HB3	2:B:348:GLY:O	1.96	0.65
2:B:69:PRO:C	2:B:71:LEU:H	2.01	0.65
2:B:64:PHE:HD1	2:B:65:ASN:N	1.95	0.64
2:B:149:HIS:O	2:B:152:PRO:HG2	1.97	0.64
1:A:58:LEU:HD11	1:A:95:LYS:HD3	1.79	0.64
1:A:294:ASN:HB3	1:A:298:GLN:HE22	1.63	0.64
2:B:23:LEU:HB3	2:B:337:GLU:OE1	1.98	0.64
1:A:112:ARG:O	1:A:144:LEU:HD11	1.98	0.64
2:B:177:LEU:HD21	2:B:210:VAL:CG1	2.27	0.64
1:A:116:ALA:O	1:A:119:LEU:HB3	1.98	0.63
1:A:355:TYR:O	1:A:358:TYR:HB3	1.97	0.63
2:B:288:PHE:CE1	2:B:305:ALA:HB2	2.34	0.63
1:A:232:ARG:CZ	2:B:45:SER:HB2	2.29	0.63
1:A:344:LEU:HD13	1:A:356:TRP:CZ2	2.34	0.63
1:A:149:GLN:NE2	1:A:149:GLN:HA	2.13	0.63
1:A:358:TYR:HB2	1:A:361:ARG:HH21	1.62	0.63
2:B:201:VAL:HG21	2:B:251:TYR:HB3	1.79	0.63
1:A:165:ASN:HD22	1:A:168:VAL:CB	2.12	0.63
1:A:165:ASN:HD22	1:A:168:VAL:H	1.43	0.63
2:B:46:ILE:O	2:B:49:ALA:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:LEU:HD23	2:B:373:ALA:HB2	1.81	0.62
2:B:214:THR:O	2:B:216:ILE:HG23	1.99	0.62
2:B:300:TYR:HA	2:B:303:TRP:HB2	1.81	0.62
1:A:224:ASP:HA	1:A:227:LEU:HD12	1.80	0.62
2:B:73:LEU:O	2:B:75:ARG:N	2.33	0.62
1:A:312:ILE:O	1:A:316:VAL:HG23	2.00	0.62
1:A:351:ILE:HD11	2:B:281:GLN:HE21	1.65	0.62
3:A:501:HFP:H102	2:B:250:GLY:HA3	1.82	0.61
2:B:370:LEU:O	2:B:374:GLN:HG3	2.01	0.61
2:B:301:SER:O	2:B:305:ALA:HB3	2.00	0.61
1:A:58:LEU:CD1	1:A:95:LYS:HD3	2.31	0.61
2:B:59:PHE:HD1	2:B:341:MET:CE	2.14	0.61
1:A:88:VAL:HG23	1:A:88:VAL:O	2.01	0.61
1:A:260:VAL:CG2	1:A:284:LEU:HD21	2.31	0.60
2:B:114:LEU:O	2:B:115:ASP:HB3	2.01	0.60
1:A:56:LEU:HD12	1:A:56:LEU:H	1.66	0.60
1:A:164:LYS:HZ2	4:A:1:TIN:H321	1.65	0.60
1:A:319:TYR:O	1:A:323:LEU:HG	2.01	0.60
2:B:73:LEU:HA	2:B:344:GLN:NE2	2.16	0.60
1:A:153:ASN:HD22	1:A:153:ASN:N	2.00	0.60
1:A:69:ARG:HB3	1:A:71:GLU:OE2	2.01	0.59
1:A:165:ASN:ND2	1:A:168:VAL:N	2.41	0.59
2:B:303:TRP:HA	2:B:303:TRP:CE3	2.36	0.59
1:A:87:VAL:O	1:A:88:VAL:C	2.41	0.59
1:A:356:TRP:C	1:A:358:TYR:H	2.03	0.59
2:B:24:TYR:HB3	2:B:337:GLU:OE2	2.03	0.59
2:B:413:THR:O	2:B:413:THR:HG22	2.02	0.59
2:B:42:THR:O	2:B:45:SER:N	2.36	0.59
2:B:163:ILE:HG22	2:B:165:THR:HG23	1.85	0.59
1:A:329:ASN:HA	1:A:331:GLU:OE2	2.03	0.59
1:A:200:TYR:CB	3:A:501:HFP:C4	2.72	0.59
2:B:89:LEU:CD1	2:B:103:LEU:HD13	2.33	0.59
1:A:296:LEU:O	1:A:300:LEU:HG	2.03	0.59
2:B:59:PHE:HA	2:B:341:MET:CE	2.31	0.59
2:B:214:THR:HA	2:B:415:PHE:CD2	2.38	0.59
1:A:159:ILE:CG1	1:A:168:VAL:HG22	2.33	0.58
2:B:109:HIS:ND1	2:B:112:GLU:OE1	2.35	0.58
1:A:80:GLN:HB2	1:A:104:ARG:CZ	2.33	0.58
2:B:265:GLU:OE1	2:B:265:GLU:N	2.29	0.58
2:B:87:ARG:HH12	2:B:122:VAL:HG12	1.67	0.58
2:B:277:VAL:HG22	2:B:307:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:HD21	1:A:168:VAL:H	1.51	0.58
1:A:200:TYR:N	3:A:501:HFP:O2P	2.37	0.58
2:B:59:PHE:CD1	2:B:341:MET:HE2	2.36	0.58
2:B:302:PHE:O	2:B:306:GLY:HA3	2.04	0.58
1:A:58:LEU:HD21	1:A:126:LEU:CD2	2.34	0.58
1:A:253:ARG:HA	1:A:253:ARG:NE	2.15	0.58
3:A:501:HFP:H142	2:B:202:ARG:CD	2.34	0.58
2:B:222:PHE:HB3	2:B:225:THR:HB	1.85	0.58
2:B:281:GLN:HE22	2:B:331:HIS:CB	2.14	0.58
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.69	0.57
2:B:251:TYR:O	2:B:254:CYS:HB2	2.04	0.57
1:A:164:LYS:HD2	4:A:1:TIN:C29	2.34	0.57
1:A:366:LYS:HG3	1:A:367:HIS:ND1	2.20	0.57
2:B:213:LEU:HD21	2:B:401:TYR:CE1	2.39	0.57
1:A:206:ARG:NH2	1:A:222:TYR:CD2	2.72	0.57
2:B:27:ARG:HB3	2:B:29:GLU:OE2	2.04	0.57
2:B:211:ALA:HA	2:B:216:ILE:HG12	1.87	0.57
2:B:247:ALA:O	2:B:291:ARG:HG2	2.05	0.57
2:B:279:SER:HB3	2:B:280:ARG:HH21	1.70	0.57
2:B:134:GLN:HB2	2:B:140:PHE:CE2	2.40	0.57
1:A:332:ASP:O	1:A:336:LYS:HB2	2.05	0.56
2:B:291:ARG:HB2	2:B:294:LYS:HD3	1.87	0.56
2:B:328:TRP:CZ2	2:B:376:PHE:HA	2.40	0.56
1:A:239:GLN:HA	1:A:239:GLN:NE2	2.14	0.56
1:A:65:LEU:O	1:A:69:ARG:HG3	2.04	0.56
1:A:70:ALA:O	1:A:72:TRP:N	2.38	0.56
1:A:167:GLN:NE2	1:A:167:GLN:N	2.53	0.56
1:A:287:ARG:N	1:A:287:ARG:NE	2.52	0.56
2:B:377:GLY:HA2	2:B:382:LEU:HD23	1.86	0.56
2:B:256:LEU:O	2:B:260:VAL:HG23	2.05	0.56
2:B:362:HIS:O	2:B:364:CYS:N	2.38	0.56
1:A:262:TYR:O	1:A:265:GLU:HB2	2.05	0.56
2:B:331:HIS:CE1	2:B:333:GLN:HB3	2.41	0.56
2:B:339:ILE:HD12	2:B:370:LEU:HD13	1.86	0.56
1:A:244:ILE:HD12	1:A:250:TYR:OH	2.05	0.56
2:B:284:PHE:HB3	2:B:285:GLU:OE1	2.06	0.56
2:B:234:ASN:HD21	2:B:236:GLU:HB2	1.71	0.56
1:A:170:HIS:O	1:A:174:VAL:HG23	2.06	0.55
2:B:352:ASP:HB3	2:B:356:LYS:HD3	1.88	0.55
1:A:56:LEU:HD12	1:A:56:LEU:N	2.21	0.55
1:A:334:LEU:O	1:A:338:LEU:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ARG:NH2	2:B:294:LYS:HE2	2.15	0.55
2:B:58:VAL:HG12	2:B:341:MET:HE2	1.89	0.55
2:B:201:VAL:HG23	2:B:202:ARG:N	2.20	0.55
2:B:79:PHE:CE2	2:B:83:LYS:HD2	2.41	0.55
2:B:151:ALA:HB3	2:B:152:PRO:CD	2.36	0.55
2:B:78:HIS:ND1	2:B:349:GLY:N	2.55	0.55
2:B:376:PHE:CZ	2:B:378:SER:HB3	2.42	0.55
2:B:361:TYR:O	2:B:364:CYS:HB3	2.07	0.55
1:A:165:ASN:HB3	1:A:168:VAL:HG12	1.87	0.54
1:A:196:ASP:C	1:A:198:LYS:H	2.10	0.54
2:B:62:TYR:HE2	2:B:341:MET:CE	2.20	0.54
1:A:289:LEU:CD1	1:A:318:ILE:HG12	2.36	0.54
1:A:323:LEU:HB3	1:A:367:HIS:CD2	2.43	0.54
1:A:351:ILE:CD1	2:B:281:GLN:HE21	2.19	0.54
1:A:144:LEU:HD12	1:A:144:LEU:N	2.23	0.54
2:B:70:ARG:C	2:B:72:VAL:H	2.10	0.54
2:B:333:GLN:HG3	2:B:387:MET:SD	2.48	0.54
1:A:253:ARG:HE	1:A:253:ARG:CA	2.18	0.54
1:A:175:LEU:O	1:A:178:TRP:HB2	2.08	0.53
1:A:344:LEU:HB3	1:A:356:TRP:CD1	2.44	0.53
1:A:164:LYS:HD2	4:A:1:TIN:H291	1.88	0.53
1:A:280:LEU:HD23	1:A:314:PHE:CE2	2.44	0.53
2:B:224:GLY:O	2:B:227:GLU:HB2	2.09	0.53
1:A:112:ARG:HA	1:A:140:LEU:CD2	2.39	0.53
2:B:26:LEU:O	2:B:27:ARG:O	2.27	0.53
2:B:62:TYR:HE2	2:B:341:MET:HE1	1.73	0.53
1:A:314:PHE:O	1:A:317:ASP:HB2	2.08	0.53
2:B:376:PHE:CD1	2:B:376:PHE:C	2.82	0.53
2:B:48:GLN:O	2:B:52:GLU:HG3	2.08	0.52
1:A:256:LEU:HD23	1:A:256:LEU:C	2.30	0.52
1:A:65:LEU:CD1	1:A:67:ARG:HH21	2.23	0.52
1:A:70:ALA:C	1:A:72:TRP:H	2.13	0.52
1:A:75:ILE:HD13	1:A:109:ARG:NH1	2.24	0.52
1:A:112:ARG:HA	1:A:140:LEU:HD21	1.91	0.52
1:A:230:ASP:CG	2:B:42:THR:HB	2.30	0.52
2:B:84:ARG:HG3	2:B:84:ARG:HH11	1.74	0.52
1:A:127:ASN:HD22	2:B:97:ASP:HB3	1.75	0.52
2:B:192:LEU:HD23	2:B:199:VAL:CG1	2.40	0.52
2:B:398:HIS:CE1	2:B:400:VAL:HB	2.45	0.52
1:A:223:VAL:HG11	1:A:240:ARG:HB2	1.91	0.52
2:B:339:ILE:HD12	2:B:370:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:NH1	2:B:45:SER:HB2	2.25	0.52
1:A:90:ILE:HB	1:A:92:TYR:CE1	2.44	0.51
3:A:501:HFP:C10	2:B:250:GLY:HA3	2.40	0.51
2:B:26:LEU:HD23	2:B:59:PHE:HB3	1.92	0.51
1:A:137:ARG:O	1:A:141:LEU:HD13	2.09	0.51
1:A:138:ARG:HG3	1:A:138:ARG:HH11	1.76	0.51
2:B:67:LEU:HG	2:B:68:VAL:HG23	1.91	0.51
2:B:258:ALA:O	2:B:262:LEU:HG	2.10	0.51
2:B:397:THR:HG22	2:B:402:ASN:HA	1.92	0.51
1:A:124:ILE:O	1:A:128:ALA:N	2.43	0.51
1:A:205:HIS:O	1:A:209:VAL:HG23	2.10	0.51
2:B:315:LEU:CD1	2:B:323:LEU:HD21	2.40	0.51
2:B:331:HIS:HE1	2:B:333:GLN:HB3	1.76	0.51
2:B:412:THR:C	2:B:414:HIS:N	2.63	0.51
1:A:85:SER:HB3	2:B:125:ASP:OD1	2.11	0.51
1:A:196:ASP:O	1:A:198:LYS:N	2.44	0.51
1:A:358:TYR:HA	1:A:361:ARG:HE	1.76	0.51
2:B:165:THR:C	2:B:167:GLU:N	2.63	0.51
1:A:358:TYR:HB2	1:A:361:ARG:NH2	2.25	0.51
2:B:381:MET:O	2:B:382:LEU:HD23	2.09	0.51
1:A:159:ILE:O	1:A:163:PRO:HG3	2.11	0.51
2:B:78:HIS:O	2:B:82:LEU:HG	2.10	0.51
2:B:398:HIS:N	2:B:405:PRO:HG3	2.26	0.51
1:A:153:ASN:N	1:A:153:ASN:ND2	2.59	0.51
2:B:134:GLN:NE2	2:B:173:ASN:H	2.05	0.51
2:B:143:GLY:N	2:B:146:GLN:NE2	2.58	0.51
2:B:280:ARG:NH1	2:B:292:CYS:N	2.59	0.51
2:B:315:LEU:CB	2:B:323:LEU:HD11	2.39	0.50
1:A:100:TYR:HE1	1:A:126:LEU:HD12	1.75	0.50
1:A:239:GLN:O	1:A:242:PHE:HB3	2.12	0.50
1:A:244:ILE:HB	1:A:250:TYR:OH	2.11	0.50
1:A:354:GLU:HG2	2:B:328:TRP:O	2.12	0.50
2:B:74:GLN:HB3	2:B:77:LYS:CB	2.31	0.50
2:B:264:LYS:O	2:B:265:GLU:C	2.49	0.50
1:A:67:ARG:HG3	1:A:68:ASP:OD1	2.11	0.50
1:A:173:ARG:HG3	1:A:208:TRP:CZ3	2.46	0.50
1:A:241:HIS:ND1	1:A:241:HIS:O	2.44	0.50
1:A:297:ASN:HA	1:A:300:LEU:HD12	1.92	0.50
1:A:323:LEU:HB3	1:A:367:HIS:HE2	1.74	0.50
2:B:23:LEU:HB2	2:B:26:LEU:HD12	1.93	0.50
2:B:190:SER:HB3	2:B:228:TRP:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PHE:O	1:A:318:ILE:HG13	2.10	0.50
2:B:303:TRP:HA	2:B:303:TRP:HE3	1.76	0.50
2:B:116:GLU:O	2:B:118:ILE:HD12	2.12	0.50
2:B:348:GLY:O	2:B:358:ARG:HD2	2.12	0.50
2:B:174:ARG:HH11	2:B:174:ARG:HB2	1.76	0.50
1:A:164:LYS:HZ2	4:A:1:TIN:C32	2.23	0.49
1:A:210:ILE:HD11	1:A:219:GLU:OE1	2.12	0.49
2:B:82:LEU:HD21	2:B:363:THR:HG21	1.94	0.49
2:B:327:HIS:O	2:B:376:PHE:CE2	2.65	0.49
2:B:396:PRO:O	2:B:405:PRO:HD3	2.12	0.49
1:A:70:ALA:C	1:A:72:TRP:N	2.66	0.49
2:B:234:ASN:ND2	2:B:236:GLU:N	2.57	0.49
2:B:362:HIS:C	2:B:364:CYS:N	2.65	0.49
2:B:389:VAL:HG22	2:B:392:ASN:HD21	1.78	0.49
1:A:287:ARG:NE	1:A:287:ARG:H	2.10	0.49
1:A:289:LEU:HD12	1:A:318:ILE:HA	1.94	0.49
1:A:231:VAL:HG13	1:A:273:ASN:ND2	2.28	0.49
2:B:175:GLU:CD	2:B:175:GLU:N	2.64	0.49
1:A:325:ASN:O	1:A:326:GLN:C	2.49	0.49
1:A:137:ARG:HG2	1:A:141:LEU:HD11	1.95	0.49
2:B:64:PHE:CD1	2:B:65:ASN:OD1	2.66	0.49
2:B:237:GLY:HA3	2:B:272:SER:O	2.12	0.49
2:B:403:ILE:O	2:B:404:GLY:C	2.49	0.49
1:A:311:LEU:O	1:A:312:ILE:C	2.50	0.49
2:B:73:LEU:HD12	2:B:344:GLN:HE21	1.75	0.49
2:B:76:GLU:O	2:B:79:PHE:HB3	2.13	0.49
1:A:58:LEU:HD21	1:A:126:LEU:HD23	1.95	0.48
1:A:165:ASN:HB3	1:A:168:VAL:CG1	2.43	0.48
2:B:276:TRP:O	2:B:277:VAL:C	2.50	0.48
1:A:351:ILE:HG12	2:B:281:GLN:NE2	2.28	0.48
2:B:70:ARG:C	2:B:72:VAL:N	2.67	0.48
2:B:84:ARG:HG3	2:B:84:ARG:NH1	2.29	0.48
2:B:316:HIS:N	2:B:323:LEU:HD11	2.29	0.48
2:B:412:THR:O	2:B:414:HIS:N	2.46	0.48
2:B:111:LEU:O	2:B:115:ASP:N	2.40	0.48
2:B:336:GLN:HG2	2:B:370:LEU:HD12	1.95	0.48
2:B:279:SER:CB	2:B:280:ARG:HH21	2.26	0.48
1:A:165:ASN:HD22	1:A:168:VAL:HB	1.78	0.48
1:A:362:SER:O	1:A:366:LYS:HG2	2.13	0.48
1:A:96:PHE:CD1	1:A:96:PHE:C	2.87	0.48
1:A:289:LEU:N	1:A:321:ASP:OD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:TYR:CD2	2:B:96:LEU:HD12	2.49	0.48
1:A:158:ILE:HG22	1:A:168:VAL:HG21	1.95	0.48
1:A:188:PHE:CZ	1:A:192:ILE:HD11	2.48	0.48
1:A:319:TYR:CD2	1:A:337:ALA:HB2	2.49	0.48
1:A:252:ASP:HB3	1:A:255:VAL:CG2	2.44	0.48
1:A:290:SER:OG	1:A:322:MET:HA	2.14	0.48
1:A:58:LEU:HD12	1:A:63:TYR:CZ	2.49	0.47
1:A:106:VAL:O	1:A:109:ARG:N	2.43	0.47
2:B:26:LEU:O	2:B:27:ARG:C	2.52	0.47
2:B:239:ILE:HG22	2:B:240:GLY:N	2.27	0.47
2:B:280:ARG:HG3	2:B:304:GLN:NE2	2.29	0.47
1:A:87:VAL:HG12	1:A:88:VAL:N	2.29	0.47
1:A:188:PHE:O	1:A:191:ASP:N	2.47	0.47
1:A:100:TYR:CE1	1:A:126:LEU:HD12	2.48	0.47
1:A:127:ASN:C	1:A:129:ALA:H	2.17	0.47
1:A:173:ARG:HG3	1:A:208:TRP:CH2	2.49	0.47
1:A:316:VAL:O	1:A:320:GLU:HG3	2.14	0.47
1:A:58:LEU:HD21	1:A:126:LEU:HD21	1.96	0.47
1:A:200:TYR:HB2	3:A:501:HFP:C4	2.40	0.47
1:A:344:LEU:HD13	1:A:356:TRP:CD2	2.48	0.47
2:B:140:PHE:O	2:B:148:PRO:HA	2.14	0.47
2:B:158:ASN:ND2	2:B:158:ASN:O	2.47	0.47
2:B:327:HIS:O	2:B:376:PHE:HE2	1.96	0.47
1:A:77:PRO:HB3	1:A:102:TYR:CE1	2.49	0.47
1:A:165:ASN:ND2	1:A:168:VAL:HG12	2.25	0.47
1:A:317:ASP:O	1:A:320:GLU:HB2	2.15	0.47
3:A:501:HFP:H142	2:B:202:ARG:HD2	1.97	0.47
2:B:69:PRO:C	2:B:71:LEU:N	2.68	0.47
2:B:87:ARG:HH11	2:B:122:VAL:HG12	1.77	0.47
2:B:109:HIS:O	2:B:112:GLU:N	2.48	0.47
2:B:287:GLY:HA2	2:B:335:LEU:CD1	2.44	0.47
2:B:296:VAL:HG22	2:B:297:ASP:N	2.30	0.47
1:A:104:ARG:O	1:A:105:ALA:C	2.53	0.47
1:A:148:LEU:O	1:A:151:GLU:HB3	2.15	0.47
1:A:250:TYR:O	1:A:256:LEU:HB2	2.15	0.47
2:B:276:TRP:O	2:B:279:SER:N	2.47	0.47
2:B:396:PRO:HG2	2:B:405:PRO:HD2	1.97	0.47
2:B:209:SER:O	2:B:213:LEU:HG	2.15	0.47
2:B:328:TRP:NE1	2:B:375:HIS:O	2.48	0.47
1:A:152:MET:O	1:A:155:ILE:HG22	2.15	0.46
1:A:265:GLU:OE2	1:A:265:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LYS:HE3	1:A:302:LEU:CD2	2.42	0.46
1:A:369:ARG:HG3	1:A:369:ARG:O	2.15	0.46
2:B:174:ARG:NH1	2:B:174:ARG:CB	2.78	0.46
1:A:138:ARG:HG3	1:A:138:ARG:NH1	2.30	0.46
1:A:165:ASN:O	1:A:169:TRP:HD1	1.98	0.46
1:A:350:THR:O	1:A:353:LYS:HB3	2.16	0.46
2:B:66:HIS:CE1	2:B:69:PRO:CG	2.98	0.46
2:B:234:ASN:ND2	2:B:234:ASN:C	2.66	0.46
2:B:401:TYR:N	2:B:401:TYR:CD2	2.84	0.46
2:B:149:HIS:ND1	2:B:152:PRO:HD2	2.30	0.46
2:B:165:THR:C	2:B:167:GLU:H	2.19	0.46
2:B:225:THR:O	2:B:229:ILE:HG13	2.15	0.46
2:B:342:CYS:O	2:B:354:PRO:HG3	2.16	0.46
1:A:297:ASN:O	1:A:300:LEU:HB2	2.16	0.46
1:A:349:ASP:OD2	1:A:352:ARG:HB2	2.15	0.46
2:B:33:GLU:HA	2:B:33:GLU:OE1	2.15	0.46
1:A:135:HIS:CD2	2:B:147:TYR:CE2	3.04	0.46
1:A:260:VAL:HG21	1:A:284:LEU:HD21	1.98	0.46
2:B:40:VAL:HG12	2:B:41:GLU:N	2.30	0.46
2:B:51:VAL:HG21	2:B:295:LEU:HD13	1.97	0.46
2:B:122:VAL:HG23	2:B:123:ALA:N	2.31	0.46
2:B:135:SER:HB2	2:B:148:PRO:HD3	1.97	0.46
2:B:315:LEU:HD13	2:B:323:LEU:HD21	1.97	0.46
1:A:78:VAL:HG11	1:A:108:GLN:HE22	1.80	0.46
1:A:154:TYR:CE1	1:A:158:ILE:HD11	2.51	0.46
2:B:108:LEU:HD23	2:B:108:LEU:HA	1.75	0.46
2:B:42:THR:O	2:B:43:VAL:C	2.53	0.46
1:A:137:ARG:HG2	1:A:141:LEU:CD1	2.45	0.46
1:A:264:LEU:HD23	1:A:267:ILE:HD12	1.98	0.46
1:A:277:TRP:CZ3	1:A:311:LEU:HA	2.50	0.46
1:A:334:LEU:HD22	1:A:367:HIS:HB3	1.98	0.46
2:B:109:HIS:O	2:B:110:SER:C	2.53	0.46
1:A:264:LEU:O	1:A:267:ILE:HB	2.15	0.46
1:A:355:TYR:CZ	1:A:359:ILE:HD11	2.51	0.46
2:B:198:GLU:CD	2:B:198:GLU:H	2.19	0.46
2:B:411:ALA:O	2:B:414:HIS:HB3	2.16	0.46
1:A:56:LEU:H	1:A:56:LEU:CD1	2.28	0.45
1:A:78:VAL:HG23	1:A:105:ALA:HB2	1.97	0.45
1:A:230:ASP:OD2	1:A:230:ASP:C	2.54	0.45
2:B:122:VAL:O	2:B:123:ALA:C	2.55	0.45
2:B:230:ALA:C	2:B:232:CYS:N	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:ILE:HG13	2:B:408:VAL:HG22	1.97	0.45
1:A:232:ARG:NH1	2:B:42:THR:OG1	2.42	0.45
2:B:64:PHE:CD1	2:B:65:ASN:N	2.82	0.45
1:A:354:GLU:HG3	2:B:329:MET:HA	1.98	0.45
2:B:193:MET:HE2	2:B:203:SER:HB2	1.97	0.45
2:B:232:CYS:CB	2:B:239:ILE:HG23	2.46	0.45
1:A:187:GLU:O	1:A:190:ALA:HB3	2.17	0.45
2:B:152:PRO:HG2	2:B:153:THR:H	1.81	0.45
2:B:321:PRO:O	2:B:323:LEU:N	2.49	0.45
2:B:239:ILE:HB	2:B:252:THR:HA	1.98	0.45
2:B:288:PHE:HB3	2:B:304:GLN:HG3	1.99	0.45
2:B:210:VAL:HG12	2:B:211:ALA:N	2.32	0.45
1:A:95:LYS:O	1:A:99:VAL:HG23	2.17	0.45
1:A:303:GLN:N	1:A:304:PRO:CD	2.79	0.45
1:A:120:THR:O	1:A:121:ARG:C	2.55	0.45
1:A:357:ARG:O	1:A:361:ARG:NE	2.50	0.45
2:B:281:GLN:NE2	2:B:331:HIS:HB3	2.19	0.45
1:A:56:LEU:HB3	1:A:57:SER:H	1.61	0.45
1:A:144:LEU:H	1:A:144:LEU:CD1	2.30	0.45
1:A:156:ILE:CG1	1:A:172:ARG:HH12	2.26	0.45
1:A:121:ARG:HH11	1:A:121:ARG:CB	2.30	0.45
1:A:127:ASN:OD1	1:A:129:ALA:HB3	2.17	0.45
1:A:286:ASP:HB2	1:A:287:ARG:NH2	2.21	0.45
1:A:351:ILE:CG1	2:B:281:GLN:HE21	2.30	0.45
4:A:1:TIN:C47	4:A:1:TIN:H192	2.45	0.45
2:B:149:HIS:CD2	2:B:194:HIS:HB3	2.52	0.45
1:A:134:TRP:CZ3	1:A:171:HIS:CD2	3.05	0.44
2:B:201:VAL:HG21	2:B:251:TYR:CB	2.46	0.44
2:B:232:CYS:HB3	2:B:239:ILE:HG23	1.98	0.44
2:B:74:GLN:HB2	2:B:78:HIS:NE2	2.31	0.44
2:B:201:VAL:CG2	2:B:251:TYR:HD1	2.30	0.44
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.29	0.44
1:A:343:ILE:O	1:A:347:GLU:N	2.48	0.44
2:B:280:ARG:HA	2:B:280:ARG:NE	2.32	0.44
1:A:123:ALA:HB3	1:A:133:VAL:HG11	2.00	0.44
2:B:403:ILE:HG13	2:B:408:VAL:CG2	2.48	0.44
1:A:274:GLU:O	1:A:274:GLU:HG2	2.18	0.44
1:A:143:SER:C	1:A:145:GLN:H	2.21	0.44
1:A:169:TRP:O	1:A:172:ARG:N	2.42	0.44
1:A:231:VAL:HG22	1:A:273:ASN:ND2	2.32	0.44
2:B:177:LEU:HD21	2:B:210:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:N	1:A:144:LEU:CD1	2.81	0.44
2:B:163:ILE:O	2:B:165:THR:HG23	2.17	0.44
1:A:274:GLU:O	1:A:278:ASN:OD1	2.36	0.43
1:A:315:LEU:O	1:A:318:ILE:N	2.51	0.43
2:B:74:GLN:HB2	2:B:78:HIS:CE1	2.53	0.43
2:B:199:VAL:HG23	2:B:199:VAL:O	2.18	0.43
1:A:260:VAL:HG22	1:A:284:LEU:HD21	1.99	0.43
2:B:152:PRO:O	2:B:155:ALA:HB3	2.18	0.43
1:A:132:THR:HG23	2:B:147:TYR:CD2	2.53	0.43
1:A:137:ARG:O	1:A:141:LEU:CD1	2.65	0.43
2:B:200:ASP:O	2:B:201:VAL:C	2.56	0.43
2:B:280:ARG:NE	2:B:280:ARG:CA	2.81	0.43
3:A:501:HFP:H62	2:B:248:HIS:CE1	2.53	0.43
2:B:230:ALA:C	2:B:232:CYS:H	2.21	0.43
2:B:201:VAL:O	2:B:202:ARG:C	2.56	0.43
1:A:57:SER:HB3	1:A:59:ASP:OD1	2.18	0.43
2:B:322:ALA:O	2:B:323:LEU:C	2.55	0.43
1:A:224:ASP:O	1:A:227:LEU:HB2	2.18	0.43
1:A:286:ASP:HB2	1:A:287:ARG:HE	1.84	0.43
1:A:320:GLU:HG2	1:A:363:LEU:HD21	2.00	0.43
1:A:329:ASN:O	1:A:331:GLU:N	2.52	0.43
1:A:353:LYS:HG3	1:A:354:GLU:N	2.34	0.43
1:A:185:GLU:O	1:A:186:LEU:C	2.57	0.43
1:A:188:PHE:O	1:A:189:ILE:C	2.57	0.43
1:A:334:LEU:O	1:A:338:LEU:CD1	2.66	0.43
2:B:77:LYS:HA	2:B:77:LYS:HD3	1.84	0.43
2:B:174:ARG:HD2	2:B:415:PHE:CE1	2.53	0.43
1:A:135:HIS:O	1:A:139:VAL:HG23	2.19	0.43
1:A:143:SER:C	1:A:145:GLN:N	2.72	0.43
1:A:182:PRO:HD3	1:A:213:PHE:CE2	2.53	0.43
1:A:216:TRP:O	1:A:218:ASN:N	2.52	0.43
2:B:108:LEU:HD22	2:B:118:ILE:HG12	2.00	0.43
2:B:214:THR:O	2:B:215:ASN:C	2.57	0.42
1:A:75:ILE:HD12	1:A:76:ASP:H	1.84	0.42
2:B:302:PHE:O	2:B:306:GLY:CA	2.65	0.42
1:A:152:MET:O	1:A:156:ILE:HG13	2.19	0.42
1:A:315:LEU:O	1:A:316:VAL:C	2.56	0.42
2:B:246:GLU:OE1	2:B:291:ARG:HD2	2.20	0.42
1:A:71:GLU:CD	1:A:71:GLU:H	2.22	0.42
2:B:138:GLY:HA3	2:B:180:TYR:HB2	2.00	0.42
2:B:389:VAL:O	2:B:391:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:VAL:O	1:A:247:THR:HG23	2.20	0.42
1:A:262:TYR:CD1	1:A:262:TYR:C	2.92	0.42
2:B:331:HIS:CE1	2:B:334:ALA:H	2.35	0.42
1:A:166:TYR:CZ	4:A:1:TIN:HC44	2.53	0.42
1:A:354:GLU:CG	2:B:329:MET:HA	2.50	0.42
2:B:153:THR:O	2:B:157:VAL:HG23	2.19	0.42
2:B:315:LEU:O	2:B:316:HIS:C	2.57	0.42
1:A:96:PHE:CE2	2:B:94:GLU:HG2	2.55	0.42
1:A:189:ILE:HD13	1:A:206:ARG:HB2	2.00	0.42
2:B:66:HIS:ND1	2:B:69:PRO:HG3	2.35	0.42
2:B:114:LEU:O	2:B:115:ASP:CB	2.65	0.42
2:B:292:CYS:O	2:B:293:ASN:HB2	2.20	0.42
2:B:389:VAL:C	2:B:391:GLU:H	2.23	0.42
1:A:80:GLN:H	1:A:104:ARG:NH1	2.17	0.42
1:A:106:VAL:O	1:A:107:LEU:C	2.58	0.42
2:B:389:VAL:N	2:B:392:ASN:ND2	2.68	0.42
3:A:501:HFP:O1	4:A:1:TIN:H292	2.20	0.42
2:B:42:THR:O	2:B:44:THR:N	2.53	0.42
2:B:201:VAL:CG2	2:B:202:ARG:N	2.83	0.42
1:A:355:TYR:OH	1:A:359:ILE:HD11	2.20	0.41
2:B:48:GLN:HE21	2:B:52:GLU:CG	2.33	0.41
2:B:160:LEU:HD13	2:B:172:ILE:HG13	2.02	0.41
1:A:170:HIS:CE1	2:B:196:GLY:O	2.73	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.92	0.41
1:A:342:GLU:O	1:A:343:ILE:C	2.59	0.41
2:B:24:TYR:CD2	2:B:334:ALA:HB2	2.56	0.41
1:A:75:ILE:HD13	1:A:109:ARG:HH11	1.84	0.41
1:A:96:PHE:CA	1:A:126:LEU:HD13	2.44	0.41
2:B:174:ARG:HB2	2:B:174:ARG:NH1	2.35	0.41
2:B:297:ASP:OD2	2:B:297:ASP:C	2.58	0.41
1:A:96:PHE:HA	1:A:126:LEU:HD11	1.99	0.41
1:A:109:ARG:O	1:A:111:GLU:N	2.53	0.41
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.91	0.41
1:A:154:TYR:O	1:A:157:ALA:HB3	2.20	0.41
1:A:311:LEU:HD23	1:A:315:LEU:HG	2.02	0.41
1:A:342:GLU:OE1	1:A:342:GLU:HA	2.20	0.41
1:A:100:TYR:O	1:A:101:ASP:C	2.57	0.41
1:A:106:VAL:HG11	1:A:116:ALA:HB1	2.02	0.41
2:B:230:ALA:HA	2:B:268:LEU:CD2	2.50	0.41
1:A:213:PHE:CD1	1:A:213:PHE:N	2.89	0.41
2:B:35:LEU:HB3	2:B:52:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:LEU:HD21	2:B:360:PHE:CE2	2.55	0.41
1:A:182:PRO:HG3	1:A:213:PHE:CD2	2.56	0.41
1:A:208:TRP:CE2	1:A:212:GLU:HG3	2.55	0.41
1:A:241:HIS:HB2	1:A:279:TYR:HE1	1.86	0.41
1:A:356:TRP:C	1:A:358:TYR:N	2.71	0.41
2:B:58:VAL:O	2:B:61:SER:HB3	2.21	0.41
2:B:69:PRO:O	2:B:71:LEU:N	2.52	0.41
2:B:261:ILE:O	2:B:263:LYS:HG3	2.21	0.41
2:B:274:LEU:HD13	2:B:311:LEU:HD13	2.03	0.41
2:B:286:GLY:HA3	2:B:334:ALA:O	2.20	0.41
1:A:161:GLU:C	1:A:163:PRO:HD3	2.41	0.41
1:A:287:ARG:N	1:A:287:ARG:HE	2.17	0.41
1:A:309:PRO:HG3	2:B:283:ARG:NH2	2.35	0.41
2:B:114:LEU:HD23	2:B:394:LEU:CD2	2.51	0.41
1:A:87:VAL:HG12	1:A:88:VAL:HG13	2.02	0.40
2:B:158:ASN:HD21	2:B:403:ILE:HG23	1.82	0.40
2:B:282:MET:C	2:B:284:PHE:H	2.25	0.40
1:A:136:PHE:CE2	1:A:140:LEU:HD11	2.57	0.40
1:A:181:ASP:OD1	1:A:181:ASP:C	2.60	0.40
1:A:196:ASP:C	1:A:198:LYS:N	2.73	0.40
2:B:289:GLN:NE2	2:B:294:LYS:H	2.20	0.40
2:B:398:HIS:HE1	2:B:400:VAL:HB	1.85	0.40
1:A:137:ARG:O	1:A:138:ARG:C	2.58	0.40
1:A:253:ARG:NE	1:A:253:ARG:CA	2.83	0.40
1:A:329:ASN:C	1:A:331:GLU:N	2.64	0.40
2:B:109:HIS:CE1	2:B:402:ASN:O	2.75	0.40
2:B:230:ALA:HA	2:B:268:LEU:HD21	2.03	0.40
2:B:362:HIS:C	2:B:364:CYS:H	2.23	0.40
1:A:100:TYR:O	1:A:103:PHE:N	2.55	0.40
1:A:179:LEU:HD22	1:A:179:LEU:N	2.37	0.40
2:B:404:GLY:C	2:B:406:ASP:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	313/315 (99%)	227 (72%)	66 (21%)	20 (6%)	1	14
2	B	395/397 (100%)	276 (70%)	96 (24%)	23 (6%)	1	16
All	All	708/712 (99%)	503 (71%)	162 (23%)	43 (6%)	1	15

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ASP
1	A	304	PRO
2	B	64	PHE
2	B	74	GLN
2	B	99	SER
2	B	322	ALA
1	A	56	LEU
1	A	71	GLU
1	A	185	GLU
1	A	197	ALA
1	A	326	GLN
1	A	365	SER
2	B	27	ARG
2	B	43	VAL
2	B	321	PRO
2	B	352	ASP
2	B	363	THR
2	B	413	THR
1	A	110	ASP
1	A	233	ASN
1	A	305	SER
1	A	330	LYS
1	A	334	LEU
1	A	357	ARG
2	B	70	ARG
2	B	115	ASP
2	B	174	ARG
2	B	246	GLU
2	B	404	GLY
2	B	61	SER
2	B	66	HIS
1	A	186	LEU
1	A	188	PHE

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Mol	Chain	Res	Type
1	A	274	GLU
2	B	110	SER
2	B	243	PRO
2	B	390	PRO
2	B	138	GLY
1	A	88	VAL
1	A	312	ILE
2	B	277	VAL
2	B	385	VAL
1	A	189	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/294 (100%)	285 (97%)	9 (3%)	40	70
2	B	335/335 (100%)	324 (97%)	11 (3%)	38	68
All	All	629/629 (100%)	609 (97%)	20 (3%)	39	69

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	GLU
1	A	167	GLN
1	A	179	LEU
1	A	181	ASP
1	A	182	PRO
1	A	239	GLN
1	A	253	ARG
1	A	287	ARG
1	A	331	GLU
2	B	29	GLU
2	B	64	PHE
2	B	70	ARG
2	B	71	LEU

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Mol	Chain	Res	Type
2	B	158	ASN
2	B	198	GLU
2	B	234	ASN
2	B	243	PRO
2	B	312	HIS
2	B	366	CYS
2	B	375	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	108	GLN
1	A	135	HIS
1	A	149	GLN
1	A	153	ASN
1	A	165	ASN
1	A	171	HIS
1	A	194	ASN
1	A	201	HIS
1	A	239	GLN
1	A	278	ASN
1	A	329	ASN
2	B	48	GLN
2	B	120	GLN
2	B	134	GLN
2	B	158	ASN
2	B	215	ASN
2	B	234	ASN
2	B	281	GLN
2	B	289	GLN
2	B	293	ASN
2	B	312	HIS
2	B	336	GLN
2	B	344	GLN
2	B	417	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	TIN	A	1	-	39,40,40	1.53	9 (23%)	47,52,52	1.57	6 (12%)
3	HFP	A	501	1	17,19,19	1.75	5 (29%)	22,25,25	2.26	7 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TIN	A	1	-	-	11/29/41/41	0/3/3/3
3	HFP	A	501	1	2/2/5/5	8/22/22/22	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HFP	C2-C3	-4.64	1.34	1.53
4	A	1	TIN	C44-C45	3.49	1.44	1.38
3	A	501	HFP	C7-C8	-3.33	1.35	1.52
4	A	1	TIN	C38-N2	3.05	1.53	1.47
4	A	1	TIN	C44-C43	2.73	1.43	1.38
4	A	1	TIN	C55-C56	2.61	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	TIN	C53-C52	2.60	1.42	1.37
4	A	1	TIN	O69-C68	-2.52	1.22	1.30
4	A	1	TIN	C43-C40	2.50	1.44	1.38
3	A	501	HFP	O1-C1	2.39	1.44	1.41
3	A	501	HFP	P-O1P	-2.30	1.46	1.49
3	A	501	HFP	C12-C13	-2.28	1.36	1.51
4	A	1	TIN	C54-C53	2.23	1.43	1.38
4	A	1	TIN	C47-C40	2.07	1.42	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HFP	C3-C2-C1	7.51	122.82	115.21
4	A	1	TIN	C66-N1-C65	5.65	135.42	121.60
4	A	1	TIN	C7-C52-C51	4.28	127.70	121.08
4	A	1	TIN	C68-C66-N1	3.29	118.33	110.55
3	A	501	HFP	C4-C3-C2	3.04	120.58	110.89
4	A	1	TIN	C7-C52-C53	-2.93	112.72	120.19
3	A	501	HFP	C2-C3-C5	2.54	120.40	111.98
3	A	501	HFP	C9-C8-C7	2.41	120.03	111.29
4	A	1	TIN	C40-C38-N2	2.26	117.51	113.12
3	A	501	HFP	C4-C3-C5	2.13	119.02	111.29
3	A	501	HFP	O1P-P-C1	-2.07	107.92	112.94
3	A	501	HFP	C9-C8-C10	2.03	118.64	111.29
4	A	1	TIN	C26-C25-N2	-2.02	108.75	113.84

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	501	HFP	C8
3	A	501	HFP	C3

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HFP	P-C1-C2-C3
3	A	501	HFP	O1-C1-C2-C3
4	A	1	TIN	C45-C65-N1-C66
4	A	1	TIN	O67-C65-N1-C66
4	A	1	TIN	C74-C66-N1-C65
3	A	501	HFP	C6-C7-C8-C9
3	A	501	HFP	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	A	1	TIN	C17-C19-N2-C25
4	A	1	TIN	C17-C19-N2-C38
4	A	1	TIN	N1-C66-C74-C76
4	A	1	TIN	C19-C17-C3-C2
4	A	1	TIN	C19-C17-C3-C4
3	A	501	HFP	C1-C2-C3-C4
3	A	501	HFP	C2-C1-P-O1P
4	A	1	TIN	C26-C25-N2-C38
3	A	501	HFP	C11-C10-C8-C9
3	A	501	HFP	C4-C3-C5-C6
4	A	1	TIN	C26-C25-N2-C19
4	A	1	TIN	C40-C38-N2-C19

There are no ring outliers.

2 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	TIN	10	0
3	A	501	HFP	20	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 TIN A 1

Bond lengths

Bond angles

Torsions

Rings

Ligand HFP A 501

Bond lengths

Bond angles

Torsions

Rings
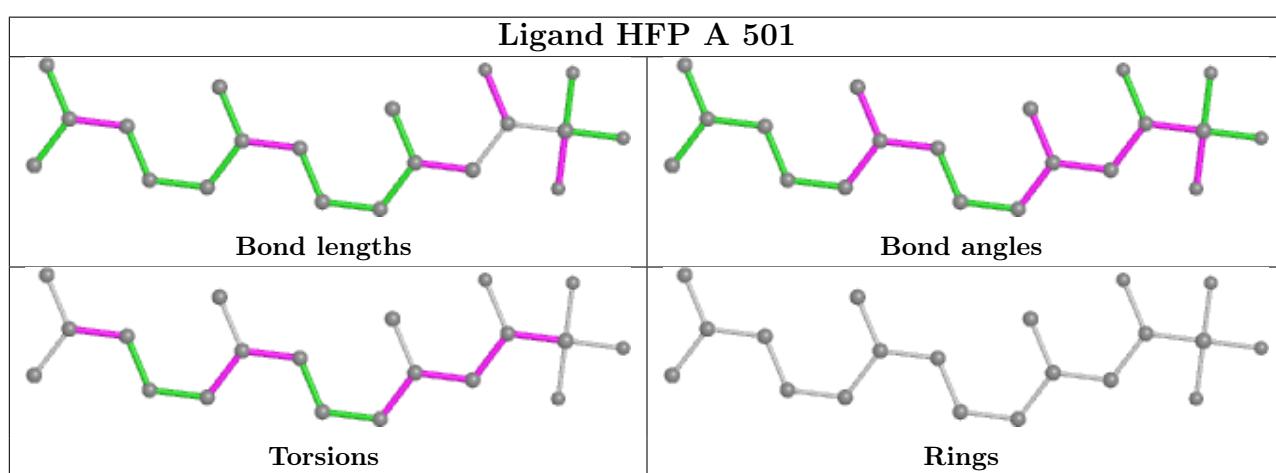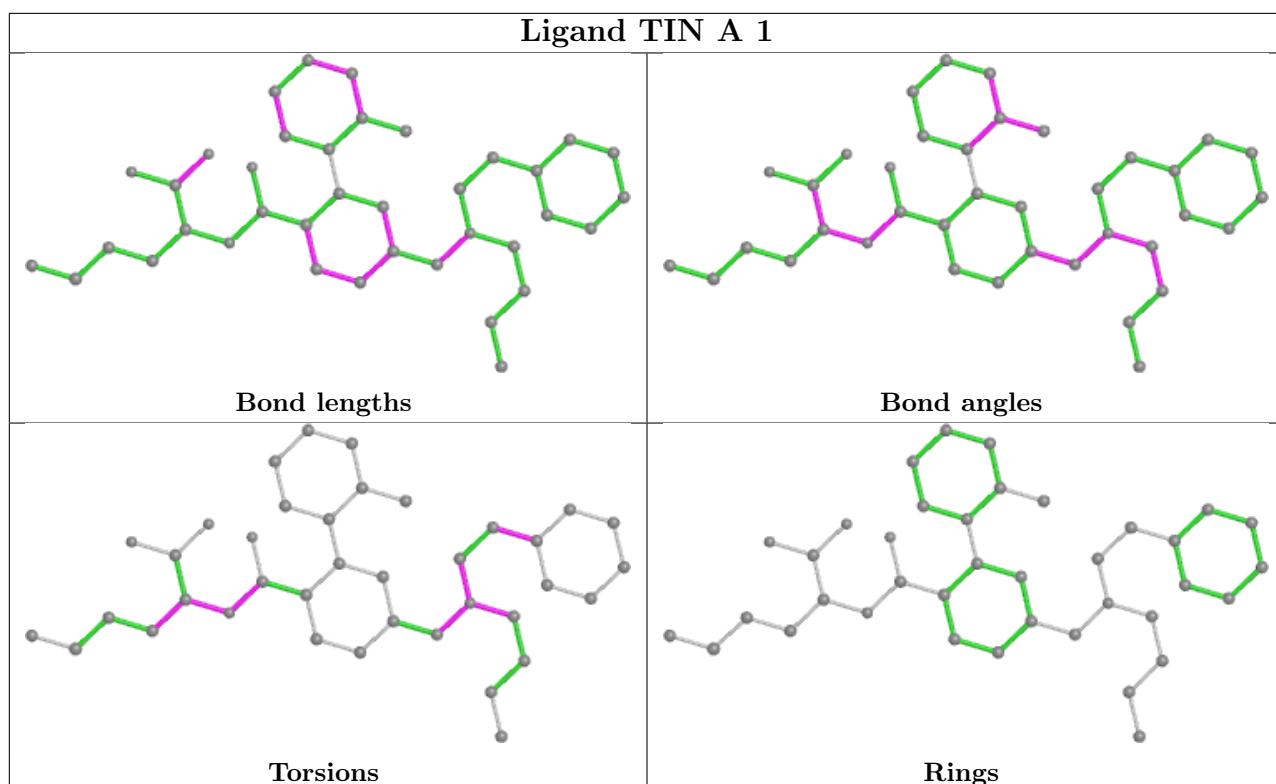
5.7 Other polymers ⓘ

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 HFP A 501:

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

Electron density around TIN A 1:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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.