



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:21 PM UTC

PDB ID : 1N94 / pdb_00001n94
Title : Aryl Tetrahydropyridine Inhibitors of Farnesyltransferase: Glycine, Phenylalanine 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

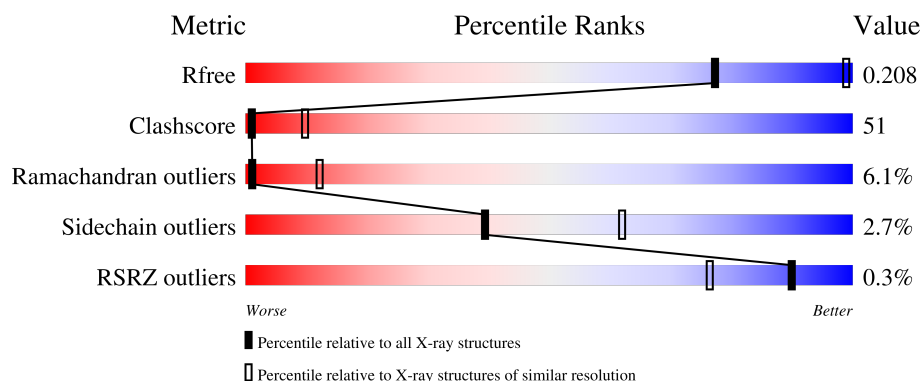
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

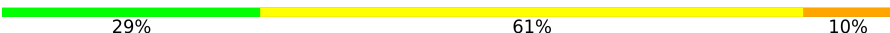
The reported resolution of this entry is 3.50 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	A	315	 29% 61% 10%
2	B	397	 34% 56% 9% .

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.

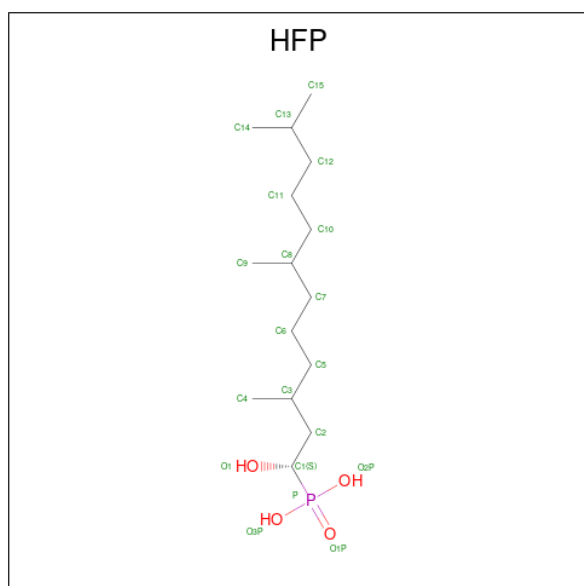
- Molecule 1 is a protein called Protein farnesyltransferase alpha subunit.

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

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

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

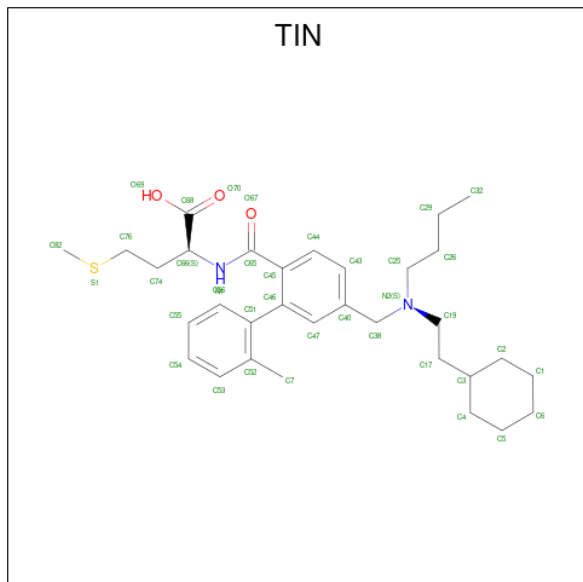
- Molecule 3 is ALPHA-HYDROXYFARNESYLPHOSPHONIC ACID (CCD ID: HFP) (formula: $C_{15}H_{33}O_4P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	15	4	1		

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

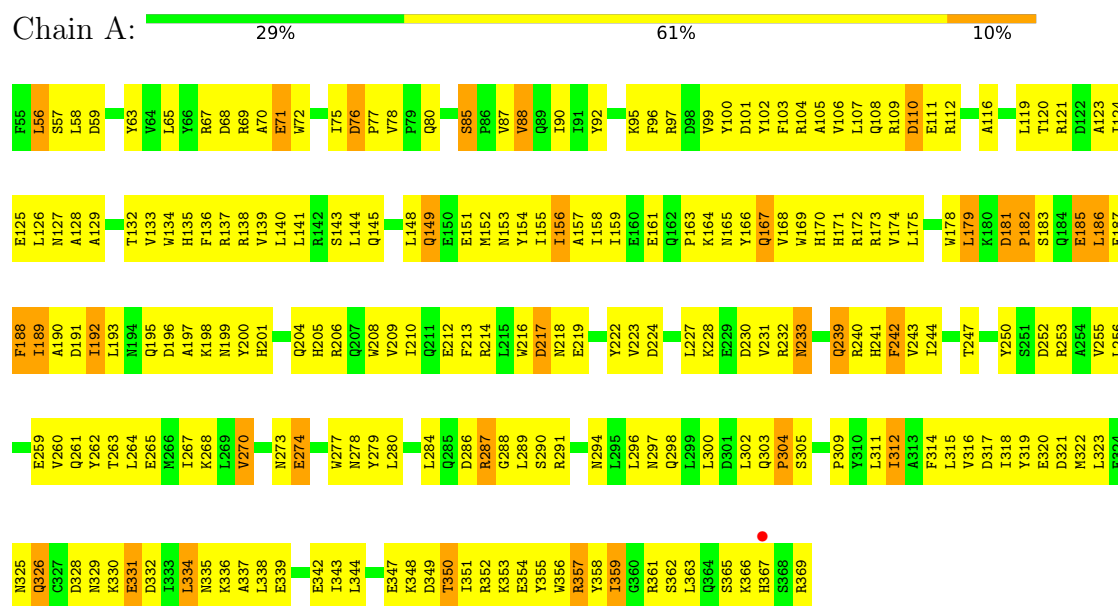
THYL-BIPHENYL-2-CARBONYL)-AMINO]-4-METHYLSULFANYL-BUTYRIC ACID
(CCD ID: TIN) (formula: C₃₂H₄₆N₂O₃S).



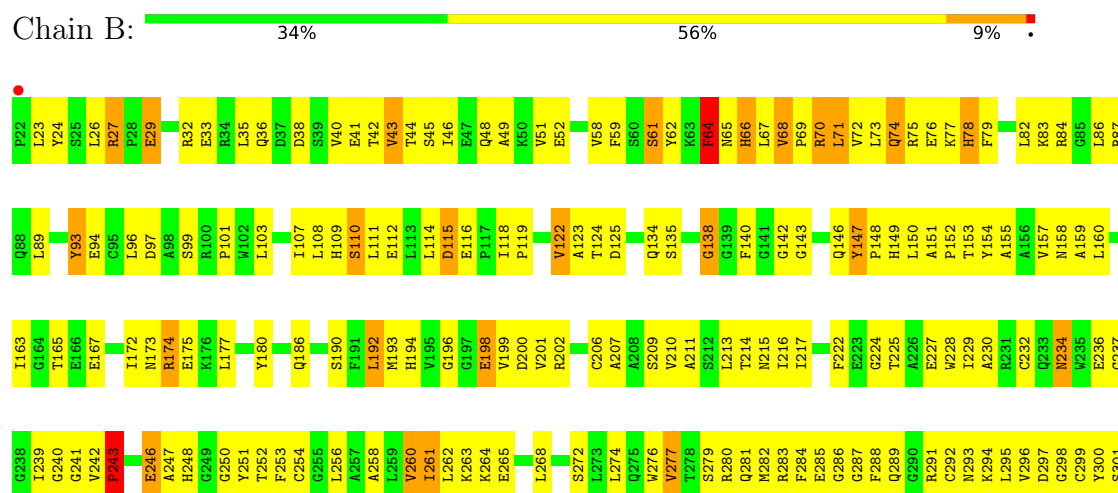
3 Residue-property plots

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 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: Protein farnesyltransferase alpha subunit



• Molecule 2: Protein farnesyltransferase beta subunit



F302	W303	Q304	A305	G306	L307	L308	P309	L310	L311	H312	L315	H316	D320	P321	A322	L323	S324	M325	S326	H327	W328	M329	F330	H331	Q332	Q333	A334	L335	Q336	E337	Y338	I339	L340	M341	C342	G343	Q344	C345	G348	G349	L350	L351	D352	K353	P354	G355	K356	S357	R358	D359	F360	Y361	H362	T363	C364	Y365
C366	L367	S368	G369	L370	A373	Q374	H375	F376	G377	S378	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	L416	Q417	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 33.94 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (33.94-3.50) 87.3 (33.94-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.18Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.295 , 0.296 0.210 , 0.208	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)	0.32 , 73.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.51	0/2755	1.03	17/3738 (0.5%)
2	B	0.50	0/3208	1.06	20/4353 (0.5%)
All	All	0.51	0/5963	1.04	37/8091 (0.5%)

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.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	ILE	N-CA-C	-9.39	101.23	110.72
2	B	32	ARG	N-CA-C	-8.36	103.60	113.88
1	A	195	GLN	N-CA-C	-7.89	103.60	113.55
1	A	348	LYS	N-CA-C	7.73	119.70	111.28
1	A	242	PHE	N-CA-C	-7.69	102.45	112.68
2	B	122	VAL	N-CA-C	-7.22	103.43	110.72
1	A	76	ASP	CA-C-N	6.97	127.38	119.92
1	A	76	ASP	C-N-CA	6.97	127.38	119.92
1	A	270	VAL	CA-C-N	6.79	127.35	119.47
1	A	270	VAL	C-N-CA	6.79	127.35	119.47
1	A	149	GLN	N-CA-C	-6.78	103.97	111.36
2	B	328	TRP	N-CA-C	-6.52	100.82	110.46
1	A	156	ILE	N-CA-C	-6.43	104.25	110.42
1	A	288	GLY	N-CA-C	-6.40	104.62	112.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	TYR	N-CA-C	-6.29	104.05	111.03
2	B	351	LEU	N-CA-C	6.17	117.25	108.74
2	B	192	LEU	N-CA-C	-6.09	102.68	110.53
2	B	150	LEU	N-CA-C	5.99	120.13	112.34
1	A	192	ILE	N-CA-C	-5.88	104.78	110.42
1	A	228	LYS	N-CA-C	-5.80	104.64	110.97
2	B	307	LEU	N-CA-C	5.70	117.17	111.07
2	B	260	VAL	N-CA-C	-5.69	103.97	111.09
2	B	370	LEU	N-CA-C	-5.64	106.06	113.12
2	B	217	ILE	N-CA-C	5.58	116.14	107.99
2	B	36	GLN	N-CA-C	-5.58	98.12	107.99
2	B	339	ILE	CB-CA-C	-5.41	104.95	112.04
1	A	350	THR	N-CA-C	5.30	117.06	111.28
2	B	68	VAL	CA-C-N	5.27	125.26	119.89
2	B	68	VAL	C-N-CA	5.27	125.26	119.89
1	A	335	ASN	N-CA-C	-5.19	106.89	113.43
2	B	147	TYR	CA-C-N	5.12	125.03	119.76
2	B	147	TYR	C-N-CA	5.12	125.03	119.76
2	B	261	ILE	N-CA-C	-5.11	105.62	110.42
1	A	85	SER	CA-C-N	5.05	125.04	119.89
1	A	85	SER	C-N-CA	5.05	125.04	119.89
2	B	193	MET	N-CA-C	-5.04	104.74	111.24
2	B	78	HIS	N-CA-C	-5.00	106.68	112.89

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	307	0
2	B	3125	0	3058	307	0
3	A	20	0	28	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	38	0	45	11	0
5	B	1	0	0	0	0
All	All	5873	0	5745	597	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 51.

All (597) 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:164:LYS:CD	3:A:501:HFP:O1P	1.80	1.28
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:59:PHE:HA	2:B:341:MET:HE1	1.42	0.98
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: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
2:B:280:ARG:NH1	2:B:292:CYS:HA	1.97	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:GLN:CD	1:A:167:GLN:H	1.94	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
1:A:156:ILE:HG23	1:A:188:PHE:CE1	2.23	0.74
2:B:175:GLU:CD	2:B:175:GLU:H	1.94	0.74
1:A:329:ASN:C	1:A:331:GLU:H	1.96	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:412:THR:C	2:B:414:HIS:H	1.99	0.71
2:B:79:PHE:CZ	2:B:83:LYS:HD2	2.26	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:69:PRO:C	2:B:71:LEU:H	2.01	0.69
1:A:96:PHE:HA	1:A:126:LEU:CD1	2.21	0.69
3:A:501:HFP:H62	2:B:248:HIS:NE2	2.08	0.69

Continued on next page...

Continued from previous page...

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
2:B:58:VAL:HG12	2:B:341:MET:HE2	1.76	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: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: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:87:VAL:O	1:A:88:VAL:C	2.41	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
1:A:356:TRP:C	1:A:358:TYR:H	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ILE:O	2:B:49:ALA:HB3	1.99	0.63
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
1:A:152:MET:HE1	1:A:172:ARG:NH2	2.17	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
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:196:ASP:C	1:A:198:LYS:H	2.10	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:70:ARG:C	2:B:72:VAL:H	2.10	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:VAL:HG22	2:B:307:LEU:HD13	1.84	0.58
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: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
2:B:376:PHE:CD1	2:B:376:PHE:C	2.82	0.57
1:A:206:ARG:NH2	1:A:222:TYR:CD2	2.72	0.57
1:A:256:LEU:HD23	1:A:256:LEU:C	2.30	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
1:A:70:ALA:C	1:A:72:TRP:H	2.13	0.57
1:A:230:ASP:CG	2:B:42:THR:HB	2.30	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:62:TYR:HE2	2:B:341:MET:HE3	1.70	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:291:ARG:NH2	2:B:294:LYS:HE2	2.15	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:165:THR:C	2:B:167:GLU:N	2.63	0.55
2:B:264:LYS:O	2:B:265:GLU:C	2.49	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:152:MET:HE1	1:A:172:ARG:CZ	2.37	0.54
1:A:165:ASN:HB3	1:A:168:VAL:HG12	1.87	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:333:GLN:HG3	2:B:387:MET:SD	2.48	0.54
2:B:412:THR:C	2:B:414:HIS:N	2.63	0.54
1:A:70:ALA:C	1:A:72:TRP:N	2.66	0.54
1:A:325:ASN:O	1:A:326:GLN:C	2.49	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:311:LEU:O	1:A:312:ILE:C	2.50	0.53
2:B:362:HIS:C	2:B:364:CYS:N	2.65	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
2:B:276:TRP:O	2:B:277:VAL:C	2.50	0.53
1:A:280:LEU:HD23	1:A:314:PHE:CE2	2.44	0.53
2:B:62:TYR:CE2	2:B:341:MET:HE3	2.44	0.53
2:B:70:ARG:C	2:B:72:VAL:N	2.67	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
1:A:314:PHE:O	1:A:317:ASP:HB2	2.08	0.53
2:B:48:GLN:O	2:B:52:GLU:HG3	2.08	0.52
2:B:403:ILE:O	2:B:404:GLY:C	2.49	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:LEU:O	2:B:27:ARG:C	2.52	0.52
1:A:65:LEU:CD1	1:A:67:ARG:HH21	2.23	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:127:ASN:C	1:A:129:ALA:H	2.17	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:175:GLU:CD	2:B:175:GLU:N	2.64	0.52
2:B:339:ILE:HD12	2:B:370:LEU:CD1	2.40	0.52
1:A:232:ARG:NH1	2:B:45:SER:HB2	2.25	0.52
2:B:69:PRO:C	2:B:71:LEU:N	2.68	0.52
1:A:90:ILE:HB	1:A:92:TYR:CE1	2.44	0.51
1:A:96:PHE:CD1	1:A:96:PHE:C	2.87	0.51
1:A:104:ARG:O	1:A:105:ALA:C	2.53	0.51
1:A:166:TYR:HH	4:A:1:TIN:HC44	1.75	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
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
1:A:358:TYR:HB2	1:A:361:ARG:NH2	2.25	0.51
2:B:165:THR:C	2:B:167:GLU:H	2.19	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:42:THR:O	2:B:43:VAL:C	2.53	0.51
2:B:134:GLN:NE2	2:B:173:ASN:H	2.05	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:HIS:O	2:B:110:SER:C	2.53	0.50
2:B:198:GLU:CD	2:B:198:GLU:H	2.19	0.50
2:B:122:VAL:O	2:B:123:ALA:C	2.55	0.50
2:B:230:ALA:C	2:B:232:CYS:N	2.68	0.50
2:B:234:ASN:ND2	2:B:234:ASN:C	2.66	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
1:A:230:ASP:OD2	1:A:230:ASP:C	2.54	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
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
1:A:120:THR:O	1:A:121:ARG:C	2.55	0.49
1:A:329:ASN:C	1:A:331:GLU:N	2.64	0.49
2:B:396:PRO:O	2:B:405:PRO:HD3	2.12	0.49
2:B:234:ASN:ND2	2:B:236:GLU:N	2.57	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:351:ILE:HG12	2:B:281:GLN:NE2	2.28	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:200:ASP:O	2:B:201:VAL:C	2.56	0.48
2:B:336:GLN:HG2	2:B:370:LEU:HD12	1.95	0.48
1:A:143:SER:C	1:A:145:GLN:H	2.21	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
2:B:230:ALA:C	2:B:232:CYS:H	2.21	0.48
1:A:289:LEU:N	1:A:321:ASP:OD2	2.47	0.48
2:B:93:TYR:CD2	2:B:96:LEU:HD12	2.49	0.48
2:B:201:VAL:O	2:B:202:ARG:C	2.56	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
2:B:322:ALA:O	2:B:323:LEU:C	2.55	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: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:185:GLU:O	1:A:186:LEU:C	2.57	0.47
1:A:188:PHE:O	1:A:189:ILE:C	2.57	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:143:SER:C	1:A:145:GLN:N	2.72	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
2:B:214:THR:O	2:B:215:ASN:C	2.57	0.47
1:A:344:LEU:HD13	1:A:356:TRP:CD2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:71:GLU:CD	1:A:71:GLU:H	2.22	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:262:TYR:CD1	1:A:262:TYR:C	2.92	0.47
1:A:315:LEU:O	1:A:316:VAL:C	2.56	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: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: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:315:LEU:O	2:B:316:HIS:C	2.57	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:106:VAL:O	1:A:107:LEU:C	2.58	0.46
1:A:152:MET:O	1:A:155:ILE:HG22	2.15	0.46
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: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: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:342:GLU:O	1:A:343:ILE:C	2.59	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
2:B:389:VAL:C	2:B:391:GLU:H	2.23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:ASP:OD2	2:B:297:ASP:C	2.58	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:100:TYR:O	1:A:101:ASP:C	2.57	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
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
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: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
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:161:GLU:C	1:A:163:PRO:HD3	2.41	0.45
1:A:354:GLU:HG3	2:B:329:MET:HA	1.98	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
1:A:265:GLU:OE2	1:A:265:GLU:HA	2.15	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
1:A:181:ASP:OD1	1:A:181:ASP:C	2.60	0.45
2:B:210:VAL:HG12	2:B:211:ALA:N	2.32	0.45
2:B:282:MET:C	2:B:284:PHE:H	2.25	0.45
1:A:95:LYS:O	1:A:99:VAL:HG23	2.17	0.45
1:A:137:ARG:O	1:A:138:ARG:C	2.58	0.45
1:A:303:GLN:N	1:A:304:PRO:CD	2.79	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
2:B:362:HIS:C	2:B:364:CYS:H	2.23	0.45
1:A:56:LEU:HB3	1:A:57:SER:H	1.61	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:404:GLY:C	2:B:406:ASP:N	2.74	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
2:B:206:CYS:O	2:B:207:ALA:C	2.58	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
1:A:240:ARG:C	1:A:242:PHE:H	2.25	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
2:B:213:LEU:C	2:B:215:ASN:H	2.25	0.44
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.29	0.44
1:A:260:VAL:O	1:A:261:GLN:C	2.58	0.44
1:A:343:ILE:O	1:A:347:GLU:N	2.48	0.44
2:B:59:PHE:HA	2:B:341:MET:CE	2.31	0.44
2:B:280:ARG:HA	2:B:280:ARG:NE	2.32	0.44
2:B:397:THR:C	2:B:405:PRO:HG3	2.42	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:181:ASP:O	1:A:181:ASP:CG	2.61	0.44
1:A:274:GLU:O	1:A:274:GLU:HG2	2.18	0.44
1:A:289:LEU:C	1:A:291:ARG:N	2.74	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
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:O	2:B:199:VAL:HG23	2.18	0.43
2:B:240:GLY:O	2:B:241:GLY:C	2.62	0.43
2:B:367:LEU:O	2:B:368:SER:C	2.60	0.43
1:A:260:VAL:HG22	1:A:284:LEU:HD21	1.99	0.43
3:A:501:HFP:H62	2:B:248:HIS:HE2	1.79	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:LEU:O	2:B:97:ASP:C	2.61	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
1:A:366:LYS:C	1:A:367:HIS:ND1	2.77	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:361:TYR:O	2:B:362:HIS:C	2.62	0.43
2:B:416:LEU:C	2:B:418:LYS:H	2.26	0.43
1:A:103:PHE:O	1:A:104:ARG:C	2.61	0.43
2:B:320:ASP:OD2	2:B:320:ASP:C	2.61	0.43
1:A:57:SER:HB3	1:A:59:ASP:OD1	2.18	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: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:182:PRO:HD3	1:A:213:PHE:CE2	2.53	0.43
1:A:216:TRP:CD1	1:A:216:TRP:H	2.36	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:234:ASN:C	2:B:234:ASN:HD22	2.27	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
2:B:246:GLU:OE1	2:B:291:ARG:HD2	2.20	0.42
2:B:138:GLY:HA3	2:B:180:TYR:HB2	2.00	0.42
2:B:362:HIS:O	2:B:363:THR:C	2.62	0.42
2:B:389:VAL:O	2:B:391:GLU:N	2.52	0.42
1:A:243:VAL:O	1:A:247:THR:HG23	2.20	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
1:A:182:PRO:O	1:A:183:SER:C	2.63	0.42
2:B:252:THR:O	2:B:253:PHE:C	2.63	0.42
1:A:96:PHE:CE2	2:B:94:GLU:HG2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:VAL:O	2:B:243:PRO:C	2.63	0.42
2:B:292:CYS:O	2:B:293:ASN:HB2	2.20	0.42
2:B:298:GLY:O	2:B:299:CYS:C	2.62	0.42
1:A:80:GLN:H	1:A:104:ARG:NH1	2.17	0.42
2:B:159:ALA:O	2:B:160:LEU:C	2.63	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:233:ASN:OD1	1:A:233:ASN:C	2.62	0.41
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:204:GLN:O	1:A:205:HIS:C	2.61	0.41
1:A:337:ALA:C	1:A:339:GLU:N	2.76	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:389:VAL:C	2:B:391:GLU:N	2.78	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:106:VAL:HG11	1:A:116:ALA:HB1	2.02	0.41
1:A:213:PHE:O	1:A:214:ARG:C	2.63	0.41
1:A:216:TRP:O	1:A:217:ASP:C	2.63	0.41
2:B:230:ALA:HA	2:B:268:LEU:CD2	2.50	0.41
1:A:100:TYR:C	1:A:102:TYR:N	2.76	0.41
1:A:213:PHE:CD1	1:A:213:PHE:N	2.89	0.41
1:A:252:ASP:CG	1:A:255:VAL:HG23	2.45	0.41
2:B:35:LEU:HB3	2:B:52:GLU:OE1	2.21	0.41
2:B:89:LEU:HD21	2:B:360:PHE:CE2	2.55	0.41
2:B:107:ILE:O	2:B:108:LEU:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:GLU:CD	2:B:291:ARG:HD2	2.46	0.41
1:A:109:ARG:C	1:A:111:GLU:N	2.77	0.41
1:A:169:TRP:O	1:A:170:HIS:C	2.63	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:262:TYR:O	1:A:263:THR:C	2.64	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
2:B:304:GLN:C	2:B:306:GLY:N	2.75	0.41
1:A:109:ARG:O	1:A:110:ASP:C	2.62	0.41
1:A:199:ASN:O	1:A:200:TYR:C	2.62	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
2:B:325:MET:O	2:B:381:MET:HE2	2.21	0.41
1:A:87:VAL:HG12	1:A:88:VAL:HG13	2.02	0.40
2:B:124:THR:O	2:B:125:ASP:C	2.64	0.40
2:B:158:ASN:HD21	2:B:403:ILE:HG23	1.82	0.40
1:A:289:LEU:C	1:A:291:ARG:H	2.29	0.40
1:A:135:HIS:C	1:A:137:ARG:N	2.78	0.40
1:A:136:PHE:CE2	1:A:140:LEU:HD11	2.57	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:200:TYR:O	1:A:201:HIS:C	2.65	0.40
1:A:253:ARG:NE	1:A:253:ARG:CA	2.83	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
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

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	11
2	B	395/397 (100%)	276 (70%)	96 (24%)	23 (6%)	1	13
All	All	708/712 (99%)	503 (71%)	162 (23%)	43 (6%)	1	12

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	286 (97%)	8 (3%)	39	62
2	B	335/335 (100%)	326 (97%)	9 (3%)	39	62
All	All	629/629 (100%)	612 (97%)	17 (3%)	39	62

All (17) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	239	GLN
1	A	287	ARG
1	A	331	GLU
2	B	29	GLU
2	B	64	PHE
2	B	71	LEU
2	B	198	GLU
2	B	234	ASN
2	B	243	PRO
2	B	312	HIS
2	B	354	PRO
2	B	366	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) 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	184	GLN
1	A	201	HIS
1	A	239	GLN
1	A	278	ASN
1	A	285	GLN
1	A	329	ASN
1	A	335	ASN
2	B	48	GLN
2	B	74	GLN
2	B	120	GLN
2	B	134	GLN
2	B	158	ASN
2	B	194	HIS
2	B	234	ASN
2	B	281	GLN
2	B	289	GLN
2	B	293	ASN
2	B	312	HIS
2	B	336	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	344	GLN
2	B	383	HIS
2	B	414	HIS
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 [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 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	-	40,40,40	1.62	10 (25%)	52,52,52	1.47	6 (11%)
3	HFP	A	501	-	16,19,19	1.81	4 (25%)	20,25,25	2.36	6 (30%)

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	-	-	13/33/41/41	0/3/3/3
3	HFP	A	501	-	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	-4.95	1.34	1.53
3	A	501	HFP	C7-C8	-3.61	1.35	1.52
4	A	1	TIN	C38-N2	3.07	1.53	1.47
4	A	1	TIN	C44-C43	3.04	1.43	1.38
4	A	1	TIN	C45-C46	2.98	1.45	1.40
4	A	1	TIN	C44-C45	2.90	1.44	1.39
4	A	1	TIN	C54-C53	2.76	1.43	1.38
4	A	1	TIN	C43-C40	2.69	1.44	1.38
4	A	1	TIN	C56-C51	2.65	1.44	1.40
4	A	1	TIN	O69-C68	-2.62	1.22	1.30
3	A	501	HFP	C12-C13	-2.48	1.36	1.51
3	A	501	HFP	P-O1P	-2.32	1.46	1.49
4	A	1	TIN	C55-C54	2.22	1.43	1.38
4	A	1	TIN	C55-C56	2.19	1.42	1.38

All (12) 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	5.78	135.42	121.56
4	A	1	TIN	C7-C52-C53	-3.92	112.72	120.28
4	A	1	TIN	C68-C66-N1	3.35	118.33	110.57
4	A	1	TIN	C7-C52-C51	3.26	127.70	122.20
3	A	501	HFP	C4-C3-C2	3.19	120.58	110.84
3	A	501	HFP	C2-C3-C5	2.61	120.40	111.86
3	A	501	HFP	C9-C8-C7	2.46	120.03	111.27
3	A	501	HFP	C4-C3-C5	2.17	119.02	111.27
4	A	1	TIN	C40-C38-N2	2.13	117.51	113.15
3	A	501	HFP	C9-C8-C10	2.07	118.64	111.27
4	A	1	TIN	C38-N2-C19	2.02	115.48	111.28

All (2) chirality outliers are listed below:

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

All (21) torsion outliers are listed below:

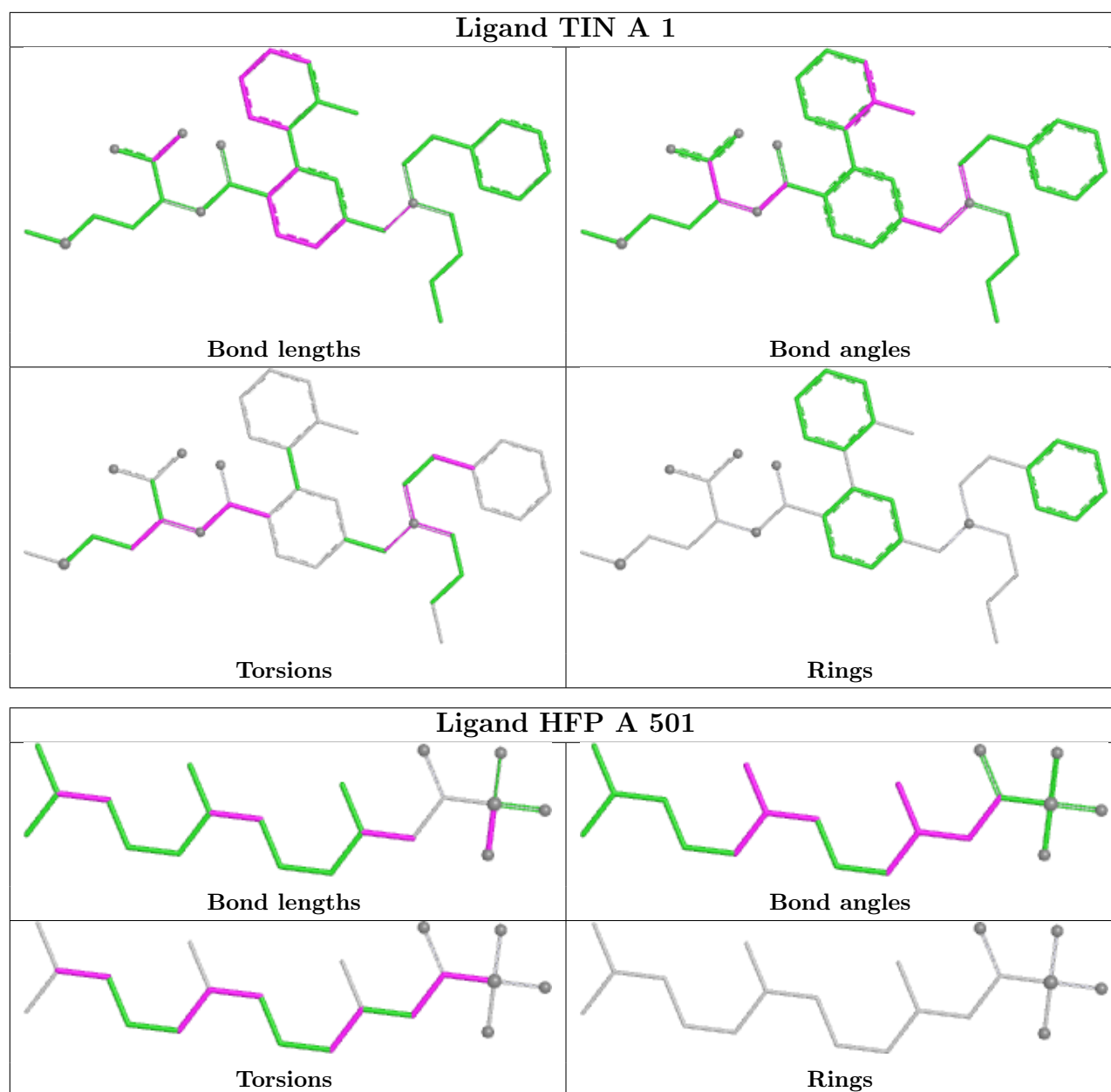
Mol	Chain	Res	Type	Atoms
3	A	501	HFP	O1-C1-P-O1P
3	A	501	HFP	P-C1-C2-C3
3	A	501	HFP	O1-C1-C2-C3
4	A	1	TIN	C19-C17-C3-C2
4	A	1	TIN	C19-C17-C3-C4
4	A	1	TIN	C45-C65-N1-C66
4	A	1	TIN	C74-C66-N1-C65
4	A	1	TIN	O67-C65-N1-C66
3	A	501	HFP	C6-C7-C8-C9
3	A	501	HFP	C11-C12-C13-C14
4	A	1	TIN	C17-C19-N2-C25
4	A	1	TIN	C17-C19-N2-C38
3	A	501	HFP	C2-C1-P-O1P
4	A	1	TIN	N1-C66-C74-C76
3	A	501	HFP	C11-C10-C8-C9
4	A	1	TIN	C26-C25-N2-C38
3	A	501	HFP	C4-C3-C5-C6
4	A	1	TIN	C44-C45-C65-O67
4	A	1	TIN	C44-C45-C65-N1
4	A	1	TIN	C40-C38-N2-C19
4	A	1	TIN	C26-C25-N2-C19

There are no ring outliers.

2 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	TIN	11	0
3	A	501	HFP	22	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 [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	A	315/315 (100%)	-0.28	1 (0%) 90 76	5, 36, 85, 99	0
2	B	397/397 (100%)	-0.29	1 (0%) 90 76	5, 32, 82, 99	0
All	All	712/712 (100%)	-0.29	2 (0%) 90 76	5, 34, 84, 99	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	22	PRO	2.6
1	A	367	HIS	2.2

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](#)

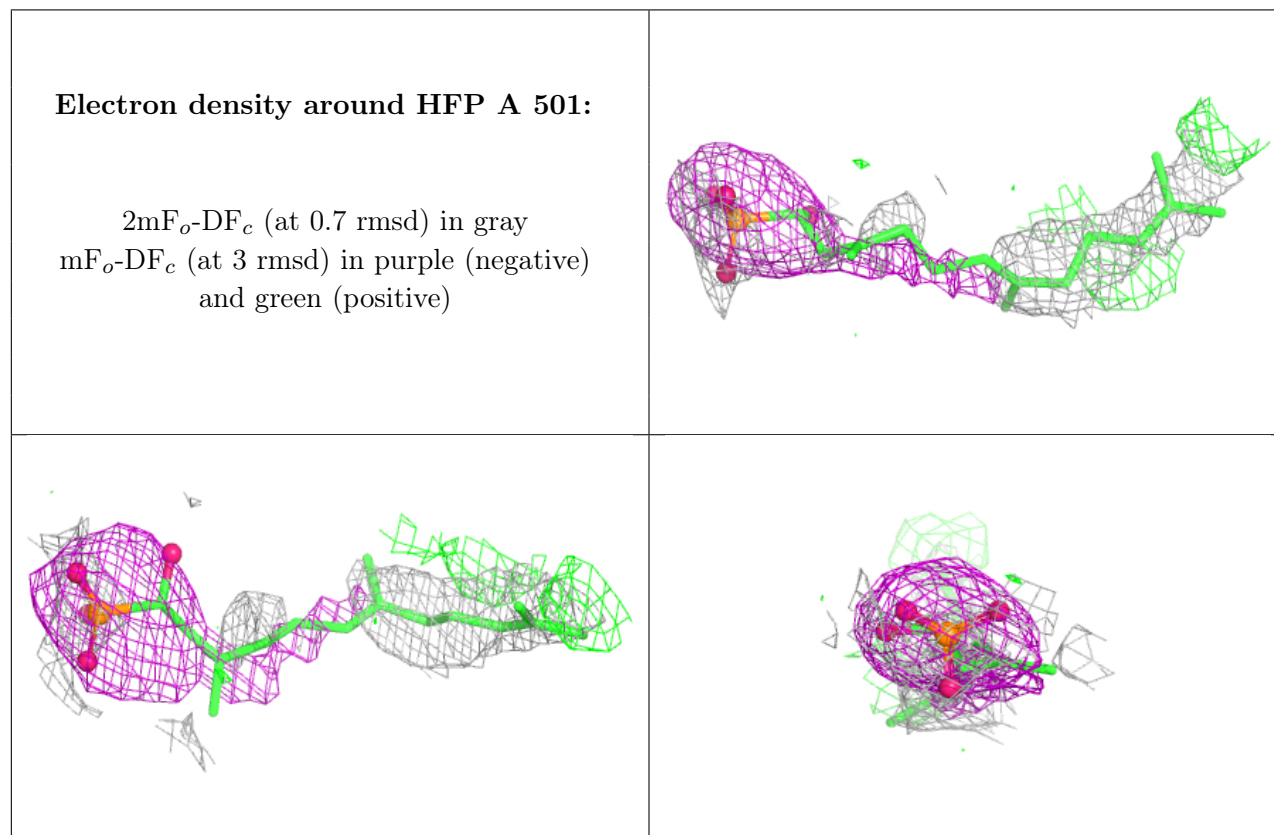
There are no oligosaccharides in this entry.

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.

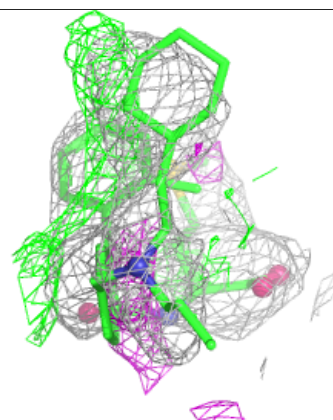
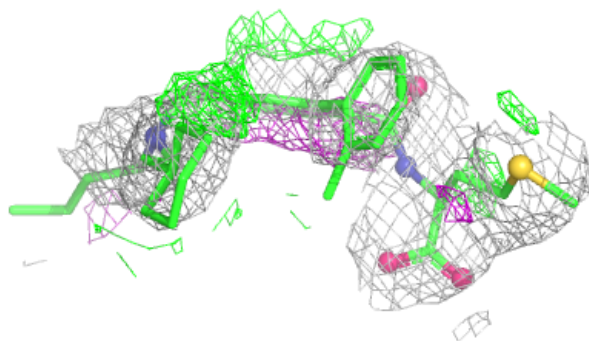
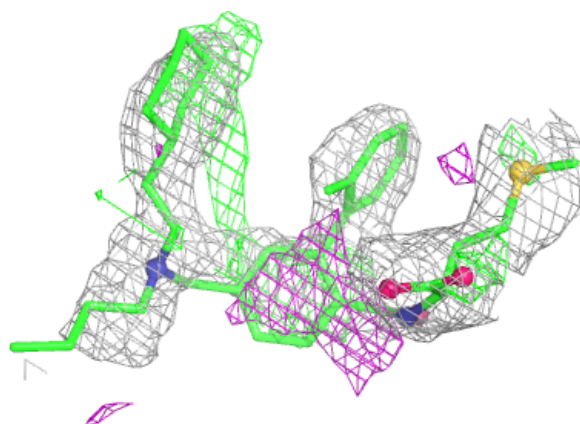
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HFP	A	501	20/20	0.72	0.31	16,34,48,53	0
4	TIN	A	1	38/38	0.79	0.21	36,36,36,36	0
5	ZN	B	2	1/1	1.00	0.01	15,15,15,15	0

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 TIN A 1:

$2mF_o-DF_c$ (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.