



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:13 AM UTC

PDB ID : 1NL4 / pdb_00001nl4
Title : Crystal Structure of Rat Farnesyl Transferase in Complex With A Potent Biphenyl Inhibitor
Authors : Curtin, M.L.; Florjancic, A.S.; Cohen, J.; Gu, W.-J.; Frost, D.J.; Muchmore, S.W.; Sham, H.L.
Deposited on : 2003-01-06
Resolution : 2.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

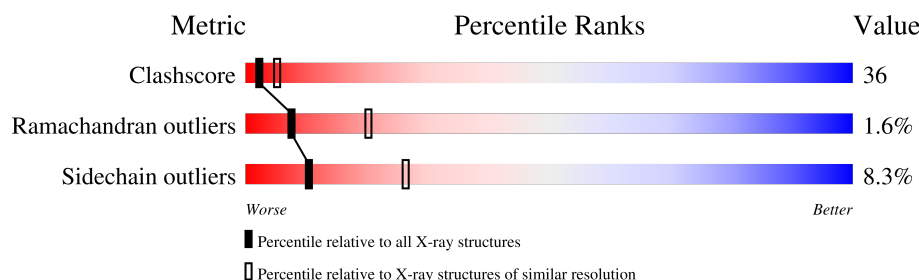
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	312	
2	B	401	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HFP	B	501	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5871 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	312	Total	C	N	O	S	0	0	0
			2661	1695	465	496	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	THR	ILE	SEE REMARK 999	UNP Q04631

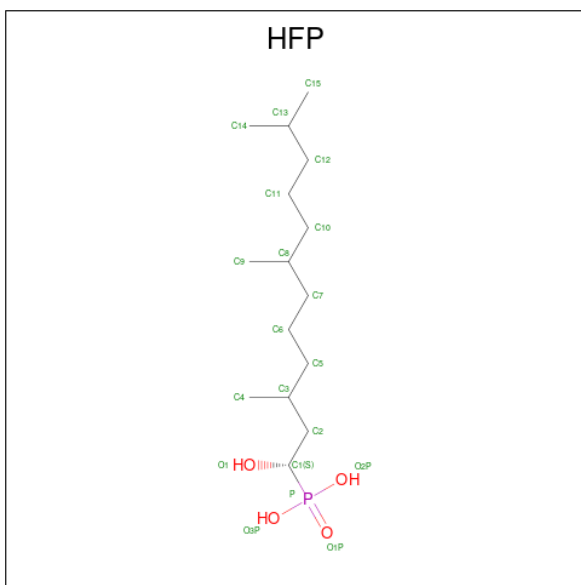
- Molecule 2 is a protein called Protein farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3154	2016	543	572	23			

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

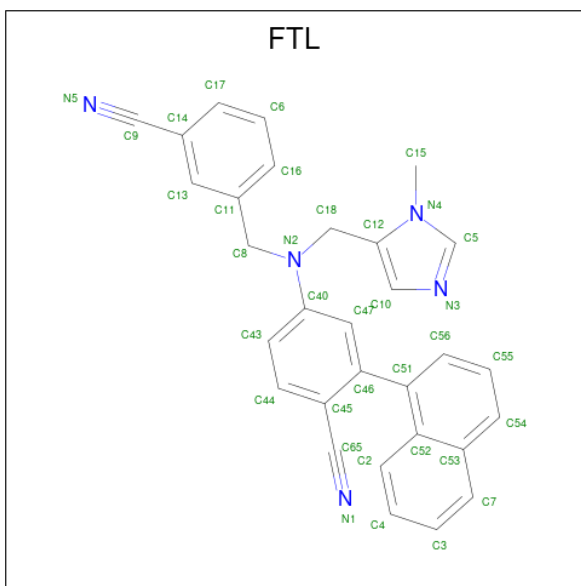
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ALPHA-HYDROXYFARNESYLPHOSPHONIC ACID (CCD ID: HFP) (formula: C₁₅H₃₃O₄P).



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

- Molecule 5 is 4-[(3-CYANO-BENZYL)-(3-METHYL-3H-IMIDAZOL-4-YLMETHYL)-AMINO]-2-NAPHTHALEN-1-YL-BENZONITRILE (CCD ID: FTL) (formula: $C_{30}H_{23}N_5$).



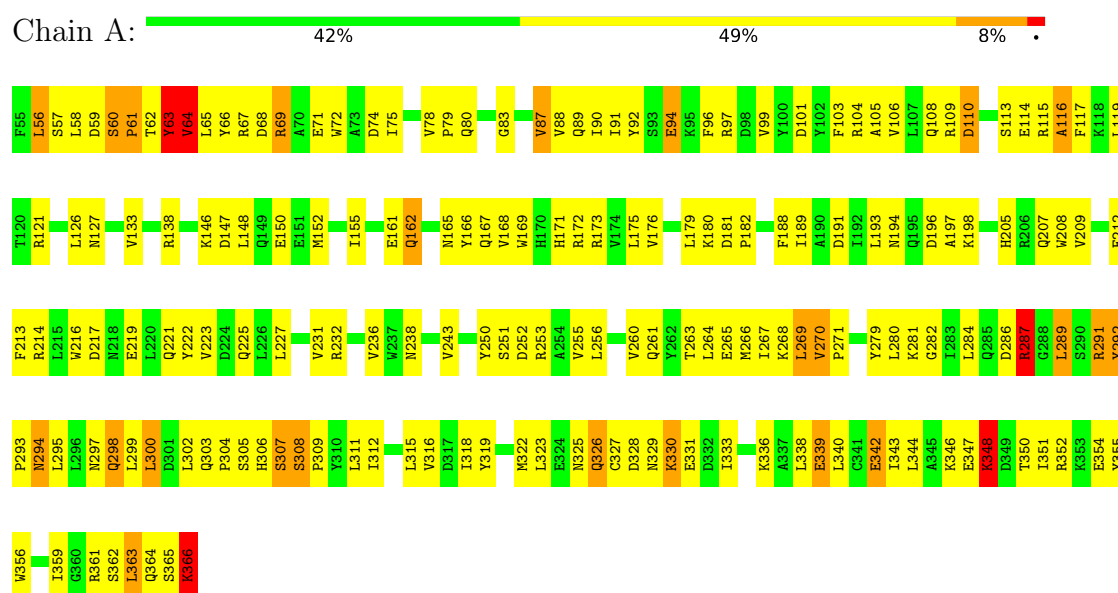
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			35	30	5		

3 Residue-property plots

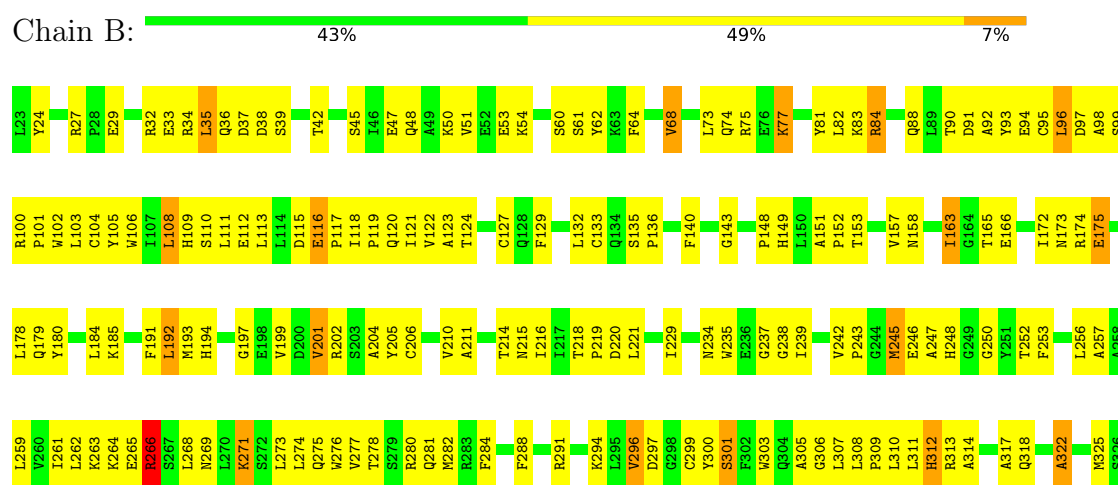
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

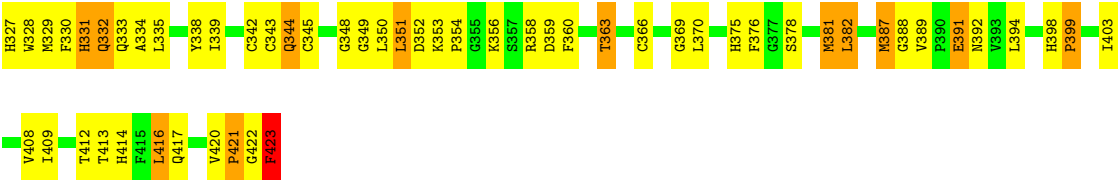
Note EDS was not executed.

• Molecule 1: Protein farnesyltransferase alpha subunit



• Molecule 2: Protein farnesyltransferase beta subunit





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	168.62Å 168.62Å 69.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70	Depositor
% Data completeness (in resolution range)	85.0 (50.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.229 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5871	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FTL, 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	0.90	3/2726 (0.1%)	1.30	32/3700 (0.9%)
2	B	0.75	2/3239 (0.1%)	1.11	21/4397 (0.5%)
All	All	0.82	5/5965 (0.1%)	1.20	53/8097 (0.7%)

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
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	ARG	NE-CZ	15.16	1.49	1.33
1	A	287	ARG	CZ-NH1	10.64	1.47	1.32
1	A	366	LYS	C-OXT	5.53	1.34	1.23
2	B	423	PHE	CA-C	5.25	1.64	1.52
2	B	423	PHE	N-CA	-5.00	1.36	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	PRO	N-CA-C	-14.65	95.55	113.86
1	A	64	VAL	N-CA-C	14.26	128.00	107.75
1	A	64	VAL	CG1-CB-CG2	-10.27	88.21	110.80
1	A	60	SER	CA-C-N	9.72	129.37	119.56
1	A	60	SER	C-N-CA	9.72	129.37	119.56
1	A	348	LYS	N-CA-C	9.05	121.15	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	GLY	CA-C-N	8.74	129.61	119.47
1	A	83	GLY	C-N-CA	8.74	129.61	119.47
1	A	69	ARG	N-CA-C	8.46	123.21	109.76
2	B	342	CYS	N-CA-C	8.30	123.70	113.50
2	B	237	GLY	N-CA-C	-7.85	105.35	114.69
1	A	292	TYR	CA-C-N	7.44	129.14	119.84
1	A	292	TYR	C-N-CA	7.44	129.14	119.84
1	A	64	VAL	CB-CA-C	-7.32	101.09	111.40
2	B	172	ILE	N-CA-C	7.30	117.90	108.12
2	B	301	SER	N-CA-C	-7.27	103.39	111.82
1	A	291	ARG	N-CA-C	-7.21	104.46	113.18
1	A	63	TYR	CA-C-N	-7.15	114.10	122.11
1	A	63	TYR	C-N-CA	-7.15	114.10	122.11
2	B	391	GLU	N-CA-C	-7.03	104.67	113.18
2	B	375	HIS	N-CA-C	6.65	119.75	108.90
1	A	243	VAL	N-CA-C	6.63	117.12	110.23
1	A	110	ASP	N-CA-C	-6.62	104.50	112.58
1	A	148	LEU	N-CA-C	6.26	118.10	111.28
1	A	270	VAL	CA-C-N	6.26	127.66	119.84
1	A	270	VAL	C-N-CA	6.26	127.66	119.84
1	A	366	LYS	CA-C-O	-6.12	102.65	121.00
1	A	217	ASP	N-CA-C	6.10	123.79	110.80
2	B	116	GLU	CA-C-N	6.06	126.56	120.14
2	B	116	GLU	C-N-CA	6.06	126.56	120.14
2	B	399	PRO	CA-C-N	-6.03	116.81	122.66
2	B	399	PRO	C-N-CA	-6.03	116.81	122.66
1	A	116	ALA	N-CA-C	-6.01	104.64	111.14
2	B	366	CYS	N-CA-C	-5.95	104.72	111.14
1	A	94	GLU	N-CA-C	-5.86	104.25	111.75
2	B	35	LEU	N-CA-C	5.83	118.78	110.10
1	A	150	GLU	N-CA-C	-5.81	104.85	111.07
2	B	27	ARG	CA-C-N	5.78	125.31	119.19
2	B	27	ARG	C-N-CA	5.78	125.31	119.19
2	B	192	LEU	N-CA-C	-5.75	102.01	110.52
2	B	351	LEU	N-CA-C	5.71	117.46	108.96
2	B	363	THR	N-CA-C	-5.58	104.89	110.97
2	B	193	MET	N-CA-C	-5.55	105.23	112.23
1	A	65	LEU	CA-C-O	5.40	126.63	120.80
2	B	163	ILE	N-CA-C	-5.35	105.39	110.42
2	B	68	VAL	N-CA-C	-5.21	104.15	108.63
1	A	307	SER	N-CA-C	5.18	118.14	110.48
1	A	216	TRP	N-CA-C	5.16	118.73	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ARG	CG-CD-NE	5.15	123.32	112.00
2	B	62	TYR	N-CA-C	5.13	116.56	110.97
1	A	308	SER	CA-C-N	-5.11	114.81	119.82
1	A	308	SER	C-N-CA	-5.11	114.81	119.82
1	A	193	LEU	N-CA-C	-5.03	106.25	112.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	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	2661	0	2585	205	0
2	B	3154	0	3085	223	0
3	B	1	0	0	0	0
4	B	20	0	28	7	0
5	B	35	0	23	5	0
All	All	5871	0	5721	420	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 36.

All (420) 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:287:ARG:HH21	1:A:291:ARG:NH1	1.35	1.23
1:A:287:ARG:NH2	1:A:291:ARG:NH1	2.04	1.05
1:A:56:LEU:CD2	1:A:63:TYR:HA	1.89	1.03
1:A:287:ARG:HE	1:A:291:ARG:CZ	1.74	0.99
1:A:286:ASP:O	1:A:287:ARG:HB2	1.64	0.97
1:A:268:LYS:HE2	1:A:302:LEU:HD11	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:501:HFP:H52	5:B:1:FTL:N1	1.80	0.97
1:A:303:GLN:O	1:A:307:SER:HB2	1.65	0.96
2:B:306:GLY:O	2:B:309:PRO:HD2	1.66	0.96
1:A:287:ARG:HH21	1:A:291:ARG:HH11	0.96	0.95
1:A:75:ILE:HD11	1:A:115:ARG:NH1	1.81	0.94
1:A:287:ARG:HE	1:A:291:ARG:NE	1.65	0.92
1:A:182:PRO:HG3	1:A:213:PHE:CD2	2.06	0.91
2:B:151:ALA:HB3	2:B:152:PRO:HD3	1.53	0.90
1:A:287:ARG:O	1:A:291:ARG:HD3	1.73	0.89
1:A:56:LEU:HD21	1:A:63:TYR:HA	1.56	0.87
2:B:381:MET:O	2:B:382:LEU:HD22	1.73	0.87
1:A:75:ILE:HD11	1:A:115:ARG:CZ	2.06	0.85
2:B:175:GLU:CD	2:B:175:GLU:H	1.83	0.84
1:A:56:LEU:HD22	1:A:63:TYR:HA	1.57	0.83
1:A:330:LYS:HG3	1:A:331:GLU:N	1.94	0.82
2:B:414:HIS:O	2:B:417:GLN:HG2	1.79	0.82
2:B:96:LEU:HD12	2:B:103:LEU:HD11	1.60	0.81
1:A:63:TYR:CD2	1:A:64:VAL:N	2.48	0.81
1:A:287:ARG:NE	1:A:291:ARG:CZ	2.45	0.79
2:B:185:LYS:HE3	2:B:221:LEU:O	1.82	0.79
1:A:366:LYS:H	1:A:366:LYS:HD3	1.49	0.78
1:A:366:LYS:HD3	1:A:366:LYS:N	1.99	0.77
1:A:58:LEU:HD23	1:A:63:TYR:CE1	2.21	0.76
1:A:63:TYR:CD2	1:A:63:TYR:C	2.61	0.76
2:B:218:THR:HB	2:B:219:PRO:HD2	1.65	0.76
2:B:282:MET:HG3	2:B:296:VAL:HG13	1.68	0.76
2:B:84:ARG:HH22	2:B:88:GLN:HG2	1.51	0.76
2:B:271:LYS:HA	2:B:271:LYS:HE3	1.68	0.75
2:B:119:PRO:O	2:B:122:VAL:HG12	1.87	0.75
1:A:284:LEU:HD22	1:A:292:TYR:CE1	2.22	0.75
2:B:73:LEU:HD12	2:B:344:GLN:OE1	1.86	0.75
1:A:61:PRO:HG2	1:A:62:THR:HG23	1.69	0.74
4:B:501:HFP:H52	5:B:1:FTL:C65	2.17	0.74
1:A:63:TYR:CD2	1:A:64:VAL:HA	2.23	0.74
1:A:260:VAL:HG13	1:A:280:LEU:CD1	2.17	0.74
2:B:253:PHE:HA	2:B:307:LEU:HD21	1.70	0.74
2:B:173:ASN:OD1	2:B:175:GLU:HG2	1.89	0.73
1:A:60:SER:OG	1:A:62:THR:OG1	2.01	0.73
2:B:35:LEU:HD12	2:B:36:GLN:N	2.03	0.73
1:A:231:VAL:HG21	1:A:266:MET:HE2	1.70	0.72
1:A:63:TYR:CG	1:A:64:VAL:N	2.58	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:VAL:HG12	2:B:391:GLU:H	1.53	0.72
1:A:287:ARG:O	1:A:287:ARG:HD3	1.89	0.72
2:B:99:SER:O	2:B:102:TRP:HB2	1.90	0.71
2:B:327:HIS:HB3	2:B:332:GLN:HE22	1.54	0.71
2:B:77:LYS:HE3	2:B:77:LYS:HA	1.72	0.71
2:B:306:GLY:C	2:B:309:PRO:HD2	2.16	0.71
1:A:319:TYR:HD2	1:A:322:MET:HE2	1.54	0.70
2:B:245:MET:CE	2:B:245:MET:HA	2.21	0.70
2:B:73:LEU:H	2:B:392:ASN:ND2	1.89	0.70
2:B:82:LEU:HD21	2:B:363:THR:HG21	1.75	0.68
1:A:80:GLN:HB2	1:A:104:ARG:CZ	2.23	0.68
1:A:268:LYS:CE	1:A:302:LEU:HD11	2.23	0.68
2:B:109:HIS:O	2:B:112:GLU:HB3	1.94	0.68
1:A:361:ARG:HB2	2:B:322:ALA:HB1	1.76	0.68
2:B:277:VAL:HG13	2:B:278:THR:N	2.06	0.68
1:A:167:GLN:CD	1:A:167:GLN:H	2.02	0.67
1:A:87:VAL:O	1:A:88:VAL:C	2.35	0.67
1:A:91:ILE:O	2:B:91:ASP:HB3	1.93	0.67
2:B:73:LEU:H	2:B:392:ASN:HD21	1.40	0.67
2:B:282:MET:CG	2:B:296:VAL:HG13	2.25	0.67
1:A:330:LYS:HG3	1:A:331:GLU:H	1.61	0.66
4:B:501:HFP:C5	5:B:1:FTL:N1	2.57	0.66
2:B:245:MET:HE2	2:B:246:GLU:H	1.60	0.66
2:B:335:LEU:O	2:B:339:ILE:HG13	1.96	0.65
2:B:96:LEU:HD22	2:B:99:SER:HB2	1.79	0.65
1:A:57:SER:O	1:A:63:TYR:HB2	1.96	0.65
2:B:84:ARG:NH2	2:B:88:GLN:HG2	2.11	0.65
2:B:96:LEU:CD1	2:B:103:LEU:HD11	2.26	0.65
2:B:266:ARG:HH22	2:B:318:GLN:HG2	1.62	0.65
1:A:289:LEU:O	1:A:292:TYR:HB2	1.97	0.64
2:B:301:SER:O	2:B:305:ALA:HB3	1.95	0.64
1:A:294:ASN:O	1:A:298:GLN:HG2	1.97	0.64
2:B:149:HIS:O	2:B:152:PRO:HD2	1.98	0.64
1:A:80:GLN:HB2	1:A:104:ARG:NH2	2.13	0.64
2:B:350:LEU:N	2:B:350:LEU:HD22	2.11	0.64
2:B:163:ILE:HG22	2:B:165:THR:HG23	1.79	0.63
1:A:327:CYS:O	1:A:330:LYS:HB3	1.97	0.62
2:B:245:MET:HA	2:B:245:MET:HE2	1.79	0.62
2:B:38:ASP:O	2:B:39:SER:HB2	2.00	0.62
1:A:231:VAL:HG21	1:A:266:MET:CE	2.30	0.62
1:A:284:LEU:HD22	1:A:292:TYR:CD1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:HB3	1:A:289:LEU:CD1	2.29	0.62
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.35	0.62
2:B:116:GLU:HB3	2:B:117:PRO:HD2	1.82	0.61
2:B:308:LEU:CD1	2:B:330:PHE:HB3	2.31	0.61
1:A:355:TYR:HA	2:B:329:MET:HE3	1.82	0.61
1:A:231:VAL:CG2	1:A:266:MET:HE2	2.31	0.60
1:A:347:GLU:HG2	1:A:348:LYS:HE3	1.83	0.60
1:A:101:ASP:OD1	1:A:104:ARG:NH1	2.34	0.60
2:B:35:LEU:HD12	2:B:36:GLN:H	1.65	0.60
2:B:333:GLN:HG3	2:B:387:MET:HE2	1.84	0.60
2:B:423:PHE:N	2:B:423:PHE:CD2	2.67	0.59
2:B:180:TYR:CZ	2:B:184:LEU:HD11	2.37	0.59
2:B:344:GLN:HA	2:B:350:LEU:HD13	1.84	0.59
1:A:167:GLN:CD	1:A:167:GLN:N	2.60	0.59
1:A:312:ILE:O	1:A:316:VAL:HG23	2.01	0.59
1:A:63:TYR:O	1:A:64:VAL:HG13	2.01	0.59
2:B:259:LEU:HD12	2:B:268:LEU:HD11	1.83	0.59
2:B:338:TYR:CE2	2:B:343:CYS:SG	2.95	0.59
2:B:273:LEU:HD12	2:B:273:LEU:O	2.02	0.59
2:B:194:HIS:CD2	2:B:197:GLY:HA3	2.37	0.59
2:B:73:LEU:O	2:B:75:ARG:N	2.33	0.59
1:A:96:PHE:HA	1:A:126:LEU:HD13	1.84	0.58
2:B:325:MET:HE3	2:B:381:MET:SD	2.43	0.58
2:B:403:ILE:HD11	2:B:408:VAL:HG22	1.85	0.58
1:A:361:ARG:O	1:A:364:GLN:HB2	2.02	0.58
1:A:56:LEU:HD21	1:A:62:THR:O	2.02	0.58
2:B:34:ARG:HD2	2:B:284:PHE:CE1	2.39	0.58
1:A:342:GLU:OE1	1:A:346:LYS:HE3	2.04	0.58
2:B:350:LEU:HB2	2:B:363:THR:HA	1.86	0.57
2:B:370:LEU:HD23	2:B:394:LEU:HD11	1.85	0.57
1:A:161:GLU:C	1:A:162:GLN:HG2	2.29	0.57
1:A:344:LEU:HD23	1:A:348:LYS:HB3	1.85	0.57
1:A:152:MET:HE1	1:A:172:ARG:CZ	2.34	0.57
1:A:302:LEU:HD22	1:A:306:HIS:CD2	2.39	0.57
1:A:359:ILE:O	1:A:363:LEU:HB2	2.05	0.57
2:B:238:GLY:HA3	2:B:247:ALA:HB1	1.85	0.57
1:A:60:SER:OG	1:A:62:THR:N	2.36	0.57
1:A:311:LEU:O	1:A:315:LEU:HG	2.04	0.57
1:A:260:VAL:O	1:A:261:GLN:C	2.48	0.56
1:A:269:LEU:HD22	1:A:269:LEU:O	2.05	0.56
1:A:354:GLU:HB3	2:B:329:MET:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:CYS:O	2:B:108:LEU:HB2	2.05	0.56
2:B:201:VAL:O	2:B:202:ARG:C	2.47	0.56
1:A:287:ARG:CZ	1:A:291:ARG:NH1	2.68	0.56
2:B:140:PHE:O	2:B:148:PRO:HA	2.06	0.56
2:B:215:ASN:CG	2:B:215:ASN:O	2.48	0.56
2:B:389:VAL:HG12	2:B:391:GLU:HB2	1.87	0.56
2:B:81:TYR:OH	2:B:358:ARG:HG3	2.06	0.56
2:B:277:VAL:CG1	2:B:278:THR:N	2.69	0.56
1:A:366:LYS:N	1:A:366:LYS:CD	2.69	0.56
1:A:67:ARG:HG3	1:A:68:ASP:N	2.20	0.56
1:A:152:MET:O	1:A:155:ILE:HG22	2.06	0.56
2:B:37:ASP:O	2:B:38:ASP:HB2	2.06	0.56
2:B:314:ALA:O	2:B:317:ALA:HB3	2.05	0.55
2:B:291:ARG:O	2:B:294:LYS:HB2	2.06	0.55
2:B:262:LEU:O	2:B:263:LYS:HB2	2.05	0.55
2:B:151:ALA:HB3	2:B:152:PRO:CD	2.33	0.55
2:B:349:GLY:C	2:B:350:LEU:HD22	2.32	0.55
1:A:267:ILE:C	1:A:269:LEU:H	2.14	0.55
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.70	0.55
1:A:63:TYR:CD2	1:A:64:VAL:CA	2.90	0.55
2:B:308:LEU:HD13	2:B:330:PHE:HB3	1.89	0.55
1:A:339:GLU:O	1:A:343:ILE:HG13	2.07	0.55
2:B:280:ARG:HH11	2:B:280:ARG:HG2	1.72	0.55
2:B:266:ARG:NH2	2:B:318:GLN:HG2	2.21	0.55
1:A:287:ARG:NH2	1:A:291:ARG:HH11	1.81	0.54
1:A:260:VAL:HG13	1:A:280:LEU:HD13	1.89	0.54
2:B:50:LYS:O	2:B:54:LYS:HG3	2.07	0.54
2:B:122:VAL:HG13	2:B:123:ALA:N	2.21	0.54
2:B:82:LEU:HB2	2:B:111:LEU:HD21	1.90	0.54
2:B:105:TYR:O	2:B:106:TRP:C	2.50	0.54
2:B:291:ARG:HB2	2:B:294:LYS:CG	2.38	0.54
1:A:223:VAL:HG13	1:A:236:VAL:HG12	1.90	0.54
1:A:304:PRO:HD2	1:A:305:SER:H	1.73	0.53
2:B:122:VAL:CG1	2:B:123:ALA:N	2.72	0.53
2:B:129:PHE:HA	2:B:132:LEU:HD12	1.91	0.53
1:A:60:SER:C	1:A:62:THR:N	2.62	0.53
1:A:75:ILE:CD1	1:A:115:ARG:CZ	2.83	0.53
1:A:294:ASN:OD1	1:A:294:ASN:N	2.39	0.53
2:B:350:LEU:N	2:B:350:LEU:CD2	2.72	0.53
1:A:94:GLU:HA	1:A:97:ARG:NH2	2.24	0.53
2:B:333:GLN:CG	2:B:387:MET:HE2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:ARG:HG2	2:B:280:ARG:NH1	2.25	0.52
1:A:196:ASP:O	1:A:198:LYS:N	2.42	0.52
2:B:266:ARG:HH12	2:B:317:ALA:HB3	1.74	0.52
2:B:353:LYS:HB2	2:B:354:PRO:HD2	1.91	0.52
2:B:75:ARG:NH2	2:B:391:GLU:O	2.41	0.52
1:A:92:TYR:HB2	1:A:97:ARG:HG3	1.92	0.52
1:A:227:LEU:HG	1:A:236:VAL:HG11	1.92	0.52
1:A:252:ASP:HB3	1:A:255:VAL:CG2	2.40	0.52
1:A:287:ARG:HD2	1:A:292:TYR:OH	2.09	0.52
2:B:121:ILE:N	2:B:121:ILE:HD12	2.24	0.52
2:B:192:LEU:HD23	2:B:199:VAL:CG2	2.39	0.52
1:A:63:TYR:C	1:A:64:VAL:HG22	2.35	0.52
2:B:165:THR:O	2:B:166:GLU:C	2.52	0.52
2:B:376:PHE:O	2:B:382:LEU:HD13	2.10	0.51
1:A:325:ASN:HD22	1:A:325:ASN:N	2.09	0.51
2:B:308:LEU:CD1	2:B:330:PHE:CD2	2.93	0.51
2:B:205:TYR:HD2	4:B:501:HFP:H153	1.74	0.51
1:A:319:TYR:CE1	1:A:336:LYS:HG3	2.46	0.51
1:A:196:ASP:C	1:A:198:LYS:H	2.19	0.51
1:A:138:ARG:NH1	1:A:171:HIS:ND1	2.55	0.51
1:A:181:ASP:OD1	1:A:181:ASP:C	2.52	0.51
2:B:206:CYS:O	2:B:210:VAL:HG22	2.11	0.51
2:B:313:ARG:O	2:B:317:ALA:N	2.42	0.51
2:B:245:MET:HE2	2:B:245:MET:CA	2.41	0.50
2:B:297:ASP:HB3	2:B:300:TYR:HD1	1.76	0.50
1:A:71:GLU:HG2	1:A:72:TRP:CD1	2.47	0.50
1:A:92:TYR:HD2	2:B:94:GLU:HG2	1.76	0.50
1:A:165:ASN:OD1	1:A:167:GLN:N	2.45	0.50
1:A:365:SER:HB2	1:A:366:LYS:HD3	1.94	0.50
1:A:308:SER:HB2	1:A:309:PRO:HD2	1.93	0.50
2:B:239:ILE:HB	2:B:252:THR:HA	1.94	0.50
2:B:178:LEU:HG	2:B:216:ILE:HB	1.93	0.49
1:A:104:ARG:O	1:A:108:GLN:HB2	2.13	0.49
2:B:47:GLU:O	2:B:50:LYS:HB2	2.12	0.49
2:B:308:LEU:HD13	2:B:330:PHE:HD2	1.76	0.49
1:A:250:TYR:O	1:A:256:LEU:HD22	2.12	0.49
2:B:124:THR:O	2:B:127:CYS:HB2	2.11	0.49
2:B:135:SER:OG	2:B:136:PRO:HD2	2.11	0.49
2:B:388:GLY:O	2:B:389:VAL:C	2.56	0.49
1:A:74:ASP:OD1	1:A:75:ILE:HG13	2.12	0.49
1:A:147:ASP:OD1	1:A:147:ASP:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ARG:HH22	2:B:53:GLU:CD	2.20	0.49
2:B:117:PRO:O	2:B:118:ILE:HD13	2.13	0.49
2:B:94:GLU:C	2:B:96:LEU:H	2.20	0.48
2:B:389:VAL:CG1	2:B:391:GLU:HB2	2.43	0.48
1:A:279:TYR:O	1:A:280:LEU:C	2.56	0.48
2:B:96:LEU:C	2:B:98:ALA:N	2.68	0.48
2:B:211:ALA:HA	2:B:216:ILE:HD11	1.94	0.48
1:A:238:ASN:HA	2:B:235:TRP:CZ2	2.48	0.48
1:A:191:ASP:O	1:A:194:ASN:HB3	2.13	0.48
1:A:284:LEU:HB3	1:A:289:LEU:HD11	1.94	0.48
2:B:352:ASP:OD1	2:B:352:ASP:C	2.57	0.48
2:B:191:PHE:O	2:B:199:VAL:HG22	2.13	0.48
2:B:308:LEU:CD1	2:B:330:PHE:HD2	2.27	0.48
2:B:33:GLU:OE2	2:B:33:GLU:HA	2.14	0.48
2:B:218:THR:HB	2:B:219:PRO:CD	2.38	0.48
1:A:302:LEU:HB3	1:A:306:HIS:HB2	1.95	0.48
1:A:344:LEU:HD13	1:A:356:TRP:CZ2	2.49	0.48
2:B:308:LEU:HD12	2:B:330:PHE:CD2	2.48	0.48
2:B:359:ASP:HB2	5:B:1:FTL:N5	2.28	0.48
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.73	0.48
2:B:331:HIS:CD2	2:B:333:GLN:HB3	2.49	0.48
1:A:57:SER:O	1:A:63:TYR:HD1	1.96	0.47
1:A:196:ASP:C	1:A:196:ASP:OD1	2.57	0.47
1:A:362:SER:C	1:A:364:GLN:N	2.72	0.47
2:B:51:VAL:HA	2:B:54:LYS:HE2	1.96	0.47
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.29	0.47
2:B:303:TRP:NE1	4:B:501:HFP:H91	2.30	0.47
2:B:381:MET:O	2:B:382:LEU:CD2	2.55	0.47
4:B:501:HFP:H21	5:B:1:FTL:HC44	1.96	0.47
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.76	0.47
2:B:96:LEU:O	2:B:98:ALA:N	2.47	0.47
1:A:227:LEU:HG	1:A:236:VAL:CG1	2.44	0.47
1:A:58:LEU:HA	1:A:63:TYR:CD1	2.49	0.47
1:A:71:GLU:CD	1:A:71:GLU:H	2.23	0.47
1:A:343:ILE:HG22	1:A:348:LYS:HB2	1.97	0.47
2:B:242:VAL:O	2:B:243:PRO:C	2.58	0.47
2:B:291:ARG:HB2	2:B:294:LYS:HG2	1.97	0.47
2:B:310:LEU:HD21	2:B:399:PRO:O	2.14	0.47
2:B:420:VAL:O	2:B:422:GLY:N	2.47	0.47
1:A:263:THR:O	1:A:267:ILE:HG13	2.15	0.47
2:B:84:ARG:HE	2:B:84:ARG:CA	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:LEU:HA	2:B:199:VAL:HG22	1.97	0.47
1:A:330:LYS:O	1:A:333:ILE:HB	2.15	0.46
2:B:257:ALA:O	2:B:261:ILE:HG13	2.16	0.46
1:A:252:ASP:O	1:A:253:ARG:C	2.58	0.46
2:B:60:SER:O	2:B:61:SER:C	2.57	0.46
2:B:273:LEU:HD12	2:B:273:LEU:C	2.38	0.46
1:A:113:SER:OG	1:A:115:ARG:HG2	2.15	0.46
1:A:293:PRO:HG2	1:A:294:ASN:OD1	2.14	0.46
2:B:37:ASP:O	2:B:37:ASP:OD2	2.33	0.46
1:A:338:LEU:HD11	1:A:364:GLN:HE22	1.79	0.46
2:B:48:GLN:HA	2:B:48:GLN:NE2	2.31	0.46
1:A:208:TRP:NE1	1:A:212:GLU:HG3	2.31	0.46
2:B:93:TYR:CZ	2:B:360:PHE:CE1	3.04	0.46
1:A:294:ASN:O	1:A:295:LEU:C	2.58	0.46
2:B:113:LEU:C	2:B:115:ASP:H	2.22	0.46
1:A:63:TYR:CE2	1:A:64:VAL:HA	2.51	0.46
2:B:331:HIS:CD2	2:B:334:ALA:H	2.34	0.46
1:A:79:PRO:HA	1:A:101:ASP:OD1	2.16	0.46
1:A:363:LEU:HD12	1:A:363:LEU:HA	1.74	0.46
1:A:205:HIS:O	1:A:209:VAL:HG23	2.15	0.46
1:A:168:VAL:HG23	1:A:169:TRP:N	2.31	0.46
1:A:325:ASN:O	1:A:326:GLN:HB2	2.15	0.46
2:B:90:THR:C	2:B:92:ALA:H	2.24	0.46
2:B:312:HIS:O	2:B:313:ARG:C	2.59	0.46
1:A:182:PRO:HG3	1:A:213:PHE:CG	2.51	0.45
2:B:245:MET:HA	2:B:245:MET:HE3	1.97	0.45
2:B:84:ARG:HE	2:B:84:ARG:HA	1.81	0.45
2:B:248:HIS:CE1	2:B:250:GLY:H	2.34	0.45
2:B:409:ILE:O	2:B:413:THR:HG23	2.16	0.45
1:A:219:GLU:OE1	1:A:219:GLU:HA	2.17	0.45
1:A:322:MET:HE3	1:A:333:ILE:HD13	1.98	0.45
1:A:354:GLU:HG3	2:B:328:TRP:O	2.16	0.45
2:B:32:ARG:C	2:B:34:ARG:H	2.24	0.45
2:B:37:ASP:C	2:B:39:SER:H	2.23	0.45
2:B:234:ASN:OD1	2:B:234:ASN:C	2.59	0.45
1:A:336:LYS:HE3	1:A:340:LEU:HD21	1.98	0.45
1:A:66:TYR:CE1	1:A:99:VAL:HG22	2.50	0.45
2:B:121:ILE:HD12	2:B:121:ILE:H	1.81	0.45
1:A:267:ILE:C	1:A:269:LEU:N	2.74	0.45
1:A:312:ILE:HD12	1:A:348:LYS:HG2	1.99	0.45
1:A:362:SER:C	1:A:364:GLN:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:LEU:HD23	2:B:307:LEU:HD22	1.99	0.45
1:A:176:VAL:O	1:A:180:LYS:N	2.50	0.45
2:B:276:TRP:O	2:B:280:ARG:HG2	2.17	0.45
1:A:270:VAL:N	1:A:271:PRO:CD	2.79	0.45
1:A:329:ASN:O	1:A:330:LYS:C	2.60	0.45
1:A:356:TRP:HA	1:A:356:TRP:CE3	2.52	0.45
1:A:364:GLN:NE2	1:A:364:GLN:HA	2.31	0.45
1:A:252:ASP:HB3	1:A:255:VAL:HG23	1.98	0.45
2:B:204:ALA:HB1	2:B:229:ILE:HD11	1.99	0.45
2:B:398:HIS:CD2	2:B:408:VAL:HG21	2.52	0.45
1:A:173:ARG:HD2	1:A:208:TRP:CD2	2.52	0.44
1:A:207:GLN:NE2	2:B:245:MET:HE3	2.31	0.44
2:B:100:ARG:O	2:B:101:PRO:C	2.59	0.44
2:B:345:CYS:O	2:B:348:GLY:N	2.45	0.44
1:A:268:LYS:HE2	1:A:302:LEU:CD1	2.33	0.44
1:A:60:SER:OG	1:A:62:THR:CA	2.66	0.44
1:A:109:ARG:O	1:A:110:ASP:HB3	2.17	0.44
1:A:152:MET:HE1	1:A:172:ARG:NH2	2.32	0.44
1:A:155:ILE:HD12	1:A:155:ILE:HA	1.90	0.44
2:B:101:PRO:O	2:B:104:CYS:HB2	2.17	0.44
2:B:173:ASN:OD1	2:B:173:ASN:C	2.60	0.44
2:B:133:CYS:SG	2:B:143:GLY:HA2	2.57	0.44
1:A:328:ASP:O	1:A:329:ASN:HB2	2.18	0.44
1:A:355:TYR:HA	2:B:329:MET:CE	2.45	0.44
2:B:37:ASP:C	2:B:39:SER:N	2.76	0.44
2:B:149:HIS:C	2:B:152:PRO:HD2	2.42	0.44
1:A:127:ASN:OD1	1:A:127:ASN:C	2.61	0.44
2:B:82:LEU:CB	2:B:111:LEU:HD21	2.47	0.44
2:B:266:ARG:NH2	2:B:318:GLN:CG	2.81	0.44
2:B:294:LYS:HD2	2:B:294:LYS:HA	1.70	0.44
1:A:319:TYR:CD2	1:A:322:MET:HE2	2.45	0.44
1:A:60:SER:O	1:A:63:TYR:HB3	2.18	0.43
1:A:222:TYR:O	1:A:225:GLN:HB3	2.18	0.43
1:A:252:ASP:O	1:A:255:VAL:N	2.51	0.43
2:B:101:PRO:HG2	2:B:152:PRO:HB3	1.99	0.43
2:B:369:GLY:O	2:B:370:LEU:C	2.58	0.43
1:A:115:ARG:HG3	1:A:116:ALA:N	2.34	0.43
1:A:325:ASN:N	1:A:325:ASN:ND2	2.66	0.43
2:B:214:THR:OG1	2:B:216:ILE:HG12	2.18	0.43
2:B:265:GLU:H	2:B:265:GLU:CD	2.21	0.43
1:A:56:LEU:HD21	1:A:63:TYR:CA	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:O	1:A:67:ARG:C	2.62	0.43
2:B:178:LEU:O	2:B:179:GLN:C	2.62	0.43
2:B:175:GLU:CD	2:B:175:GLU:N	2.62	0.43
2:B:303:TRP:CE2	4:B:501:HFP:H91	2.54	0.43
2:B:416:LEU:HD12	2:B:416:LEU:HA	1.67	0.43
1:A:90:ILE:HB	1:A:92:TYR:CE2	2.54	0.43
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.84	0.43
2:B:110:SER:O	2:B:111:LEU:C	2.62	0.43
1:A:175:LEU:O	1:A:176:VAL:C	2.61	0.43
1:A:78:VAL:O	1:A:101:ASP:HA	2.19	0.42
1:A:232:ARG:NH1	2:B:42:THR:HG23	2.33	0.42
1:A:295:LEU:HD12	1:A:295:LEU:HA	1.74	0.42
2:B:82:LEU:O	2:B:83:LYS:C	2.59	0.42
1:A:279:TYR:O	1:A:282:GLY:N	2.52	0.42
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.93	0.42
2:B:281:GLN:HB2	2:B:288:PHE:CE2	2.54	0.42
1:A:284:LEU:HB3	1:A:289:LEU:HD12	2.01	0.42
2:B:220:ASP:O	2:B:221:LEU:C	2.62	0.42
1:A:78:VAL:HG23	1:A:105:ALA:HB2	2.01	0.42
2:B:245:MET:HE2	2:B:246:GLU:N	2.32	0.42
1:A:114:GLU:O	1:A:117:PHE:HB3	2.20	0.42
1:A:116:ALA:O	1:A:119:LEU:HB3	2.20	0.42
1:A:292:TYR:O	1:A:295:LEU:HB2	2.20	0.42
2:B:96:LEU:C	2:B:98:ALA:H	2.27	0.42
2:B:157:VAL:O	2:B:158:ASN:C	2.61	0.42
2:B:178:LEU:HD12	2:B:421:PRO:HB2	2.02	0.42
1:A:173:ARG:HD2	1:A:208:TRP:CE2	2.55	0.42
1:A:292:TYR:HA	1:A:293:PRO:HD2	1.70	0.42
1:A:336:LYS:NZ	1:A:340:LEU:HD21	2.34	0.42
2:B:178:LEU:HD23	2:B:178:LEU:HA	1.85	0.41
2:B:398:HIS:ND1	2:B:399:PRO:HD2	2.34	0.41
1:A:67:ARG:CG	1:A:68:ASP:N	2.83	0.41
2:B:24:TYR:H	2:B:333:GLN:NE2	2.18	0.41
2:B:93:TYR:CZ	2:B:360:PHE:HE1	2.38	0.41
2:B:308:LEU:HD13	2:B:330:PHE:CD2	2.53	0.41
1:A:60:SER:C	1:A:62:THR:H	2.22	0.41
1:A:64:VAL:O	1:A:69:ARG:NH2	2.50	0.41
1:A:179:LEU:O	1:A:180:LYS:C	2.63	0.41
2:B:274:LEU:O	2:B:277:VAL:HG12	2.20	0.41
1:A:188:PHE:O	1:A:191:ASP:HB3	2.21	0.41
2:B:96:LEU:O	2:B:97:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:VAL:CG1	2:B:278:THR:H	2.33	0.41
2:B:291:ARG:HB2	2:B:294:LYS:HG3	2.01	0.41
2:B:119:PRO:C	2:B:121:ILE:H	2.29	0.41
2:B:299:CYS:C	2:B:301:SER:H	2.28	0.41
2:B:331:HIS:HD2	2:B:334:ALA:H	1.67	0.41
2:B:211:ALA:HA	2:B:216:ILE:CG1	2.50	0.41
1:A:57:SER:O	1:A:63:TYR:CD1	2.74	0.41
1:A:300:LEU:HA	1:A:300:LEU:HD12	1.66	0.41
1:A:351:ILE:O	2:B:331:HIS:HB2	2.20	0.41
2:B:24:TYR:HB2	2:B:333:GLN:NE2	2.35	0.41
2:B:113:LEU:C	2:B:115:ASP:N	2.78	0.41
1:A:87:VAL:C	1:A:88:VAL:HG22	2.45	0.41
1:A:351:ILE:HD12	1:A:351:ILE:HA	1.90	0.41
1:A:59:ASP:O	1:A:60:SER:C	2.63	0.41
1:A:87:VAL:C	1:A:88:VAL:CG2	2.94	0.41
1:A:238:ASN:OD1	2:B:235:TRP:NE1	2.46	0.41
1:A:318:ILE:O	1:A:319:TYR:C	2.64	0.41
2:B:119:PRO:C	2:B:121:ILE:N	2.79	0.41
2:B:276:TRP:O	2:B:280:ARG:NH1	2.54	0.41
2:B:311:LEU:HA	2:B:311:LEU:HD23	1.70	0.41
2:B:331:HIS:HD2	2:B:333:GLN:HB3	1.85	0.41
2:B:352:ASP:HB3	2:B:356:LYS:HG3	2.02	0.41
2:B:273:LEU:HG	2:B:311:LEU:HD11	2.01	0.41
1:A:116:ALA:O	1:A:117:PHE:C	2.63	0.40
1:A:297:ASN:O	1:A:300:LEU:N	2.54	0.40
2:B:24:TYR:HB2	2:B:333:GLN:CD	2.46	0.40
2:B:64:PHE:HD1	2:B:64:PHE:N	2.19	0.40
2:B:94:GLU:C	2:B:96:LEU:N	2.79	0.40
2:B:345:CYS:HB3	2:B:349:GLY:O	2.21	0.40
2:B:174:ARG:NH2	2:B:215:ASN:O	2.50	0.40
2:B:382:LEU:HD13	2:B:382:LEU:HA	1.88	0.40
1:A:179:LEU:O	1:A:180:LYS:HB2	2.21	0.40
2:B:266:ARG:NH1	2:B:317:ALA:HB3	2.35	0.40
2:B:269:ASN:OD1	2:B:269:ASN:C	2.63	0.40
2:B:408:VAL:O	2:B:412:THR:HG23	2.22	0.40
1:A:61:PRO:CD	1:A:62:THR:H	2.33	0.40
1:A:146:LYS:HE3	1:A:146:LYS:HB3	1.90	0.40
1:A:223:VAL:HG13	1:A:236:VAL:CG1	2.51	0.40
1:A:304:PRO:CD	1:A:305:SER:H	2.32	0.40
1:A:330:LYS:HE3	1:A:330:LYS:HB2	1.59	0.40
2:B:64:PHE:N	2:B:64:PHE:CD1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:HIS:HB3	2:B:152:PRO:CD	2.51	0.40
2:B:264:LYS:O	2:B:265:GLU:C	2.64	0.40
2:B:277:VAL:O	2:B:280:ARG:HB2	2.22	0.40
2:B:153:THR:O	2:B:157:VAL:HG23	2.22	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	310/312 (99%)	259 (84%)	48 (16%)	3 (1%)	12	32
2	B	399/401 (100%)	349 (88%)	42 (10%)	8 (2%)	6	16
All	All	709/713 (99%)	608 (86%)	90 (13%)	11 (2%)	7	20

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ALA
1	A	287	ARG
2	B	74	GLN
2	B	322	ALA
2	B	378	SER
1	A	326	GLN
2	B	95	CYS
2	B	331	HIS
2	B	421	PRO
2	B	120	GLN
2	B	266	ARG

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	291/291 (100%)	262 (90%)	29 (10%)	7	19
2	B	338/338 (100%)	315 (93%)	23 (7%)	14	35
All	All	629/629 (100%)	577 (92%)	52 (8%)	10	26

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	63	TYR
1	A	64	VAL
1	A	87	VAL
1	A	89	GLN
1	A	106	VAL
1	A	121	ARG
1	A	162	GLN
1	A	214	ARG
1	A	221	GLN
1	A	251	SER
1	A	265	GLU
1	A	269	LEU
1	A	281	LYS
1	A	287	ARG
1	A	289	LEU
1	A	294	ASN
1	A	298	GLN
1	A	299	LEU
1	A	300	LEU
1	A	323	LEU
1	A	330	LYS
1	A	339	GLU
1	A	342	GLU
1	A	348	LYS
1	A	350	THR
1	A	352	ARG

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Mol	Chain	Res	Type
1	A	363	LEU
1	A	366	LYS
2	B	29	GLU
2	B	45	SER
2	B	68	VAL
2	B	77	LYS
2	B	84	ARG
2	B	96	LEU
2	B	108	LEU
2	B	175	GLU
2	B	201	VAL
2	B	245	MET
2	B	266	ARG
2	B	271	LYS
2	B	275	GLN
2	B	296	VAL
2	B	312	HIS
2	B	332	GLN
2	B	344	GLN
2	B	351	LEU
2	B	381	MET
2	B	382	LEU
2	B	387	MET
2	B	416	LEU
2	B	423	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	204	GLN
1	A	246	ASN
1	A	285	GLN
1	A	306	HIS
1	A	325	ASN
1	A	329	ASN
1	A	335	ASN
1	A	364	GLN
2	B	48	GLN
2	B	56	GLN
2	B	146	GLN
2	B	327	HIS

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Mol	Chain	Res	Type
2	B	331	HIS
2	B	332	GLN
2	B	333	GLN
2	B	392	ASN
2	B	410	GLN
2	B	414	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	HFP	B	501	-	16,19,19	1.42	3 (18%)	20,25,25	2.96	5 (25%)
5	FTL	B	1	3	39,39,39	1.54	6 (15%)	49,54,54	2.13	6 (12%)

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	HFP	B	501	-	2/2/5/5	11/22/22/22	-
5	FTL	B	1	3	-	1/20/20/20	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	FTL	C10-C12	4.63	1.42	1.36
4	B	501	HFP	C7-C8	-3.41	1.36	1.52
4	B	501	HFP	C2-C3	-2.88	1.42	1.53
5	B	1	FTL	C18-C12	2.73	1.53	1.50
5	B	1	FTL	C5-N3	2.52	1.38	1.32
4	B	501	HFP	C12-C13	-2.48	1.36	1.51
5	B	1	FTL	C3-C7	2.28	1.41	1.36
5	B	1	FTL	C4-C2	2.18	1.41	1.36
5	B	1	FTL	C55-C54	2.18	1.41	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	FTL	N4-C5-N3	-11.10	106.33	112.94
4	B	501	HFP	C3-C2-C1	10.84	126.20	115.21
5	B	1	FTL	C11-C8-N2	6.77	125.10	114.13
5	B	1	FTL	C10-N3-C5	4.27	110.82	105.24
4	B	501	HFP	C4-C3-C2	3.70	122.14	110.84
4	B	501	HFP	C2-C3-C5	2.96	121.53	111.86
5	B	1	FTL	C12-C10-N3	-2.62	104.23	109.79
4	B	501	HFP	C9-C8-C7	2.49	120.14	111.27
5	B	1	FTL	C8-C11-C13	-2.46	115.63	120.27
5	B	1	FTL	C8-C11-C16	2.25	124.89	120.75
4	B	501	HFP	C9-C8-C10	2.24	119.25	111.27

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	501	HFP	C3
4	B	501	HFP	C8

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	HFP	O1-C1-P-O1P
4	B	501	HFP	O1-C1-P-O2P

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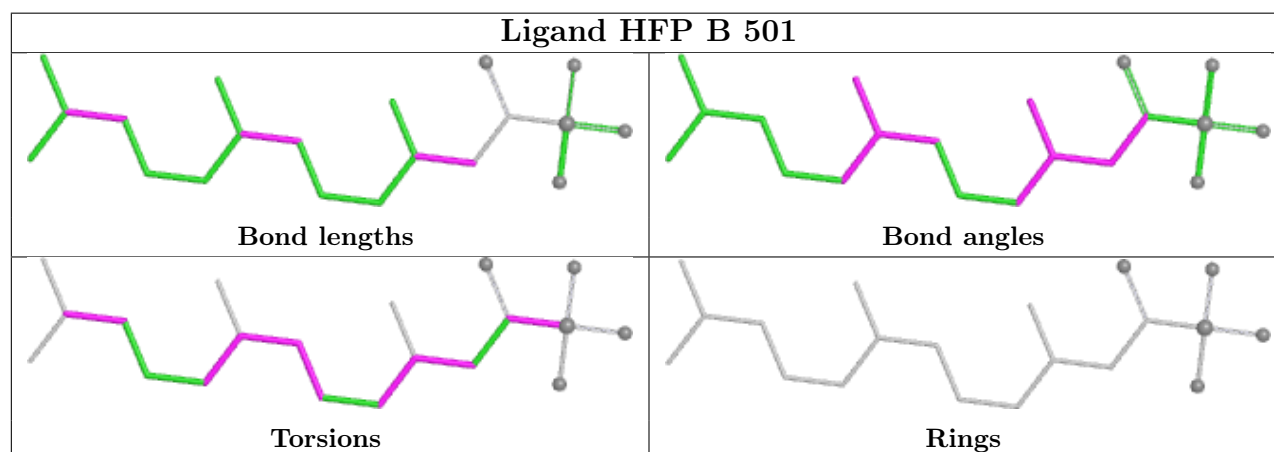
Mol	Chain	Res	Type	Atoms
4	B	501	HFP	O1-C1-P-O3P
4	B	501	HFP	C1-C2-C3-C4
4	B	501	HFP	C6-C7-C8-C9
4	B	501	HFP	C11-C12-C13-C14
4	B	501	HFP	C2-C1-P-O1P
4	B	501	HFP	C11-C10-C8-C9
4	B	501	HFP	C4-C3-C5-C6
4	B	501	HFP	C5-C6-C7-C8
4	B	501	HFP	C2-C3-C5-C6
5	B	1	FTL	C46-C45-C65-N1

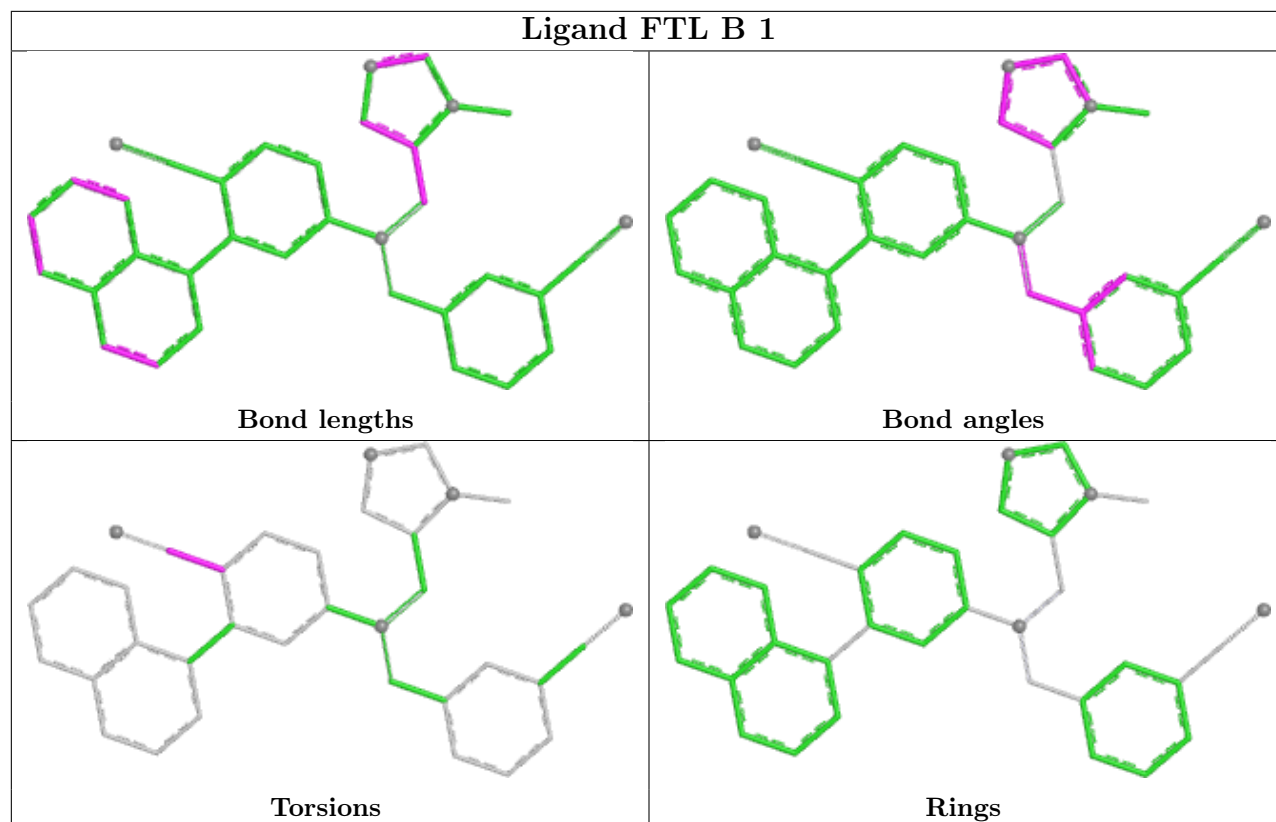
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	HFP	7	0
5	B	1	FTL	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.