



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:53 PM UTC

PDB ID : 1UBX / pdb_00001ubx
Title : STRUCTURE OF FARNESYL PYROPHOSPHATE SYNTHETASE
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Deposited on : 1996-10-14
Resolution : 2.50 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)	:	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

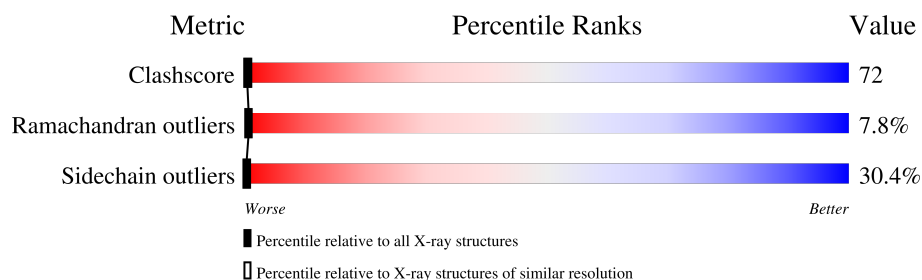
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	367	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2874 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 FARNESYL DIPHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2804	1786	477	527	14			

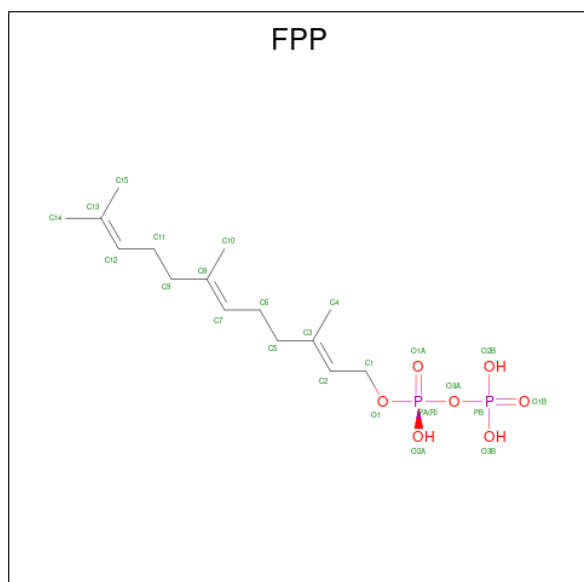
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	PHE	conflict	UNP P08836
A	113	SER	PHE	conflict	UNP P08836

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is FARNESYL DIPHOSPHATE (CCD ID: FPP) (formula: C₁₅H₂₈O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			24	15	7	2		

- Molecule 4 is water.

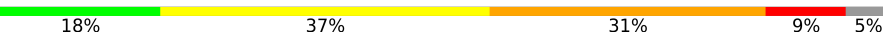
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		

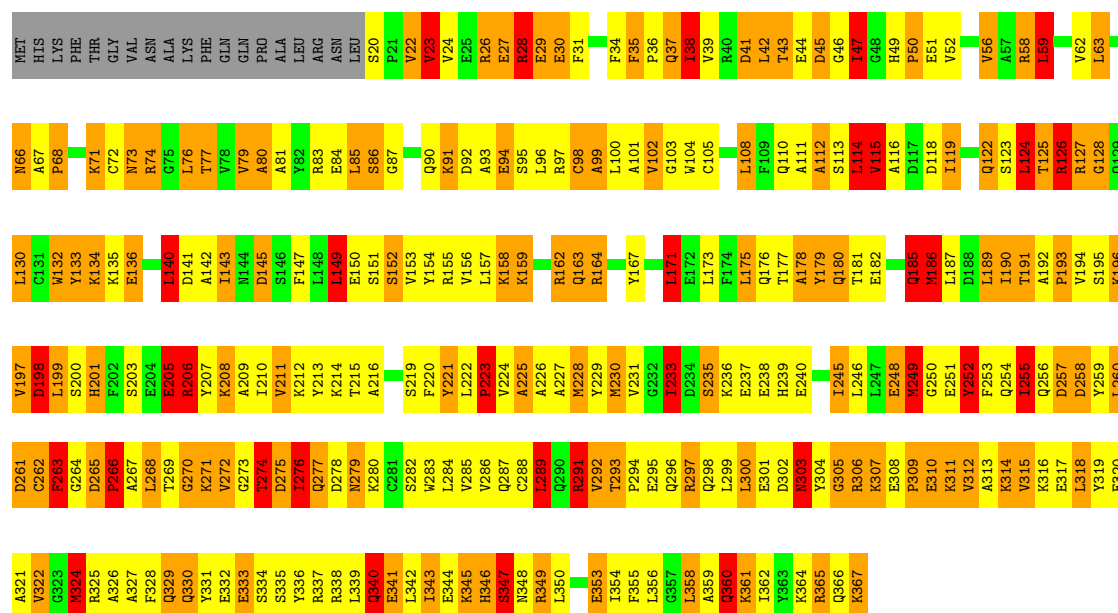
3 Residue-property plots

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: FARNESYL DIPHOSPHATE SYNTHASE

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	88.70Å 88.70Å 276.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2874	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: MG, FPP

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	1.41	9/2859 (0.3%)	1.91	83/3856 (2.2%)

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	16

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	MET	SD-CE	7.42	1.98	1.79
1	A	209	ALA	CA-CB	-7.22	1.42	1.53
1	A	228	MET	SD-CE	-7.01	1.62	1.79
1	A	255	ILE	CA-CB	-6.13	1.47	1.54
1	A	205	GLU	C-O	-5.50	1.17	1.24
1	A	176	GLN	CG-CD	5.45	1.65	1.52
1	A	178	ALA	CA-CB	-5.34	1.44	1.53
1	A	233	ILE	CA-CB	-5.24	1.47	1.54
1	A	229	TYR	CA-C	5.09	1.59	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ILE	CB-CA-C	-12.22	95.65	112.14
1	A	291	ARG	N-CA-C	-11.48	95.71	111.56
1	A	324	MET	N-CA-C	10.66	122.48	111.07
1	A	275	ASP	N-CA-C	10.25	123.32	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	PHE	N-CA-C	9.48	126.45	113.37
1	A	66	ASN	N-CA-C	9.46	125.60	112.45
1	A	119	ILE	CB-CA-C	-9.11	100.11	112.04
1	A	185	GLN	N-CA-C	-8.85	101.60	111.07
1	A	62	VAL	N-CA-C	-8.69	102.08	110.42
1	A	38	ILE	N-CA-C	-8.36	102.09	110.62
1	A	30	GLU	N-CA-C	-8.35	102.12	111.14
1	A	99	ALA	N-CA-C	-8.32	101.12	111.11
1	A	115	VAL	N-CA-C	-8.15	102.40	110.30
1	A	199	LEU	N-CA-C	-8.08	100.34	112.54
1	A	195	SER	N-CA-C	-7.92	102.59	111.14
1	A	343	ILE	CB-CA-C	-7.48	102.23	112.04
1	A	114	LEU	N-CA-C	7.26	121.39	112.54
1	A	132	TRP	N-CA-C	-7.17	103.55	111.36
1	A	230	MET	N-CA-C	-7.06	104.47	113.23
1	A	258	ASP	N-CA-C	6.96	119.89	111.82
1	A	128	GLY	CA-C-N	-6.85	111.50	122.53
1	A	128	GLY	C-N-CA	-6.85	111.50	122.53
1	A	190	ILE	CB-CA-C	-6.70	103.09	111.94
1	A	270	GLY	N-CA-C	-6.70	97.30	113.18
1	A	42	LEU	N-CA-C	6.65	120.85	112.87
1	A	347	SER	N-CA-C	6.64	121.28	112.25
1	A	354	ILE	N-CA-C	6.61	116.77	110.42
1	A	27	GLU	N-CA-C	-6.45	104.17	111.07
1	A	140	LEU	CA-CB-CG	-6.33	94.13	116.30
1	A	29	GLU	N-CA-C	6.24	120.97	113.23
1	A	176	GLN	N-CA-C	-6.23	104.41	111.14
1	A	47	ILE	CB-CA-C	-6.15	101.21	111.29
1	A	341	GLU	N-CA-C	6.12	118.49	111.02
1	A	274	THR	CB-CA-C	-5.89	98.69	110.42
1	A	266	PRO	N-CA-C	5.89	124.59	112.47
1	A	124	LEU	N-CA-C	-5.88	105.36	113.18
1	A	37	GLN	N-CA-C	-5.87	104.57	110.97
1	A	198	ASP	N-CA-C	5.84	123.24	110.80
1	A	149	LEU	N-CA-C	-5.84	105.00	111.36
1	A	257	ASP	N-CA-C	-5.81	105.45	112.54
1	A	79	VAL	CA-C-N	-5.77	113.03	120.65
1	A	79	VAL	C-N-CA	-5.77	113.03	120.65
1	A	190	ILE	N-CA-C	-5.76	105.50	110.74
1	A	152	SER	CA-CB-OG	-5.73	99.63	111.10
1	A	157	LEU	N-CA-C	-5.73	105.12	111.71
1	A	248	GLU	N-CA-C	-5.68	104.78	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	TYR	CB-CA-C	-5.68	101.93	110.90
1	A	23	VAL	N-CA-CB	5.66	117.17	110.55
1	A	206	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	A	81	ALA	N-CA-C	5.61	117.40	111.28
1	A	35	PHE	N-CA-C	5.56	122.10	109.81
1	A	272	VAL	N-CA-C	5.55	116.57	108.58
1	A	158	LYS	N-CA-C	-5.51	105.35	111.36
1	A	62	VAL	CB-CA-C	-5.51	104.92	111.97
1	A	255	ILE	N-CA-C	-5.51	104.50	110.23
1	A	346	HIS	N-CA-C	-5.49	106.43	114.39
1	A	85	LEU	N-CA-C	5.48	120.09	113.41
1	A	130	LEU	CB-CG-CD2	-5.44	94.39	110.70
1	A	145	ASP	N-CA-C	-5.42	105.53	111.82
1	A	141	ASP	N-CA-C	-5.41	105.31	112.34
1	A	364	LYS	O-C-N	5.39	129.76	122.59
1	A	214	LYS	CA-C-N	-5.38	111.35	121.63
1	A	214	LYS	C-N-CA	-5.38	111.35	121.63
1	A	59	LEU	CB-CA-C	-5.38	101.81	110.74
1	A	118	ASP	N-CA-C	5.34	117.52	111.11
1	A	249	MET	CB-CG-SD	-5.34	96.69	112.70
1	A	68	PRO	N-CA-C	-5.33	102.19	112.01
1	A	153	VAL	CB-CA-C	-5.31	104.90	112.22
1	A	76	LEU	CB-CG-CD1	-5.30	94.80	110.70
1	A	276	ILE	CB-CA-C	-5.29	102.62	111.29
1	A	171	LEU	CB-CA-C	-5.26	102.39	110.81
1	A	108	LEU	CB-CG-CD2	-5.23	95.00	110.70
1	A	303	ASN	N-CA-C	5.21	119.35	113.15
1	A	276	ILE	CG1-CB-CG2	-5.10	95.41	110.70
1	A	140	LEU	N-CA-C	5.08	118.74	112.54
1	A	176	GLN	CB-CG-CD	5.08	121.24	112.60
1	A	41	ASP	N-CA-C	-5.04	104.88	111.02
1	A	73	ASN	CA-C-N	-5.03	113.79	120.63
1	A	73	ASN	C-N-CA	-5.03	113.79	120.63
1	A	208	LYS	N-CA-C	5.02	118.89	112.87
1	A	98	CYS	CB-CA-C	-5.02	102.46	110.79
1	A	223	PRO	CA-C-N	-5.01	114.25	120.56
1	A	223	PRO	C-N-CA	-5.01	114.25	120.56

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	VAL	Mainchain
1	A	112	ALA	Mainchain
1	A	115	VAL	Mainchain
1	A	126	ARG	Mainchain
1	A	133	TYR	Sidechain
1	A	135	LYS	Mainchain
1	A	149	LEU	Mainchain
1	A	179	TYR	Mainchain
1	A	221	TYR	Sidechain
1	A	225	ALA	Mainchain
1	A	252	TYR	Sidechain
1	A	263	PHE	Sidechain
1	A	28	ARG	Mainchain
1	A	340	GLN	Mainchain
1	A	80	ALA	Mainchain
1	A	98	CYS	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2804	0	2790	404	0
2	A	1	0	0	0	0
3	A	24	0	25	3	0
4	A	45	0	0	8	0
All	All	2874	0	2815	404	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 72.

All (404) 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:299:LEU:HD13	1:A:318:LEU:HD22	1.24	1.14
1:A:298:GLN:HA	1:A:301:GLU:HG2	1.31	1.08
1:A:249:MET:HE1	1:A:358:LEU:HB3	1.41	1.03
1:A:296:GLN:HB3	1:A:318:LEU:HD21	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HD13	1:A:301:GLU:H	1.18	1.02
1:A:300:LEU:HD13	1:A:301:GLU:N	1.73	1.02
1:A:249:MET:CE	1:A:358:LEU:HB3	1.89	1.01
1:A:366:GLN:HG2	1:A:367:LYS:HE3	1.39	1.00
1:A:275:ASP:HB2	1:A:280:LYS:HZ2	1.29	0.96
1:A:80:ALA:HA	1:A:83:ARG:NH1	1.83	0.94
1:A:293:THR:HG23	1:A:296:GLN:HE22	1.37	0.90
1:A:277:GLN:HB2	1:A:307:LYS:HB3	1.57	0.87
1:A:185:GLN:HE21	1:A:185:GLN:HA	1.39	0.87
1:A:332:GLU:OE1	1:A:365:ARG:HG2	1.74	0.87
1:A:191:THR:O	1:A:193:PRO:HD3	1.75	0.86
1:A:298:GLN:HA	1:A:301:GLU:CG	2.05	0.86
1:A:329:GLN:NE2	1:A:365:ARG:NE	2.25	0.85
1:A:205:GLU:HB2	4:A:438:HOH:O	1.76	0.84
1:A:80:ALA:HA	1:A:83:ARG:HH12	1.43	0.83
1:A:329:GLN:HE21	1:A:365:ARG:HE	1.26	0.82
1:A:220:PHE:CE2	1:A:250:GLY:HA2	2.16	0.81
1:A:198:ASP:C	1:A:199:LEU:HD12	2.08	0.79
1:A:328:PHE:HZ	1:A:365:ARG:HB2	1.46	0.79
1:A:111:ALA:O	1:A:115:VAL:HG23	1.83	0.79
1:A:312:VAL:O	1:A:315:VAL:HG23	1.83	0.78
1:A:177:THR:O	1:A:181:THR:HG23	1.82	0.78
1:A:92:ASP:OD2	1:A:94:GLU:HB3	1.83	0.77
1:A:79:VAL:HG21	1:A:100:LEU:HD23	1.66	0.77
1:A:318:LEU:HA	1:A:321:ALA:HB3	1.66	0.77
1:A:277:GLN:HG3	1:A:278:ASP:N	1.98	0.76
1:A:298:GLN:CA	1:A:301:GLU:HG2	2.15	0.76
1:A:190:ILE:HG22	1:A:191:THR:N	2.01	0.76
1:A:285:VAL:HG22	1:A:319:TYR:OH	1.85	0.75
1:A:292:VAL:CG1	1:A:297:ARG:HB2	2.16	0.75
1:A:328:PHE:CZ	1:A:365:ARG:HB2	2.21	0.75
1:A:252:TYR:CE2	1:A:332:GLU:HG3	2.21	0.75
1:A:296:GLN:HB3	1:A:318:LEU:CD2	2.15	0.75
1:A:318:LEU:O	1:A:322:VAL:HG23	1.87	0.74
1:A:283:TRP:O	1:A:287:GLN:HG2	1.88	0.74
1:A:330:GLN:HA	1:A:333:GLU:HG2	1.70	0.74
1:A:22:VAL:O	1:A:26:ARG:HG2	1.88	0.73
1:A:317:GLU:O	1:A:321:ALA:N	2.20	0.73
1:A:38:ILE:O	1:A:41:ASP:HB2	1.88	0.73
1:A:255:ILE:HG22	1:A:256:GLN:N	2.04	0.73
1:A:278:ASP:C	1:A:280:LYS:H	1.97	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:OE1	1:A:338:ARG:HG2	1.88	0.72
1:A:275:ASP:HB2	1:A:280:LYS:NZ	2.02	0.72
1:A:226:ALA:O	1:A:230:MET:HG3	1.89	0.72
1:A:314:LYS:O	1:A:317:GLU:HB3	1.90	0.72
1:A:245:ILE:HG13	1:A:246:LEU:N	2.04	0.72
1:A:163:GLN:C	1:A:164:ARG:HG2	2.14	0.71
1:A:35:PHE:HB3	1:A:36:PRO:HD3	1.72	0.71
1:A:329:GLN:NE2	1:A:365:ARG:HE	1.87	0.71
1:A:284:LEU:CD2	1:A:324:MET:HG3	2.20	0.70
1:A:276:ILE:N	1:A:280:LYS:HD3	2.06	0.70
1:A:282:SER:O	1:A:286:VAL:HG23	1.90	0.70
1:A:249:MET:HE2	1:A:358:LEU:HB3	1.73	0.70
1:A:249:MET:HE1	1:A:358:LEU:CB	2.21	0.70
1:A:38:ILE:CG2	1:A:42:LEU:HD12	2.22	0.70
1:A:245:ILE:HA	1:A:342:LEU:HD23	1.74	0.69
1:A:274:THR:HG23	1:A:275:ASP:N	2.03	0.69
1:A:200:SER:OG	1:A:201:HIS:N	2.25	0.69
1:A:303:ASN:HD22	1:A:311:LYS:HG2	1.56	0.69
1:A:336:TYR:O	1:A:340:GLN:HG2	1.92	0.69
1:A:211:VAL:HG12	1:A:212:LYS:N	2.08	0.69
1:A:293:THR:HG23	1:A:296:GLN:NE2	2.07	0.69
1:A:245:ILE:HD11	1:A:355:PHE:HB3	1.75	0.69
1:A:295:GLU:HG2	1:A:296:GLN:OE1	1.92	0.69
1:A:41:ASP:HA	4:A:432:HOH:O	1.93	0.68
1:A:186:MET:HE2	1:A:186:MET:HA	1.76	0.68
1:A:196:LYS:O	1:A:198:ASP:N	2.27	0.68
1:A:196:LYS:HG3	1:A:198:ASP:OD2	1.93	0.68
1:A:220:PHE:O	1:A:223:PRO:HD2	1.93	0.68
1:A:299:LEU:HD13	1:A:318:LEU:CD2	2.14	0.68
1:A:191:THR:C	1:A:193:PRO:HD3	2.19	0.68
1:A:365:ARG:HG3	1:A:365:ARG:HH11	1.60	0.67
1:A:311:LYS:O	1:A:314:LYS:N	2.23	0.67
1:A:317:GLU:O	1:A:320:GLU:HB2	1.94	0.67
1:A:203:SER:O	1:A:206:ARG:N	2.27	0.67
1:A:356:LEU:O	1:A:359:ALA:HB3	1.95	0.66
1:A:28:ARG:HE	1:A:73:ASN:HD21	1.44	0.66
1:A:329:GLN:HA	1:A:329:GLN:OE1	1.91	0.66
1:A:303:ASN:HB3	1:A:311:LYS:CB	2.25	0.66
1:A:278:ASP:O	1:A:280:LYS:HG2	1.95	0.65
1:A:259:TYR:OH	1:A:325:ARG:HG2	1.96	0.65
1:A:71:LYS:HE3	4:A:431:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLU:HA	1:A:344:GLU:OE2	1.97	0.65
1:A:154:TYR:CZ	1:A:175:LEU:HD13	2.32	0.65
1:A:285:VAL:O	1:A:288:CYS:N	2.30	0.65
1:A:349:ARG:O	1:A:350:LEU:HD23	1.96	0.65
1:A:196:LYS:O	1:A:196:LYS:HE3	1.96	0.64
1:A:264:GLY:HA3	1:A:367:LYS:HZ1	1.62	0.64
1:A:296:GLN:O	1:A:299:LEU:N	2.30	0.64
1:A:329:GLN:HE21	1:A:365:ARG:NE	1.90	0.64
1:A:338:ARG:CG	1:A:342:LEU:HD13	2.27	0.64
1:A:245:ILE:CD1	1:A:355:PHE:HB3	2.28	0.64
1:A:92:ASP:O	1:A:95:SER:N	2.31	0.64
1:A:304:TYR:O	1:A:306:ARG:N	2.31	0.64
1:A:312:VAL:HG12	1:A:313:ALA:N	2.11	0.64
1:A:255:ILE:O	1:A:258:ASP:HB2	1.99	0.63
1:A:59:LEU:O	1:A:59:LEU:HD22	1.99	0.63
1:A:125:THR:HG23	4:A:418:HOH:O	1.98	0.63
1:A:275:ASP:HB3	1:A:280:LYS:CD	2.29	0.63
1:A:252:TYR:HE2	1:A:332:GLU:HG3	1.64	0.63
1:A:173:LEU:O	1:A:177:THR:HG23	1.99	0.62
1:A:185:GLN:HE21	1:A:185:GLN:CA	2.12	0.62
1:A:228:MET:HE2	1:A:239:HIS:CE1	2.34	0.62
1:A:102:VAL:O	1:A:105:CYS:HB2	1.99	0.62
1:A:263:PHE:CE2	1:A:324:MET:HB2	2.34	0.62
1:A:338:ARG:HD3	4:A:428:HOH:O	1.98	0.62
1:A:366:GLN:O	1:A:367:LYS:NZ	2.32	0.62
1:A:303:ASN:HB3	1:A:311:LYS:HB3	1.81	0.62
1:A:154:TYR:CE1	1:A:175:LEU:HD13	2.33	0.62
1:A:294:PRO:HD2	1:A:295:GLU:OE1	2.00	0.62
1:A:342:LEU:O	1:A:346:HIS:HB2	2.00	0.62
1:A:309:PRO:O	1:A:313:ALA:HB3	2.00	0.62
1:A:147:PHE:O	1:A:150:GLU:HB3	1.99	0.61
1:A:327:ALA:HB1	4:A:424:HOH:O	1.99	0.61
1:A:194:VAL:HA	1:A:197:VAL:HA	1.81	0.61
1:A:285:VAL:HG21	1:A:304:TYR:CZ	2.35	0.61
1:A:293:THR:CG2	1:A:296:GLN:HE22	2.12	0.61
1:A:318:LEU:O	1:A:321:ALA:N	2.33	0.61
1:A:74:ARG:O	1:A:77:THR:HB	2.00	0.61
1:A:126:ARG:HG3	1:A:127:ARG:N	2.15	0.61
1:A:303:ASN:HB3	1:A:311:LYS:CG	2.31	0.61
1:A:338:ARG:HG2	1:A:342:LEU:HD13	1.83	0.61
1:A:110:GLN:O	1:A:114:LEU:HG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASP:CB	1:A:280:LYS:HZ2	2.08	0.60
1:A:275:ASP:HB3	1:A:280:LYS:HD2	1.81	0.60
1:A:22:VAL:HG12	1:A:23:VAL:N	2.17	0.60
1:A:46:GLY:HA3	1:A:56:VAL:HG21	1.82	0.60
1:A:340:GLN:O	1:A:344:GLU:OE1	2.18	0.60
1:A:366:GLN:C	1:A:367:LYS:HG3	2.25	0.60
1:A:38:ILE:HG22	1:A:42:LEU:HD12	1.82	0.60
1:A:284:LEU:HD22	1:A:324:MET:HG3	1.83	0.59
1:A:154:TYR:CZ	1:A:175:LEU:CD1	2.85	0.59
1:A:296:GLN:OE1	1:A:296:GLN:N	2.21	0.59
1:A:345:LYS:O	1:A:345:LYS:HG2	2.01	0.59
1:A:318:LEU:HD12	1:A:318:LEU:C	2.28	0.59
1:A:278:ASP:O	1:A:280:LYS:N	2.33	0.59
1:A:277:GLN:OE1	1:A:307:LYS:HD2	2.03	0.59
1:A:284:LEU:HD22	1:A:324:MET:CG	2.33	0.59
1:A:20:SER:C	1:A:22:VAL:H	2.10	0.58
1:A:46:GLY:C	1:A:56:VAL:HG21	2.28	0.58
1:A:86:SER:OG	1:A:91:LYS:HE3	2.03	0.58
1:A:101:ALA:O	1:A:103:GLY:N	2.37	0.58
1:A:274:THR:O	1:A:275:ASP:OD1	2.21	0.58
1:A:220:PHE:HE2	1:A:250:GLY:HA2	1.66	0.58
1:A:353:GLU:OE1	1:A:353:GLU:N	2.36	0.58
1:A:332:GLU:CD	1:A:365:ARG:HG2	2.28	0.58
1:A:26:ARG:HG3	1:A:26:ARG:HH11	1.68	0.58
1:A:43:THR:O	1:A:47:ILE:HG12	2.04	0.57
1:A:35:PHE:O	1:A:39:VAL:HG23	2.04	0.57
1:A:277:GLN:C	1:A:277:GLN:HE21	2.12	0.57
1:A:259:TYR:CE2	1:A:263:PHE:HB3	2.40	0.57
1:A:31:PHE:CE1	1:A:104:TRP:CD1	2.92	0.57
1:A:104:TRP:O	1:A:108:LEU:HG	2.04	0.57
1:A:266:PRO:O	1:A:267:ALA:HB3	2.05	0.57
1:A:66:ASN:HD21	1:A:132:TRP:HB2	1.70	0.56
1:A:296:GLN:O	1:A:300:LEU:HD12	2.05	0.56
1:A:26:ARG:HG3	1:A:26:ARG:NH1	2.19	0.56
1:A:255:ILE:O	1:A:258:ASP:N	2.39	0.56
1:A:292:VAL:HG11	1:A:297:ARG:HB2	1.85	0.56
1:A:235:SER:OG	1:A:238:GLU:HB2	2.04	0.56
1:A:233:ILE:HD13	1:A:350:LEU:CD2	2.35	0.56
1:A:311:LYS:O	1:A:315:VAL:HG22	2.05	0.56
1:A:326:ALA:O	1:A:329:GLN:N	2.39	0.56
1:A:279:ASN:OD1	1:A:304:TYR:HD2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:O	1:A:112:ALA:C	2.48	0.56
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.71	0.56
1:A:31:PHE:HD1	1:A:100:LEU:HD22	1.71	0.55
1:A:265:ASP:O	1:A:268:LEU:HB2	2.07	0.55
1:A:71:LYS:O	1:A:72:CYS:HB2	2.06	0.55
1:A:270:GLY:CA	1:A:271:LYS:HE3	2.36	0.55
1:A:298:GLN:HA	1:A:301:GLU:CD	2.32	0.55
1:A:35:PHE:HB3	1:A:36:PRO:CD	2.36	0.55
1:A:278:ASP:HB2	1:A:280:LYS:HD2	1.88	0.55
1:A:275:ASP:CB	1:A:280:LYS:NZ	2.68	0.55
1:A:318:LEU:O	1:A:322:VAL:N	2.40	0.55
1:A:275:ASP:OD2	1:A:278:ASP:OD2	2.26	0.54
1:A:224:VAL:HG21	1:A:246:LEU:HD11	1.90	0.54
1:A:220:PHE:CD2	1:A:250:GLY:HA2	2.43	0.54
1:A:252:TYR:CD1	1:A:252:TYR:C	2.86	0.54
1:A:104:TRP:O	1:A:108:LEU:N	2.37	0.54
1:A:259:TYR:CZ	1:A:263:PHE:HB3	2.43	0.54
1:A:259:TYR:C	1:A:261:ASP:H	2.15	0.54
1:A:263:PHE:CE2	1:A:324:MET:CB	2.91	0.54
1:A:297:ARG:O	1:A:301:GLU:HB3	2.08	0.54
1:A:339:LEU:HD23	1:A:340:GLN:OE1	2.08	0.54
1:A:248:GLU:HG3	1:A:338:ARG:CZ	2.37	0.54
1:A:262:CYS:HB2	1:A:316:LYS:NZ	2.23	0.54
1:A:262:CYS:SG	1:A:263:PHE:CD1	3.01	0.53
1:A:215:THR:O	1:A:219:SER:OG	2.23	0.53
1:A:285:VAL:HG21	1:A:304:TYR:OH	2.08	0.53
1:A:349:ARG:O	1:A:349:ARG:HG2	2.08	0.53
1:A:190:ILE:O	1:A:193:PRO:HG3	2.09	0.53
1:A:316:LYS:O	1:A:319:TYR:HB2	2.07	0.53
1:A:287:GLN:HB3	1:A:324:MET:CE	2.38	0.53
1:A:277:GLN:HG3	1:A:278:ASP:OD1	2.09	0.53
1:A:365:ARG:HH11	1:A:365:ARG:CG	2.22	0.52
1:A:113:SER:O	1:A:116:ALA:HB3	2.09	0.52
1:A:252:TYR:CZ	1:A:332:GLU:HG3	2.43	0.52
1:A:318:LEU:HD12	1:A:322:VAL:CG2	2.40	0.52
1:A:35:PHE:CE2	1:A:39:VAL:HG21	2.44	0.51
1:A:49:HIS:C	1:A:51:GLU:H	2.17	0.51
1:A:185:GLN:HA	1:A:185:GLN:NE2	2.19	0.51
1:A:259:TYR:O	1:A:261:ASP:N	2.43	0.51
1:A:248:GLU:O	1:A:251:GLU:N	2.43	0.51
1:A:259:TYR:CE2	1:A:325:ARG:HG2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:PHE:HZ	1:A:365:ARG:CB	2.19	0.51
1:A:127:ARG:N	4:A:417:HOH:O	2.27	0.51
1:A:298:GLN:HA	1:A:301:GLU:OE2	2.10	0.51
1:A:311:LYS:O	1:A:312:VAL:C	2.53	0.51
1:A:46:GLY:CA	1:A:56:VAL:HG21	2.41	0.51
1:A:181:THR:HA	1:A:213:TYR:O	2.10	0.51
1:A:287:GLN:OE1	1:A:291:ARG:NH1	2.43	0.51
1:A:233:ILE:HD13	1:A:350:LEU:HD21	1.93	0.51
1:A:293:THR:OG1	1:A:295:GLU:HG2	2.11	0.51
1:A:304:TYR:CD2	1:A:305:GLY:N	2.78	0.51
1:A:252:TYR:OH	1:A:332:GLU:HG3	2.11	0.51
1:A:34:PHE:CD2	1:A:100:LEU:HB3	2.46	0.50
1:A:59:LEU:HD22	1:A:63:LEU:HD22	1.92	0.50
1:A:278:ASP:C	1:A:280:LYS:N	2.68	0.50
1:A:329:GLN:C	1:A:331:TYR:H	2.19	0.50
1:A:259:TYR:CZ	1:A:325:ARG:HG2	2.46	0.50
1:A:111:ALA:C	1:A:115:VAL:HG23	2.34	0.50
1:A:333:GLU:HG3	1:A:334:SER:N	2.26	0.50
1:A:27:GLU:O	1:A:30:GLU:N	2.45	0.50
1:A:366:GLN:CG	1:A:367:LYS:HE3	2.28	0.50
1:A:222:LEU:N	1:A:223:PRO:CD	2.75	0.50
1:A:262:CYS:SG	1:A:263:PHE:N	2.84	0.50
1:A:203:SER:O	1:A:206:ARG:HB3	2.12	0.49
1:A:262:CYS:HB2	1:A:316:LYS:HZ2	1.77	0.49
1:A:220:PHE:CD2	1:A:250:GLY:CA	2.95	0.49
1:A:339:LEU:O	1:A:340:GLN:C	2.54	0.49
1:A:77:THR:HG22	1:A:223:PRO:HB2	1.94	0.49
1:A:97:ARG:O	1:A:100:LEU:HB2	2.13	0.49
1:A:119:ILE:O	1:A:122:GLN:NE2	2.45	0.49
1:A:318:LEU:HA	1:A:321:ALA:CB	2.41	0.49
1:A:116:ALA:HB3	3:A:401:FPP:H102	1.94	0.49
1:A:191:THR:HG22	1:A:192:ALA:N	2.28	0.49
1:A:299:LEU:HD22	1:A:318:LEU:HD23	1.95	0.49
1:A:101:ALA:C	1:A:103:GLY:N	2.69	0.49
1:A:125:THR:HG23	1:A:126:ARG:N	2.28	0.48
1:A:292:VAL:HG13	1:A:293:THR:N	2.27	0.48
1:A:186:MET:HE2	1:A:186:MET:CA	2.43	0.48
1:A:296:GLN:CB	1:A:318:LEU:HD21	2.29	0.48
1:A:122:GLN:HA	1:A:133:TYR:OH	2.12	0.48
1:A:293:THR:CB	1:A:294:PRO:CD	2.91	0.48
1:A:304:TYR:C	1:A:306:ARG:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:O	1:A:99:ALA:HB3	2.14	0.48
1:A:248:GLU:OE1	1:A:342:LEU:HD22	2.13	0.48
1:A:79:VAL:HG21	1:A:100:LEU:CD2	2.42	0.48
1:A:275:ASP:C	1:A:280:LYS:HD3	2.38	0.48
1:A:338:ARG:HG3	1:A:342:LEU:HD13	1.94	0.48
1:A:293:THR:OG1	1:A:295:GLU:OE1	2.32	0.48
1:A:178:ALA:O	1:A:182:GLU:HG3	2.13	0.48
1:A:263:PHE:CD2	1:A:325:ARG:HG3	2.49	0.48
1:A:35:PHE:N	1:A:36:PRO:HD2	2.28	0.47
1:A:296:GLN:O	1:A:299:LEU:HB3	2.14	0.47
1:A:27:GLU:OE2	1:A:83:ARG:NH1	2.47	0.47
1:A:299:LEU:C	1:A:299:LEU:HD23	2.39	0.47
1:A:84:GLU:OE1	1:A:353:GLU:HB2	2.14	0.47
1:A:285:VAL:CG2	1:A:304:TYR:CE1	2.98	0.47
1:A:297:ARG:NH1	1:A:301:GLU:OE1	2.48	0.47
1:A:20:SER:O	1:A:24:VAL:HG12	2.15	0.47
1:A:59:LEU:HD13	1:A:63:LEU:HD22	1.97	0.47
1:A:207:TYR:O	1:A:210:ILE:HB	2.15	0.47
1:A:365:ARG:CG	1:A:365:ARG:NH1	2.78	0.47
1:A:292:VAL:CG1	1:A:293:THR:N	2.76	0.47
1:A:270:GLY:HA3	1:A:271:LYS:HE3	1.97	0.47
1:A:280:LYS:O	1:A:304:TYR:OH	2.31	0.47
1:A:45:ASP:OD1	1:A:45:ASP:N	2.47	0.47
1:A:266:PRO:N	1:A:366:GLN:HE22	2.11	0.46
1:A:274:THR:HG23	1:A:275:ASP:HA	1.96	0.46
1:A:312:VAL:C	1:A:314:LYS:H	2.23	0.46
1:A:110:GLN:O	1:A:113:SER:OG	2.26	0.46
1:A:189:LEU:HD13	1:A:189:LEU:N	2.28	0.46
1:A:275:ASP:O	1:A:276:ILE:HG13	2.16	0.46
1:A:74:ARG:HH21	1:A:219:SER:CB	2.28	0.46
1:A:196:LYS:HD2	1:A:196:LYS:HA	1.77	0.46
1:A:311:LYS:O	1:A:314:LYS:HB3	2.16	0.46
1:A:259:TYR:HD1	1:A:260:LEU:HD23	1.80	0.46
1:A:300:LEU:C	1:A:302:ASP:N	2.72	0.46
1:A:101:ALA:O	1:A:102:VAL:C	2.57	0.46
1:A:329:GLN:NE2	1:A:365:ARG:CZ	2.79	0.46
1:A:182:GLU:HG2	3:A:401:FPP:C12	2.45	0.46
1:A:329:GLN:C	1:A:331:TYR:N	2.73	0.46
1:A:49:HIS:HB3	1:A:52:VAL:HG22	1.97	0.46
1:A:340:GLN:O	1:A:343:ILE:N	2.41	0.46
1:A:264:GLY:CA	1:A:367:LYS:NZ	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLU:C	1:A:320:GLU:HB2	2.40	0.46
1:A:304:TYR:CG	1:A:305:GLY:N	2.84	0.45
1:A:123:SER:O	1:A:133:TYR:OH	2.32	0.45
1:A:42:LEU:C	1:A:43:THR:HG23	2.41	0.45
1:A:92:ASP:CG	1:A:95:SER:H	2.25	0.45
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.49	0.45
1:A:203:SER:C	1:A:206:ARG:H	2.24	0.45
1:A:253:PHE:CD1	1:A:253:PHE:C	2.94	0.45
1:A:276:ILE:HG21	1:A:315:VAL:HG21	1.98	0.45
1:A:158:LYS:O	1:A:162:ARG:HB2	2.17	0.45
1:A:224:VAL:O	1:A:227:ALA:HB3	2.16	0.45
1:A:310:GLU:O	1:A:314:LYS:HB3	2.15	0.45
1:A:289:LEU:HD23	1:A:289:LEU:O	2.15	0.45
1:A:287:GLN:HA	1:A:291:ARG:NH1	2.32	0.45
1:A:126:ARG:O	1:A:127:ARG:C	2.59	0.44
1:A:304:TYR:C	1:A:306:ARG:N	2.72	0.44
1:A:275:ASP:HB2	1:A:280:LYS:CE	2.47	0.44
1:A:49:HIS:CD2	1:A:50:PRO:HD2	2.51	0.44
1:A:63:LEU:HD13	1:A:149:LEU:CD2	2.48	0.44
1:A:67:ALA:N	1:A:68:PRO:CD	2.79	0.44
1:A:86:SER:HA	1:A:90:GLN:OE1	2.17	0.44
1:A:308:GLU:HA	1:A:309:PRO:HD2	1.44	0.44
1:A:360:GLN:O	1:A:360:GLN:HG2	2.17	0.44
1:A:151:SER:O	1:A:152:SER:C	2.61	0.44
1:A:327:ALA:O	1:A:331:TYR:N	2.51	0.44
1:A:329:GLN:O	1:A:333:GLU:HB3	2.18	0.44
1:A:124:LEU:HD13	1:A:124:LEU:HA	1.68	0.44
1:A:189:LEU:HA	1:A:189:LEU:HD12	1.33	0.44
1:A:303:ASN:OD1	1:A:303:ASN:N	2.50	0.44
1:A:140:LEU:HA	1:A:140:LEU:HD12	0.89	0.44
1:A:198:ASP:HB3	1:A:200:SER:OG	2.18	0.44
1:A:343:ILE:O	1:A:347:SER:HB2	2.18	0.44
1:A:196:LYS:HG3	1:A:198:ASP:CG	2.43	0.43
1:A:300:LEU:HD13	1:A:300:LEU:C	2.34	0.43
1:A:186:MET:HA	1:A:186:MET:CE	2.46	0.43
1:A:285:VAL:O	1:A:288:CYS:HB3	2.18	0.43
1:A:300:LEU:C	1:A:302:ASP:H	2.26	0.43
1:A:134:LYS:HA	1:A:134:LYS:HD3	1.65	0.43
1:A:208:LYS:HA	1:A:211:VAL:HB	1.99	0.43
1:A:252:TYR:HE1	1:A:256:GLN:CD	2.26	0.43
1:A:279:ASN:OD1	1:A:304:TYR:CD2	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:OH	1:A:175:LEU:HD12	2.18	0.43
1:A:318:LEU:HD12	1:A:322:VAL:HG22	2.00	0.43
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.72	0.43
1:A:228:MET:CE	1:A:239:HIS:CE1	3.01	0.43
1:A:303:ASN:HB3	1:A:311:LYS:HG2	2.01	0.43
1:A:79:VAL:O	1:A:80:ALA:C	2.57	0.43
1:A:108:LEU:HA	1:A:108:LEU:HD23	1.66	0.43
1:A:149:LEU:O	1:A:152:SER:HB2	2.19	0.43
1:A:259:TYR:CE2	1:A:263:PHE:CB	3.02	0.43
1:A:177:THR:HA	1:A:180:GLN:HG3	2.00	0.43
1:A:119:ILE:O	1:A:119:ILE:HG22	2.15	0.43
1:A:191:THR:CG2	1:A:192:ALA:N	2.78	0.43
1:A:274:THR:HG23	1:A:275:ASP:CA	2.48	0.43
1:A:58:ARG:NH1	1:A:145:ASP:OD2	2.53	0.42
1:A:332:GLU:OE2	1:A:365:ARG:HB3	2.19	0.42
1:A:26:ARG:O	1:A:27:GLU:C	2.62	0.42
1:A:116:ALA:HB3	3:A:401:FPP:C10	2.49	0.42
1:A:276:ILE:O	1:A:305:GLY:HA2	2.20	0.42
1:A:56:VAL:O	1:A:59:LEU:HB3	2.19	0.42
1:A:318:LEU:O	1:A:321:ALA:HB3	2.19	0.42
1:A:126:ARG:C	1:A:128:GLY:N	2.77	0.42
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.71	0.42
1:A:127:ARG:O	1:A:127:ARG:HG3	2.20	0.42
1:A:266:PRO:O	1:A:267:ALA:CB	2.68	0.42
1:A:335:SER:O	1:A:336:TYR:C	2.62	0.42
1:A:339:LEU:O	1:A:342:LEU:HB2	2.19	0.42
1:A:344:GLU:OE1	1:A:344:GLU:N	2.51	0.42
1:A:186:MET:CA	1:A:186:MET:CE	2.96	0.42
1:A:276:ILE:HG21	1:A:276:ILE:HD13	1.45	0.42
1:A:262:CYS:HB2	1:A:316:LYS:HE3	2.01	0.42
1:A:292:VAL:HG13	1:A:297:ARG:HB2	1.99	0.42
1:A:331:TYR:O	1:A:334:SER:N	2.53	0.42
1:A:348:ASN:OD1	1:A:348:ASN:O	2.38	0.42
1:A:359:ALA:C	1:A:361:LYS:H	2.27	0.42
1:A:206:ARG:HE	1:A:206:ARG:HB2	1.66	0.42
1:A:191:THR:OG1	1:A:206:ARG:NH1	2.53	0.41
1:A:262:CYS:CB	1:A:316:LYS:HZ2	2.33	0.41
1:A:273:GLY:O	1:A:274:THR:HB	2.20	0.41
1:A:275:ASP:CB	1:A:280:LYS:CE	2.97	0.41
1:A:318:LEU:O	1:A:322:VAL:CG2	2.65	0.41
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLU:H	1:A:344:GLU:CD	2.29	0.41
1:A:254:GLN:HE21	1:A:254:GLN:HA	1.84	0.41
1:A:342:LEU:O	1:A:346:HIS:CD2	2.74	0.41
1:A:49:HIS:HA	1:A:50:PRO:HD2	1.86	0.41
1:A:87:GLY:O	1:A:90:GLN:N	2.53	0.41
1:A:159:LYS:O	1:A:159:LYS:HG3	2.21	0.41
1:A:206:ARG:HG3	1:A:207:TYR:N	2.29	0.41
1:A:207:TYR:O	1:A:210:ILE:N	2.54	0.41
1:A:222:LEU:N	1:A:223:PRO:HD3	2.35	0.41
1:A:248:GLU:CD	1:A:338:ARG:HG2	2.45	0.41
1:A:291:ARG:O	1:A:322:VAL:CG1	2.69	0.41
1:A:349:ARG:O	1:A:349:ARG:CG	2.68	0.41
1:A:49:HIS:C	1:A:51:GLU:N	2.77	0.41
1:A:126:ARG:HG2	1:A:127:ARG:HG2	2.03	0.41
1:A:335:SER:C	1:A:337:ARG:N	2.73	0.41
1:A:47:ILE:N	1:A:56:VAL:HG21	2.36	0.41
1:A:142:ALA:O	1:A:143:ILE:C	2.64	0.41
1:A:221:TYR:CE1	1:A:225:ALA:HB2	2.56	0.41
1:A:299:LEU:O	1:A:303:ASN:OD1	2.39	0.41
1:A:359:ALA:C	1:A:361:LYS:N	2.78	0.41
1:A:283:TRP:NE1	1:A:287:GLN:HG3	2.36	0.40
1:A:248:GLU:HG3	1:A:338:ARG:NH1	2.36	0.40
1:A:336:TYR:CE1	1:A:340:GLN:OE1	2.74	0.40
1:A:26:ARG:HG2	1:A:26:ARG:H	1.68	0.40
1:A:140:LEU:C	1:A:142:ALA:N	2.78	0.40
1:A:156:VAL:O	1:A:156:VAL:HG12	2.21	0.40
1:A:212:LYS:O	1:A:216:ALA:HB3	2.22	0.40
1:A:276:ILE:HG13	1:A:316:LYS:NZ	2.37	0.40
1:A:312:VAL:C	1:A:314:LYS:N	2.80	0.40
1:A:348:ASN:ND2	4:A:447:HOH:O	2.50	0.40
1:A:85:LEU:HB3	1:A:231:VAL:HG11	2.03	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	346/367 (94%)	253 (73%)	66 (19%)	27 (8%)	1	0

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	ARG
1	A	193	PRO
1	A	198	ASP
1	A	276	ILE
1	A	279	ASN
1	A	309	PRO
1	A	349	ARG
1	A	136	GLU
1	A	162	ARG
1	A	197	VAL
1	A	260	LEU
1	A	265	ASP
1	A	305	GLY
1	A	311	LYS
1	A	360	GLN
1	A	47	ILE
1	A	167	TYR
1	A	223	PRO
1	A	233	ILE
1	A	266	PRO
1	A	274	THR
1	A	22	VAL
1	A	43	THR
1	A	289	LEU
1	A	50	PRO
1	A	93	ALA
1	A	345	LYS

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	299/315 (95%)	208 (70%)	91 (30%)	0 0

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	26	ARG
1	A	28	ARG
1	A	29	GLU
1	A	37	GLN
1	A	38	ILE
1	A	44	GLU
1	A	45	ASP
1	A	56	VAL
1	A	58	ARG
1	A	59	LEU
1	A	63	LEU
1	A	71	LYS
1	A	74	ARG
1	A	76	LEU
1	A	77	THR
1	A	86	SER
1	A	91	LYS
1	A	94	GLU
1	A	114	LEU
1	A	115	VAL
1	A	122	GLN
1	A	124	LEU
1	A	125	THR
1	A	126	ARG
1	A	130	LEU
1	A	134	LYS
1	A	136	GLU
1	A	140	LEU
1	A	143	ILE
1	A	159	LYS
1	A	163	GLN
1	A	164	ARG
1	A	171	LEU
1	A	175	LEU
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	185	GLN
1	A	186	MET
1	A	189	LEU
1	A	191	THR
1	A	196	LYS
1	A	201	HIS
1	A	205	GLU
1	A	206	ARG
1	A	211	VAL
1	A	235	SER
1	A	236	LYS
1	A	237	GLU
1	A	240	GLU
1	A	245	ILE
1	A	249	MET
1	A	252	TYR
1	A	255	ILE
1	A	257	ASP
1	A	261	ASP
1	A	262	CYS
1	A	268	LEU
1	A	269	THR
1	A	271	LYS
1	A	272	VAL
1	A	274	THR
1	A	276	ILE
1	A	277	GLN
1	A	289	LEU
1	A	291	ARG
1	A	292	VAL
1	A	293	THR
1	A	297	ARG
1	A	300	LEU
1	A	303	ASN
1	A	306	ARG
1	A	307	LYS
1	A	310	GLU
1	A	312	VAL
1	A	314	LYS
1	A	315	VAL
1	A	318	LEU
1	A	322	VAL

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Mol	Chain	Res	Type
1	A	324	MET
1	A	329	GLN
1	A	330	GLN
1	A	333	GLU
1	A	340	GLN
1	A	347	SER
1	A	353	GLU
1	A	358	LEU
1	A	360	GLN
1	A	361	LYS
1	A	362	ILE
1	A	365	ARG
1	A	367	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	73	ASN
1	A	169	HIS
1	A	185	GLN
1	A	254	GLN
1	A	329	GLN
1	A	330	GLN
1	A	346	HIS
1	A	348	ASN

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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$
3	FPP	A	401	-	22,23,23	1.56	1 (4%)	27,31,31	1.78	6 (22%)

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
3	FPP	A	401	-	-	4/25/25/25	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	FPP	PA-O3A	-4.98	1.54	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	FPP	O3B-PB-O3A	4.65	120.24	104.64
3	A	401	FPP	O3A-PA-O1A	-4.41	97.43	110.70
3	A	401	FPP	C4-C3-C5	2.92	120.30	115.23
3	A	401	FPP	C10-C8-C9	2.75	120.00	115.23
3	A	401	FPP	O3B-PB-O1B	-2.45	101.30	110.83
3	A	401	FPP	O2A-PA-O3A	2.37	113.69	107.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	FPP	C1-O1-PA-O1A

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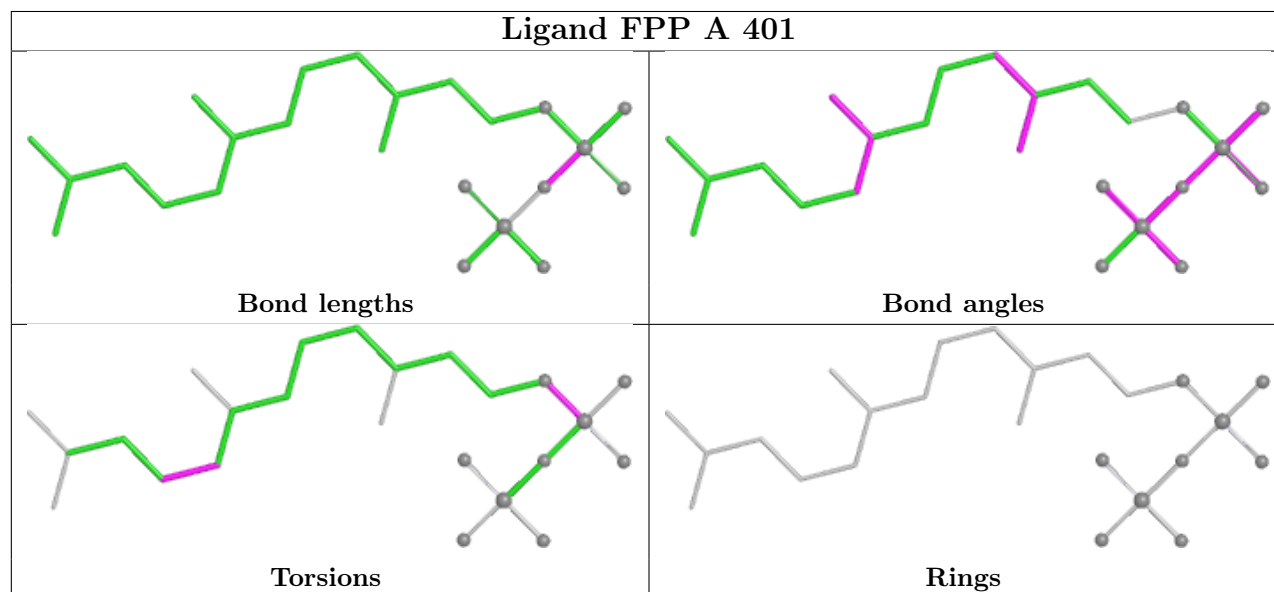
Mol	Chain	Res	Type	Atoms
3	A	401	FPP	C1-O1-PA-O2A
3	A	401	FPP	C1-O1-PA-O3A
3	A	401	FPP	C12-C11-C9-C8

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	FPP	3	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 ⓘ

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

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.