Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 07:38 AM EST

PDB ID : 1UBX
Title : STRUCTURE OF FARNESYL PYROPHOSPHATE SYNTHETASE
Authors : Tarshis, L.C.; Proteau, P.; Poulter, C.D.; Sacchettini, J.C.
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 (i) 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 (i)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
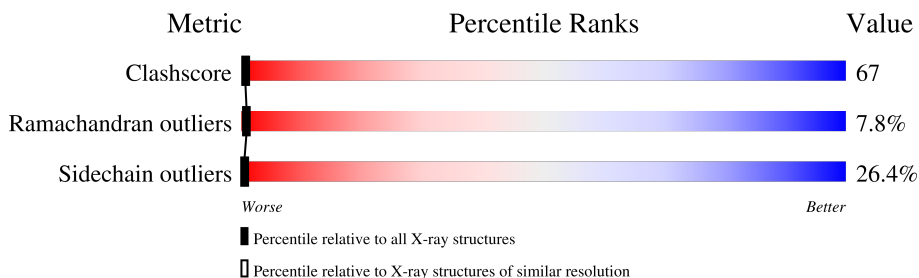Validation Pipeline (wwPDB-VP) : 2.36

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	Percentile Ranks	Value
Clashscore		67
Ramachandran outliers		7.8%
Sidechain outliers		26.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	367	22% 41% 25% 7% 5%

2 Entry composition ⓘ

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.

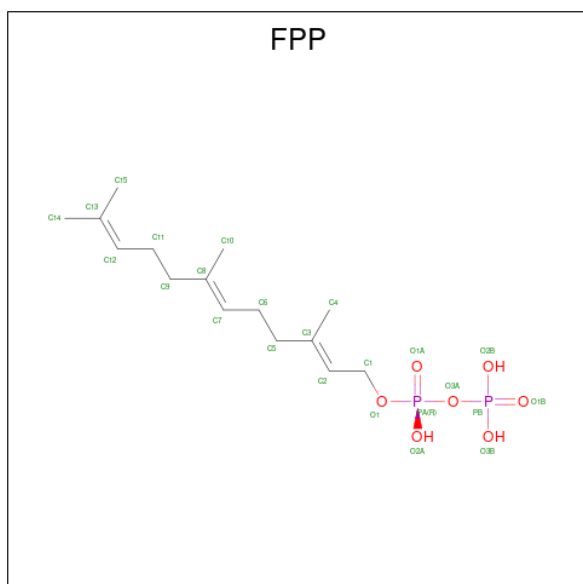| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total 2804	C 1786	N 477	O 527	S 14	0	0	0

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: $C_{15}H_{28}O_7P_2$).

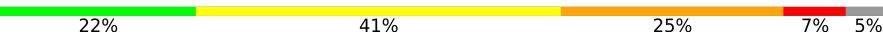| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 24	C 15	O 7	P 2	0	0

- Molecule 4 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: FARNESYL DIPHOSPHATE SYNTHASE
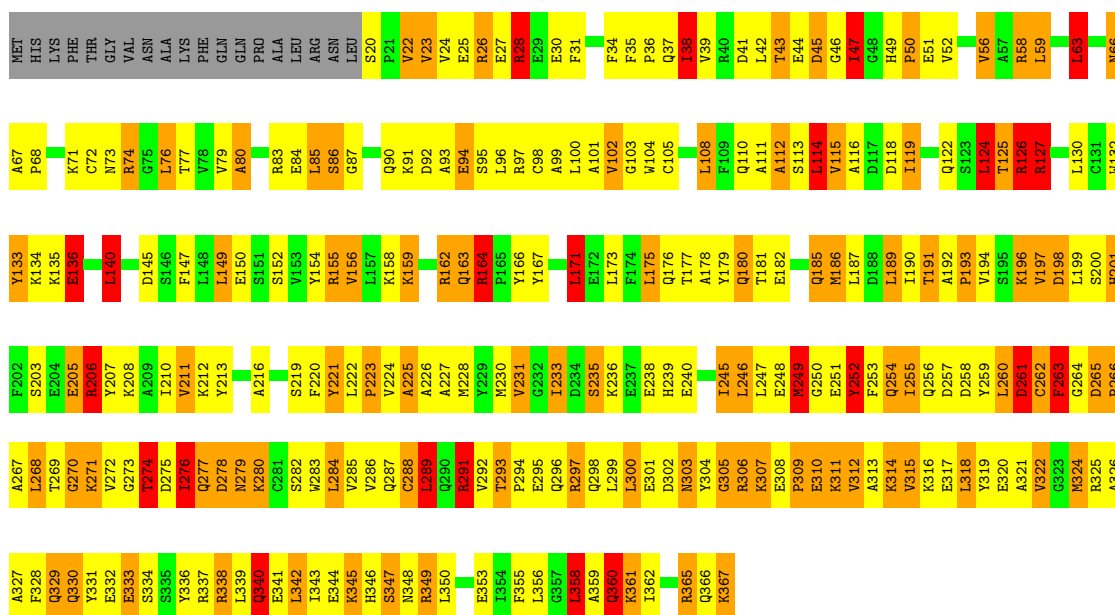
4 Data and refinement statistics (i)

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	1.20	9/2859 (0.3%)	1.53	41/3856 (1.1%)

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	136	GLU	CG-CD	7.32	1.62	1.51
1	A	25	GLU	CG-CD	6.74	1.62	1.51
1	A	176	GLN	CG-CD	6.36	1.65	1.51
1	A	361	LYS	CD-CE	6.12	1.66	1.51
1	A	166	TYR	CD1-CE1	-5.66	1.30	1.39
1	A	156	VAL	CB-CG1	-5.47	1.41	1.52
1	A	205	GLU	CG-CD	5.22	1.59	1.51
1	A	263	PHE	CB-CG	-5.05	1.42	1.51
1	A	25	GLU	CB-CG	5.03	1.61	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	LEU	CB-CG-CD2	-9.77	94.39	111.00
1	A	76	LEU	CB-CG-CD1	-9.53	94.80	111.00
1	A	108	LEU	CB-CG-CD2	-9.41	95.00	111.00
1	A	140	LEU	CA-CB-CG	-9.20	94.13	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	LEU	CB-CG-CD1	-8.50	96.54	111.00
1	A	38	ILE	CB-CA-C	-7.98	95.65	111.60
1	A	206	ARG	NE-CZ-NH2	7.97	124.29	120.30
1	A	284	LEU	CB-CG-CD1	7.66	124.02	111.00
1	A	63	LEU	CA-CB-CG	7.40	132.32	115.30
1	A	276	ILE	CG1-CB-CG2	-7.27	95.41	111.40
1	A	246	LEU	CB-CG-CD2	7.23	123.30	111.00
1	A	127	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	155	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	A	342	LEU	CA-CB-CG	6.92	131.21	115.30
1	A	164	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	231	VAL	CB-CA-C	-6.39	99.25	111.40
1	A	270	GLY	N-CA-C	-6.32	97.30	113.10
1	A	118	ASP	CB-CG-OD1	-6.27	112.65	118.30
1	A	288	CYS	CA-CB-SG	6.25	125.26	114.00
1	A	342	LEU	CB-CG-CD1	6.15	121.45	111.00
1	A	155	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	263	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	A	280	LYS	CD-CE-NZ	5.84	125.13	111.70
1	A	278	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	85	LEU	CB-CG-CD2	5.80	120.85	111.00
1	A	247	LEU	CB-CG-CD2	5.78	120.83	111.00
1	A	289	LEU	CA-CB-CG	-5.76	102.05	115.30
1	A	119	ILE	CB-CA-C	-5.75	100.11	111.60
1	A	263	PHE	N-CA-C	5.72	126.45	111.00
1	A	291	ARG	N-CA-C	-5.66	95.71	111.00
1	A	261	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	358	LEU	CB-CG-CD1	-5.49	101.66	111.00
1	A	66	ASN	N-CA-C	5.41	125.60	111.00
1	A	289	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	A	338	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	249	MET	CB-CG-SD	-5.24	96.69	112.40
1	A	124	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	A	47	ILE	CB-CA-C	-5.20	101.21	111.60
1	A	206	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	A	114	LEU	CB-CG-CD1	-5.14	102.27	111.00
1	A	114	LEU	CB-CG-CD2	-5.05	102.42	111.00

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 ⓘ

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	380	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	380	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 67.

All (380) 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:296:GLN:HB3	1:A:318:LEU:HD21	1.39	1.02
1:A:300:LEU:HD13	1:A:301:GLU:H	1.18	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: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:249:MET:HE2	1:A:358:LEU:HB3	1.48	0.93
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: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:249:MET:HE1	1:A:358:LEU:HB3	1.66	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:198:ASP:C	1:A:199:LEU:HD12	2.08	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

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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:264:GLY:HA3	1:A:367:LYS:HZ1	1.53	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: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: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:278:ASP:C	1:A:280:LYS:H	1.97	0.68
1:A:41:ASP:HA	4:A:432:HOH:O	1.93	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:163:GLN:C	1:A:164:ARG:HG2	2.14	0.67
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:191:THR:C	1:A:193:PRO:HD3	2.19	0.63
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:186:MET:HE2	1:A:186:MET:HA	1.81	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: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: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:126:ARG:HG3	1:A:127:ARG:N	2.15	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: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
1:A:275:ASP:CB	1:A:280:LYS:HZ2	2.08	0.60
1:A:228:MET:HE2	1:A:239:HIS:CE1	2.36	0.60
1:A:275:ASP:HB3	1:A:280:LYS:HD2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:367:LYS:NZ	2.32	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: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:86:SER:OG	1:A:91:LYS:HE3	2.03	0.58
1:A:264:GLY:CA	1:A:367:LYS:HZ1	2.16	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: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: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
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.71	0.56
1:A:366:GLN:C	1:A:367:LYS:HG3	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:318:LEU:HD12	1:A:318:LEU:C	2.28	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:46:GLY:C	1:A:56:VAL:HG21	2.28	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: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:20:SER:C	1:A:22:VAL:H	2.10	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:332:GLU:CD	1:A:365:ARG:HG2	2.28	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:293:THR:HG1	1:A:295:GLU:HG2	1.74	0.53
1:A:316:LYS:O	1:A:319:TYR:HB2	2.07	0.53
1:A:262:CYS:SG	1:A:263:PHE:CD1	3.01	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: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
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:111:ALA:O	1:A:112:ALA:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:277:GLN:HE21	1:A:277:GLN:C	2.12	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:259:TYR:CZ	1:A:325:ARG:HG2	2.46	0.50
1:A:298:GLN:HA	1:A:301:GLU:CD	2.32	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:220:PHE:CD2	1:A:250:GLY:CA	2.95	0.49
1:A:252:TYR:CD1	1:A:252:TYR:C	2.86	0.49
1:A:259:TYR:C	1:A:261:ASP:H	2.15	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLU:OE1	1:A:353:GLU:HB2	2.14	0.47
1:A:262:CYS:HB2	1:A:316:LYS:HZ2	1.80	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:49:HIS:C	1:A:51:GLU:H	2.17	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:45:ASP:OD1	1:A:45:ASP:N	2.47	0.47
1:A:119:ILE:O	1:A:119:ILE:HG22	2.15	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: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:311:LYS:O	1:A:312:VAL:C	2.53	0.46
1:A:74:ARG:HH21	1:A:219:SER:CB	2.28	0.46
1:A:191:THR:CG2	1:A:192:ALA:N	2.78	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: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:49:HIS:HB3	1:A:52:VAL:HG22	1.97	0.46
1:A:206:ARG:HG3	1:A:207:TYR:N	2.29	0.46
1:A:329:GLN:C	1:A:331:TYR:H	2.19	0.46
1:A:340:GLN:O	1:A:343:ILE:N	2.41	0.46
1:A:111:ALA:C	1:A:115:VAL:HG23	2.34	0.45
1:A:264:GLY:CA	1:A:367:LYS:NZ	2.79	0.45
1:A:304:TYR:CG	1:A:305:GLY:N	2.84	0.45
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.49	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:339:LEU:O	1:A:340:GLN:C	2.54	0.45
1:A:211:VAL:CG1	1:A:212:LYS:N	2.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:101:ALA:C	1:A:103:GLY:N	2.69	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: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: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: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:279:ASN:OD1	1:A:304:TYR:CD2	2.69	0.43
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:275:ASP:C	1:A:280:LYS:HD3	2.38	0.43
1:A:303:ASN:HB3	1:A:311:LYS:HG2	2.01	0.43
1:A:304:TYR:C	1:A:306:ARG:H	2.21	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:274:THR:HG23	1:A:275:ASP:CA	2.48	0.43
1:A:278:ASP:C	1:A:280:LYS:N	2.68	0.43
1:A:299:LEU:C	1:A:299:LEU:HD23	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:C	1:A:302:ASP:N	2.72	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: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:CE	1:A:186:MET:CA	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:312:VAL:C	1:A:314:LYS:H	2.23	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:206:ARG:HE	1:A:206:ARG:HB2	1.66	0.42
1:A:329:GLN:C	1:A:331:TYR:N	2.73	0.42
1:A:186:MET:HB2	1:A:186:MET:HE3	1.47	0.41
1:A:191:THR:OG1	1:A:206:ARG:NH1	2.53	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
1:A:101:ALA:O	1:A:102:VAL:C	2.57	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: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: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:126:ARG:HG2	1:A:127:ARG:HG2	2.03	0.41
1:A:47:ILE:N	1:A:56:VAL:HG21	2.36	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:317:GLU:C	1:A:320:GLU:HB2	2.40	0.41
1:A:42:LEU:C	1:A:43:THR:HG23	2.41	0.40
1:A:92:ASP:CG	1:A:95:SER:H	2.25	0.40
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:253:PHE:CD1	1:A:253:PHE:C	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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 1

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

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Mol	Chain	Res	Type
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%)	220 (74%)	79 (26%)	0	0

All (79) 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	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	74	ARG
1	A	76	LEU

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Mol	Chain	Res	Type
1	A	86	SER
1	A	94	GLU
1	A	114	LEU
1	A	124	LEU
1	A	125	THR
1	A	126	ARG
1	A	136	GLU
1	A	140	LEU
1	A	159	LYS
1	A	163	GLN
1	A	164	ARG
1	A	171	LEU
1	A	175	LEU
1	A	180	GLN
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	206	ARG
1	A	211	VAL
1	A	235	SER
1	A	236	LYS
1	A	240	GLU
1	A	245	ILE
1	A	249	MET
1	A	252	TYR
1	A	254	GLN
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	277	GLN
1	A	289	LEU
1	A	291	ARG
1	A	293	THR

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Mol	Chain	Res	Type
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
1	A	324	MET
1	A	329	GLN
1	A	330	GLN
1	A	333	GLU
1	A	337	ARG
1	A	340	GLN
1	A	347	SER
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	73	ASN
1	A	185	GLN
1	A	239	HIS
1	A	254	GLN
1	A	329	GLN
1	A	330	GLN
1	A	346	HIS
1	A	348	ASN
1	A	360	GLN

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 monosaccharides 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	-	21,23,23	1.15	0	27,31,31	1.76	5 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FPP	A	401	-	-	4/25/25/25	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	FPP	O3B-PB-O3A	4.65	120.24	104.64
3	A	401	FPP	PA-O3A-PB	-4.31	118.03	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	FPP	C4-C3-C5	2.99	120.30	115.27
3	A	401	FPP	C10-C8-C9	2.81	120.00	115.27
3	A	401	FPP	O3B-PB-O1B	-2.40	101.30	110.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	FPP	C1-O1-PA-O3A
3	A	401	FPP	C1-O1-PA-O1A
3	A	401	FPP	C1-O1-PA-O2A
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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FPP A 401

Bond lengths

Bond angles

Torsions

Rings
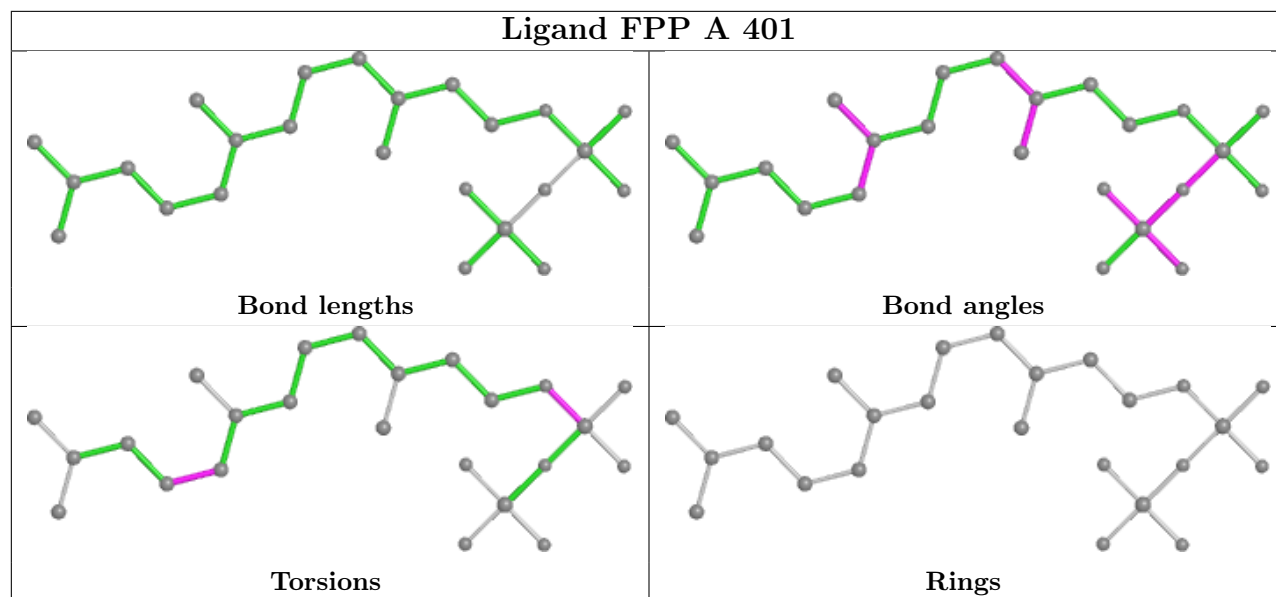
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.