



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:33 PM UTC

PDB ID : 1UBY / pdb_00001uby
Title : STRUCTURE OF FARNESYL PYROPHOSPHATE SYNTHETASE
Authors : Tarshis, L.C.; Proteau, P.; Poulter, C.D.; Sacchettini, J.C.
Deposited on : 1996-10-14
Resolution : 2.40 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
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

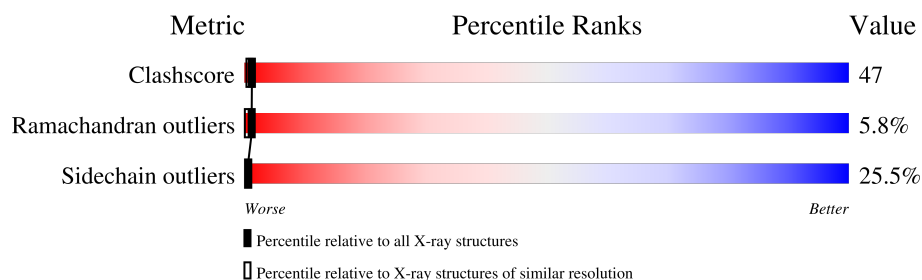
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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

There are 4 unique types of molecules in this entry. The entry contains 2888 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
			2800	1783	476	527	14			

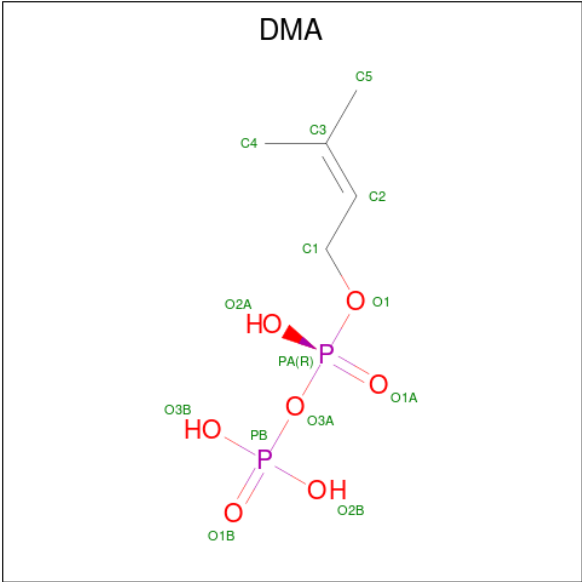
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	PHE	conflict	UNP P08836
A	113	SER	PHE	conflict	UNP P08836
A	271	ALA	LYS	conflict	UNP P08836

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

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

- Molecule 3 is DIMETHYLALLYL DIPHOSPHATE (CCD ID: DMA) (formula: C₅H₁₂O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 4 is water.

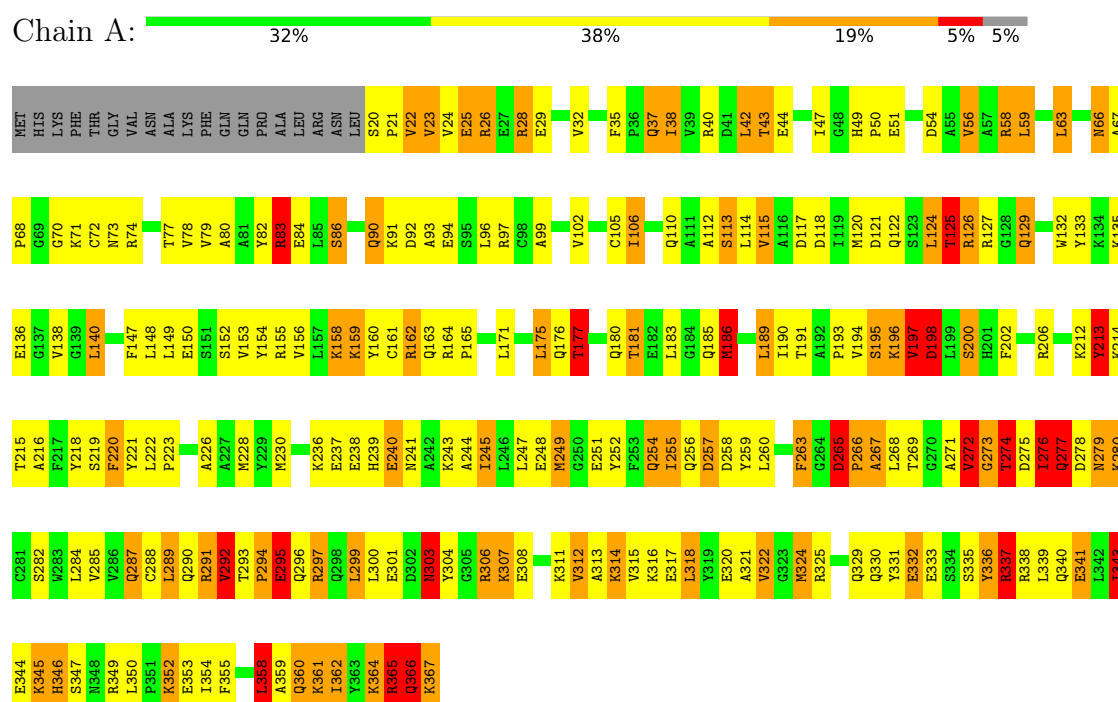
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		

3 Residue-property plots [i](#)

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

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	88.30Å 88.30Å 274.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	0.05	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	2888	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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, DMA

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	1.13	2/2855 (0.1%)	1.67	57/3852 (1.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	MET	SD-CE	13.12	2.12	1.79
1	A	244	ALA	CA-C	-5.32	1.46	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	VAL	N-CA-C	11.71	122.41	110.23
1	A	213	TYR	N-CA-C	10.15	122.11	111.14
1	A	66	ASN	N-CA-C	9.50	125.00	113.41
1	A	129	GLN	N-CA-C	-9.28	95.30	109.41
1	A	346	HIS	N-CA-C	8.95	125.30	113.30
1	A	292	VAL	N-CA-C	8.61	119.94	110.21
1	A	272	VAL	CB-CA-C	8.34	121.78	112.19
1	A	206	ARG	N-CA-C	-8.24	101.34	111.40
1	A	263	PHE	N-CA-C	8.19	121.83	112.57
1	A	238	GLU	N-CA-C	-8.14	103.14	113.23
1	A	277	GLN	N-CA-C	-8.06	102.49	111.28
1	A	32	VAL	CB-CA-C	-7.69	102.04	111.88
1	A	272	VAL	N-CA-C	-7.69	105.07	111.91
1	A	332	GLU	N-CA-C	-7.31	103.31	111.71
1	A	295	GLU	N-CA-C	-7.07	100.08	111.04
1	A	276	ILE	N-CA-C	-6.86	104.91	112.80
1	A	343	ILE	N-CA-C	-6.84	102.54	111.09
1	A	263	PHE	CA-C-N	-6.72	116.17	121.82
1	A	263	PHE	C-N-CA	-6.72	116.17	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	GLU	N-CA-C	-6.56	103.96	112.23
1	A	115	VAL	N-CA-CB	6.51	118.60	110.47
1	A	83	ARG	CA-C-N	-6.37	110.21	122.06
1	A	83	ARG	C-N-CA	-6.37	110.21	122.06
1	A	90	GLN	N-CA-C	6.35	119.75	112.57
1	A	257	ASP	N-CA-C	-6.26	103.60	111.11
1	A	112	ALA	N-CA-C	-6.25	104.38	111.07
1	A	82	TYR	N-CA-C	-6.17	104.47	111.07
1	A	190	ILE	CB-CA-C	-6.00	104.38	111.94
1	A	177	THR	N-CA-C	-5.79	104.97	111.28
1	A	42	LEU	N-CA-C	5.75	118.49	111.82
1	A	35	PHE	N-CA-C	5.70	120.66	113.25
1	A	343	ILE	CB-CA-C	-5.68	103.06	112.26
1	A	147	PHE	N-CA-C	-5.64	105.13	111.28
1	A	118	ASP	N-CA-C	5.62	117.40	111.28
1	A	149	LEU	N-CA-C	-5.56	104.85	111.69
1	A	159	LYS	N-CA-C	5.52	117.10	111.14
1	A	125	THR	N-CA-C	5.44	118.09	109.50
1	A	28	ARG	N-CA-C	5.38	117.56	111.11
1	A	38	ILE	CB-CA-C	-5.35	104.92	112.14
1	A	99	ALA	N-CA-C	-5.33	105.37	111.07
1	A	358	LEU	N-CA-C	-5.33	105.37	111.07
1	A	265	ASP	N-CA-C	5.33	121.58	109.81
1	A	70	GLY	N-CA-C	-5.32	103.52	112.77
1	A	294	PRO	CA-C-N	-5.30	112.93	120.89
1	A	294	PRO	C-N-CA	-5.30	112.93	120.89
1	A	78	VAL	CB-CA-C	-5.23	105.28	111.97
1	A	280	LYS	N-CA-C	5.18	117.20	109.59
1	A	360	GLN	CA-C-N	-5.17	114.05	122.26
1	A	360	GLN	C-N-CA	-5.17	114.05	122.26
1	A	43	THR	N-CA-C	5.15	121.10	114.56
1	A	292	VAL	CB-CA-C	-5.13	105.70	111.45
1	A	29	GLU	N-CA-C	5.12	116.87	111.28
1	A	220	PHE	N-CA-C	5.11	119.27	112.72
1	A	263	PHE	CB-CA-C	-5.07	103.21	111.06
1	A	22	VAL	N-CA-C	5.07	116.39	110.62
1	A	303	ASN	N-CA-C	5.05	121.56	110.80
1	A	306	ARG	N-CA-C	5.03	116.60	108.41

There are no chirality outliers.

There are no planarity outliers.

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	2800	0	2782	265	0
2	A	2	0	0	0	0
3	A	14	0	9	2	0
4	A	72	0	0	13	0
All	All	2888	0	2791	265	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 47.

All (265) 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:186:MET:SD	1:A:186:MET:CE	2.12	1.38
1:A:162:ARG:HH11	1:A:162:ARG:HG2	1.12	1.04
1:A:277:GLN:HG2	1:A:307:LYS:HE2	1.36	1.03
1:A:290:GLN:NE2	1:A:291:ARG:HH12	1.57	1.02
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.27	0.99
1:A:59:LEU:HD22	1:A:63:LEU:HD22	1.44	0.94
1:A:276:ILE:HG21	1:A:316:LYS:NZ	1.84	0.91
1:A:276:ILE:HD12	1:A:316:LYS:HZ3	1.35	0.89
1:A:318:LEU:O	1:A:322:VAL:HG23	1.75	0.87
1:A:276:ILE:HD12	1:A:316:LYS:CE	2.05	0.87
1:A:77:THR:HG22	1:A:223:PRO:HB2	1.57	0.86
1:A:276:ILE:HD12	1:A:316:LYS:HE2	1.58	0.84
1:A:311:LYS:O	1:A:315:VAL:HG23	1.78	0.84
1:A:315:VAL:HB	1:A:316:LYS:HD3	1.59	0.84
1:A:276:ILE:HD12	1:A:316:LYS:NZ	1.92	0.84
1:A:77:THR:CG2	1:A:223:PRO:HB2	2.08	0.83
1:A:290:GLN:HB2	1:A:291:ARG:NH1	1.93	0.83
1:A:126:ARG:O	1:A:129:GLN:HG2	1.79	0.82
1:A:276:ILE:HG12	1:A:276:ILE:O	1.79	0.81
1:A:292:VAL:CG2	1:A:296:GLN:HB2	2.10	0.81
1:A:308:GLU:OE1	1:A:311:LYS:HE2	1.81	0.81
1:A:265:ASP:HB3	1:A:266:PRO:HD3	1.62	0.81
1:A:276:ILE:HG21	1:A:316:LYS:HZ1	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ARG:NE	1:A:306:ARG:HA	1.96	0.81
1:A:158:LYS:HB2	4:A:408:HOH:O	1.80	0.80
1:A:290:GLN:HE21	1:A:291:ARG:HH12	1.25	0.80
1:A:287:GLN:O	1:A:291:ARG:HD2	1.83	0.78
1:A:140:LEU:HB2	4:A:462:HOH:O	1.83	0.78
1:A:293:THR:HB	1:A:294:PRO:HD2	1.66	0.78
1:A:274:THR:HG23	1:A:275:ASP:N	1.99	0.77
1:A:330:GLN:O	1:A:333:GLU:HB3	1.85	0.77
1:A:191:THR:O	1:A:193:PRO:HD3	1.85	0.77
1:A:340:GLN:HA	1:A:343:ILE:HG13	1.67	0.77
1:A:289:LEU:CD2	1:A:297:ARG:HH11	1.98	0.76
1:A:162:ARG:HG2	1:A:162:ARG:NH1	1.86	0.76
1:A:96:LEU:N	1:A:96:LEU:HD23	2.01	0.75
1:A:276:ILE:HG21	1:A:316:LYS:CE	2.15	0.75
1:A:198:ASP:OD1	1:A:200:SER:HB3	1.86	0.75
1:A:364:LYS:HG2	4:A:489:HOH:O	1.85	0.75
1:A:265:ASP:C	1:A:268:LEU:HD23	2.12	0.74
1:A:277:GLN:CG	1:A:307:LYS:HE2	2.15	0.73
1:A:365:ARG:HB2	4:A:437:HOH:O	1.88	0.73
1:A:186:MET:HE3	1:A:186:MET:HB2	1.68	0.73
1:A:66:ASN:HD21	1:A:132:TRP:HB2	1.54	0.72
1:A:292:VAL:HG22	1:A:296:GLN:HB2	1.71	0.72
1:A:276:ILE:CD1	1:A:315:VAL:HG11	2.20	0.72
1:A:276:ILE:HD11	1:A:315:VAL:HG11	1.71	0.71
1:A:186:MET:CE	1:A:186:MET:HB2	2.22	0.70
1:A:275:ASP:OD1	1:A:278:ASP:N	2.22	0.70
1:A:237:GLU:HA	1:A:240:GLU:HG3	1.73	0.69
1:A:177:THR:O	1:A:181:THR:HG23	1.93	0.68
1:A:197:VAL:O	1:A:279:ASN:ND2	2.26	0.68
1:A:364:LYS:O	1:A:365:ARG:HB2	1.93	0.68
1:A:186:MET:CE	1:A:186:MET:CB	2.72	0.68
1:A:291:ARG:HB3	1:A:322:VAL:CG1	2.24	0.67
1:A:312:VAL:HG12	1:A:313:ALA:N	2.10	0.67
1:A:59:LEU:HD22	1:A:59:LEU:O	1.95	0.66
1:A:58:ARG:HH11	1:A:58:ARG:CG	2.07	0.66
1:A:276:ILE:CD1	1:A:316:LYS:HZ3	2.08	0.65
1:A:236:LYS:O	1:A:240:GLU:HG2	1.96	0.65
1:A:318:LEU:O	1:A:321:ALA:HB3	1.97	0.65
1:A:278:ASP:O	1:A:280:LYS:N	2.28	0.64
1:A:275:ASP:O	1:A:280:LYS:HE2	1.96	0.64
1:A:290:GLN:NE2	1:A:291:ARG:NH1	2.39	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLN:HG3	1:A:278:ASP:N	2.13	0.64
1:A:306:ARG:HA	1:A:306:ARG:CZ	2.27	0.64
1:A:23:VAL:HG12	1:A:24:VAL:N	2.12	0.64
1:A:290:GLN:HB2	1:A:291:ARG:HH12	1.61	0.64
1:A:293:THR:HB	1:A:294:PRO:CD	2.27	0.63
1:A:80:ALA:O	1:A:83:ARG:HB3	1.98	0.63
1:A:265:ASP:CA	1:A:268:LEU:HD23	2.27	0.63
1:A:195:SER:O	1:A:196:LYS:HB2	1.98	0.63
1:A:120:MET:SD	1:A:189:LEU:HD21	2.39	0.62
1:A:226:ALA:O	1:A:230:MET:HG3	1.99	0.62
1:A:290:GLN:HE21	1:A:291:ARG:NH1	1.94	0.62
1:A:251:GLU:O	1:A:255:ILE:HD13	2.00	0.62
1:A:94:GLU:OE2	1:A:97:ARG:NH1	2.33	0.62
1:A:155:ARG:NH1	4:A:477:HOH:O	2.31	0.62
1:A:275:ASP:C	1:A:280:LYS:HE2	2.25	0.61
1:A:236:LYS:NZ	1:A:237:GLU:OE1	2.33	0.61
1:A:314:LYS:O	1:A:317:GLU:HB3	2.00	0.61
1:A:354:ILE:HG22	1:A:355:PHE:N	2.15	0.61
1:A:92:ASP:O	1:A:96:LEU:HG	2.01	0.61
1:A:117:ASP:CG	3:A:401:DMA:H11	2.26	0.60
1:A:292:VAL:HG23	1:A:296:GLN:HB2	1.82	0.60
1:A:265:ASP:CG	1:A:272:VAL:HG21	2.27	0.60
1:A:285:VAL:HG21	1:A:304:TYR:OH	2.01	0.60
1:A:185:GLN:HE21	1:A:185:GLN:HA	1.67	0.60
1:A:158:LYS:HE2	4:A:442:HOH:O	2.02	0.60
1:A:289:LEU:HD22	1:A:297:ARG:HH11	1.64	0.60
1:A:136:GLU:CD	1:A:136:GLU:H	2.09	0.59
1:A:312:VAL:O	1:A:316:LYS:HG2	2.02	0.59
1:A:49:HIS:ND1	1:A:50:PRO:HD2	2.17	0.59
1:A:237:GLU:HA	1:A:240:GLU:CG	2.33	0.59
1:A:365:ARG:CD	1:A:367:LYS:H	2.16	0.59
1:A:292:VAL:HG22	1:A:293:THR:O	2.03	0.58
1:A:254:GLN:O	1:A:254:GLN:NE2	2.35	0.58
1:A:277:GLN:HG2	1:A:307:LYS:CE	2.23	0.58
1:A:66:ASN:ND2	4:A:460:HOH:O	2.36	0.58
1:A:315:VAL:CB	1:A:316:LYS:HD3	2.32	0.58
1:A:58:ARG:HG2	1:A:58:ARG:NH1	2.07	0.58
1:A:365:ARG:HD2	1:A:367:LYS:H	1.67	0.58
1:A:345:LYS:HD2	1:A:346:HIS:NE2	2.19	0.58
1:A:122:GLN:HA	1:A:133:TYR:OH	2.03	0.58
1:A:214:LYS:HD2	3:A:401:DMA:H43	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:HIS:CG	1:A:50:PRO:HD2	2.39	0.57
1:A:22:VAL:HG13	1:A:26:ARG:HD2	1.86	0.57
1:A:292:VAL:HG22	1:A:293:THR:N	2.19	0.57
1:A:47:ILE:HD13	1:A:56:VAL:HG22	1.86	0.57
1:A:243:LYS:O	1:A:247:LEU:HG	2.04	0.57
1:A:293:THR:OG1	1:A:296:GLN:HG3	2.04	0.57
1:A:245:ILE:C	1:A:245:ILE:HD12	2.29	0.57
1:A:263:PHE:HB3	1:A:325:ARG:NH2	2.19	0.57
1:A:318:LEU:C	1:A:318:LEU:HD23	2.29	0.57
1:A:255:ILE:O	1:A:258:ASP:HB2	2.04	0.57
1:A:292:VAL:HG22	1:A:293:THR:H	1.68	0.57
1:A:241:ASN:HB3	1:A:346:HIS:O	2.04	0.56
1:A:316:LYS:CD	1:A:316:LYS:N	2.68	0.56
1:A:49:HIS:CE1	1:A:51:GLU:HB2	2.41	0.56
1:A:43:THR:O	1:A:47:ILE:HG12	2.05	0.56
1:A:329:GLN:O	1:A:333:GLU:HB2	2.05	0.56
1:A:306:ARG:HG2	4:A:433:HOH:O	2.05	0.55
1:A:332:GLU:OE2	1:A:365:ARG:HA	2.07	0.55
1:A:277:GLN:HG3	1:A:278:ASP:OD1	2.07	0.55
1:A:284:LEU:HD23	1:A:324:MET:HG3	1.87	0.55
1:A:213:TYR:N	1:A:213:TYR:CD1	2.75	0.55
1:A:291:ARG:HB3	1:A:322:VAL:HG11	1.88	0.55
1:A:335:SER:O	1:A:336:TYR:O	2.26	0.55
1:A:308:GLU:HB2	1:A:311:LYS:HG3	1.89	0.54
1:A:38:ILE:HG22	1:A:42:LEU:HD12	1.89	0.54
1:A:59:LEU:O	1:A:63:LEU:HD22	2.08	0.54
1:A:316:LYS:HD3	1:A:316:LYS:N	2.23	0.54
1:A:289:LEU:HD22	1:A:297:ARG:NH1	2.23	0.53
1:A:303:ASN:O	1:A:306:ARG:HB2	2.08	0.53
1:A:259:TYR:CD2	1:A:260:LEU:HD23	2.43	0.53
1:A:288:CYS:HA	1:A:324:MET:HE1	1.91	0.53
1:A:74:ARG:HE	1:A:219:SER:CB	2.21	0.53
1:A:293:THR:HG1	1:A:296:GLN:HG3	1.73	0.53
1:A:273:GLY:O	1:A:274:THR:HB	2.08	0.53
1:A:260:LEU:HD23	1:A:260:LEU:N	2.21	0.53
1:A:59:LEU:HD22	1:A:63:LEU:CD2	2.28	0.53
1:A:176:GLN:O	1:A:180:GLN:HG3	2.09	0.53
1:A:71:LYS:O	1:A:72:CYS:HB2	2.08	0.52
1:A:228:MET:HE2	1:A:239:HIS:CE1	2.44	0.52
1:A:110:GLN:O	1:A:113:SER:HB2	2.08	0.52
1:A:79:VAL:HG12	1:A:80:ALA:N	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASP:HB3	1:A:266:PRO:CD	2.36	0.52
1:A:339:LEU:O	1:A:343:ILE:HG12	2.08	0.52
1:A:360:GLN:O	1:A:360:GLN:HG2	2.09	0.52
1:A:287:GLN:HA	1:A:287:GLN:NE2	2.25	0.52
1:A:317:GLU:O	1:A:321:ALA:N	2.35	0.51
1:A:274:THR:O	1:A:275:ASP:HB2	2.09	0.51
1:A:265:ASP:O	1:A:268:LEU:HB2	2.11	0.51
1:A:154:TYR:CZ	1:A:175:LEU:HD13	2.46	0.50
1:A:293:THR:HG23	1:A:296:GLN:OE1	2.12	0.50
1:A:186:MET:CE	1:A:186:MET:HA	2.42	0.49
1:A:299:LEU:HD13	1:A:318:LEU:CD1	2.42	0.49
1:A:180:GLN:O	1:A:213:TYR:HB3	2.13	0.49
1:A:152:SER:O	1:A:156:VAL:HG23	2.13	0.49
1:A:285:VAL:HG21	1:A:304:TYR:CZ	2.48	0.49
1:A:164:ARG:HD2	1:A:165:PRO:HD2	1.95	0.48
1:A:276:ILE:CD1	1:A:316:LYS:HE2	2.38	0.48
1:A:263:PHE:HD2	1:A:325:ARG:HH21	1.61	0.48
1:A:241:ASN:O	1:A:245:ILE:HG23	2.13	0.48
1:A:92:ASP:OD1	1:A:92:ASP:N	2.47	0.48
1:A:329:GLN:HG2	1:A:367:LYS:O	2.13	0.48
1:A:306:ARG:NH1	1:A:307:LYS:H	2.11	0.48
1:A:318:LEU:O	1:A:318:LEU:HD23	2.14	0.48
1:A:277:GLN:OE1	1:A:307:LYS:HD2	2.13	0.48
1:A:341:GLU:N	1:A:341:GLU:OE1	2.47	0.48
1:A:186:MET:CE	1:A:186:MET:CG	2.90	0.47
1:A:77:THR:HG21	1:A:223:PRO:HB2	1.94	0.47
1:A:220:PHE:O	1:A:223:PRO:HD2	2.13	0.47
1:A:276:ILE:HG13	1:A:304:TYR:CE1	2.49	0.47
1:A:284:LEU:O	1:A:288:CYS:HB2	2.15	0.47
1:A:278:ASP:C	1:A:280:LYS:N	2.71	0.47
1:A:121:ASP:C	1:A:122:GLN:HG2	2.38	0.47
1:A:268:LEU:CD2	1:A:366:GLN:NE2	2.78	0.47
1:A:340:GLN:O	1:A:343:ILE:HB	2.15	0.47
1:A:221:TYR:OH	1:A:239:HIS:HD2	1.98	0.46
1:A:293:THR:OG1	1:A:295:GLU:OE1	2.26	0.46
1:A:25:GLU:OE1	1:A:28:ARG:NH1	2.46	0.46
1:A:93:ALA:O	1:A:97:ARG:HG3	2.15	0.46
1:A:265:ASP:HA	1:A:268:LEU:HD23	1.97	0.46
1:A:272:VAL:O	1:A:273:GLY:O	2.34	0.46
1:A:185:GLN:HA	1:A:185:GLN:NE2	2.31	0.46
1:A:249:MET:CE	1:A:359:ALA:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HE	1:A:365:ARG:HB3	1.68	0.46
1:A:245:ILE:HD12	1:A:245:ILE:O	2.16	0.45
1:A:287:GLN:NE2	1:A:287:GLN:CA	2.78	0.45
1:A:265:ASP:OD1	1:A:272:VAL:HG21	2.16	0.45
1:A:58:ARG:CG	1:A:58:ARG:NH1	2.73	0.45
1:A:336:TYR:O	1:A:337:ARG:C	2.60	0.45
1:A:249:MET:HE1	1:A:355:PHE:O	2.17	0.45
1:A:255:ILE:N	1:A:255:ILE:CD1	2.80	0.45
1:A:329:GLN:HE21	1:A:329:GLN:HA	1.82	0.45
1:A:126:ARG:O	1:A:127:ARG:C	2.59	0.45
1:A:158:LYS:O	1:A:162:ARG:HB2	2.16	0.45
1:A:365:ARG:NE	1:A:366:GLN:H	2.14	0.45
1:A:212:LYS:O	1:A:216:ALA:HB3	2.17	0.44
1:A:266:PRO:O	1:A:267:ALA:HB3	2.17	0.44
1:A:191:THR:C	1:A:193:PRO:HD3	2.41	0.44
1:A:49:HIS:CG	1:A:50:PRO:CD	3.00	0.44
1:A:125:THR:HG23	1:A:126:ARG:N	2.32	0.44
1:A:252:TYR:CD1	1:A:252:TYR:C	2.96	0.44
1:A:343:ILE:CG2	1:A:352:LYS:HG2	2.48	0.44
1:A:74:ARG:O	1:A:77:THR:HB	2.18	0.44
1:A:265:ASP:OD2	1:A:272:VAL:HG21	2.18	0.44
1:A:74:ARG:HB2	4:A:457:HOH:O	2.18	0.44
1:A:186:MET:HE3	1:A:186:MET:CB	2.38	0.44
1:A:303:ASN:HA	1:A:311:LYS:HD2	2.00	0.44
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.82	0.43
1:A:276:ILE:HD11	1:A:315:VAL:HG21	2.00	0.43
1:A:183:LEU:O	1:A:186:MET:HB3	2.18	0.43
1:A:263:PHE:CD1	1:A:263:PHE:N	2.86	0.43
1:A:336:TYR:O	1:A:339:LEU:N	2.52	0.43
1:A:215:THR:HA	1:A:218:TYR:CE1	2.54	0.43
1:A:265:ASP:N	1:A:268:LEU:HD23	2.33	0.43
1:A:106:ILE:HD13	1:A:222:LEU:HG	2.01	0.43
1:A:37:GLN:NE2	1:A:37:GLN:HA	2.34	0.43
1:A:293:THR:CB	1:A:294:PRO:CD	2.96	0.43
1:A:161:CYS:O	1:A:164:ARG:HB2	2.19	0.42
1:A:181:THR:O	1:A:185:GLN:N	2.49	0.42
1:A:220:PHE:C	1:A:223:PRO:HD2	2.44	0.42
1:A:127:ARG:NH1	4:A:456:HOH:O	2.26	0.42
1:A:255:ILE:N	1:A:255:ILE:HD12	2.34	0.42
1:A:67:ALA:N	1:A:68:PRO:CD	2.82	0.42
1:A:186:MET:HA	1:A:186:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASN:HB2	1:A:361:LYS:HE3	2.02	0.42
1:A:102:VAL:O	1:A:105:CYS:HB2	2.20	0.42
1:A:186:MET:CE	1:A:186:MET:CA	2.98	0.42
1:A:249:MET:CE	1:A:359:ALA:CA	2.98	0.42
1:A:358:LEU:HD12	1:A:362:ILE:CD1	2.50	0.42
1:A:124:LEU:HD13	1:A:124:LEU:HA	1.73	0.42
1:A:331:TYR:C	1:A:333:GLU:N	2.76	0.42
1:A:358:LEU:HD12	1:A:358:LEU:O	2.19	0.42
1:A:49:HIS:HA	1:A:50:PRO:HD3	1.59	0.41
1:A:285:VAL:HG23	4:A:428:HOH:O	2.20	0.41
1:A:288:CYS:SG	1:A:300:LEU:HD11	2.60	0.41
1:A:268:LEU:HB3	1:A:272:VAL:HB	2.03	0.41
1:A:349:ARG:N	4:A:452:HOH:O	2.49	0.41
1:A:202:PHE:N	1:A:202:PHE:HD1	2.17	0.41
1:A:277:GLN:HB2	1:A:307:LYS:HG3	2.03	0.41
1:A:202:PHE:N	1:A:202:PHE:CD1	2.88	0.41
1:A:365:ARG:HB3	1:A:366:GLN:H	1.26	0.41
1:A:114:LEU:O	1:A:115:VAL:C	2.64	0.41
1:A:277:GLN:CD	1:A:307:LYS:HD2	2.46	0.41
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.96	0.41
1:A:277:GLN:CD	1:A:307:LYS:HE2	2.45	0.41
1:A:367:LYS:HB2	1:A:367:LYS:HE2	1.47	0.41
1:A:74:ARG:HE	1:A:219:SER:HB3	1.84	0.41
1:A:86:SER:OG	1:A:91:LYS:NZ	2.54	0.41
1:A:318:LEU:CD2	1:A:322:VAL:CG2	2.98	0.41
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.77	0.40
1:A:280:LYS:HE3	4:A:484:HOH:O	2.22	0.40
1:A:159:LYS:HG2	1:A:160:TYR:CE1	2.56	0.40
1:A:358:LEU:HD12	1:A:358:LEU:C	2.45	0.40
1:A:84:GLU:OE2	1:A:353:GLU:HB2	2.21	0.40
1:A:20:SER:HA	1:A:21:PRO:HD2	1.79	0.40
1:A:38:ILE:HG22	1:A:42:LEU:CD1	2.50	0.40
1:A:215:THR:HA	1:A:218:TYR:CD1	2.56	0.40
1:A:73:ASN:OD1	1:A:73:ASN:N	2.52	0.40
1:A:285:VAL:O	1:A:288:CYS:HB3	2.22	0.40
1:A:303:ASN:HB3	1:A:311:LYS:HB3	2.03	0.40
1:A:318:LEU:O	1:A:322:VAL:N	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	298 (86%)	28 (8%)	20 (6%)	1 0

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	THR
1	A	279	ASN
1	A	336	TYR
1	A	337	ARG
1	A	364	LYS
1	A	365	ARG
1	A	196	LYS
1	A	198	ASP
1	A	265	ASP
1	A	271	ALA
1	A	273	GLY
1	A	274	THR
1	A	289	LEU
1	A	366	GLN
1	A	266	PRO
1	A	267	ALA
1	A	113	SER
1	A	303	ASN
1	A	194	VAL
1	A	138	VAL

5.3.2 Protein sidechains [i](#)

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	298/314 (95%)	222 (74%)	76 (26%)	0 0

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	25	GLU
1	A	26	ARG
1	A	37	GLN
1	A	44	GLU
1	A	54	ASP
1	A	56	VAL
1	A	58	ARG
1	A	59	LEU
1	A	63	LEU
1	A	83	ARG
1	A	86	SER
1	A	90	GLN
1	A	106	ILE
1	A	124	LEU
1	A	125	THR
1	A	126	ARG
1	A	135	LYS
1	A	140	LEU
1	A	150	GLU
1	A	153	VAL
1	A	158	LYS
1	A	162	ARG
1	A	163	GLN
1	A	171	LEU
1	A	175	LEU
1	A	177	THR
1	A	181	THR
1	A	186	MET
1	A	189	LEU
1	A	195	SER
1	A	197	VAL
1	A	198	ASP
1	A	200	SER
1	A	213	TYR
1	A	240	GLU

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Mol	Chain	Res	Type
1	A	245	ILE
1	A	248	GLU
1	A	249	MET
1	A	254	GLN
1	A	255	ILE
1	A	256	GLN
1	A	257	ASP
1	A	272	VAL
1	A	274	THR
1	A	276	ILE
1	A	277	GLN
1	A	282	SER
1	A	287	GLN
1	A	291	ARG
1	A	292	VAL
1	A	295	GLU
1	A	297	ARG
1	A	299	LEU
1	A	301	GLU
1	A	307	LYS
1	A	312	VAL
1	A	314	LYS
1	A	318	LEU
1	A	322	VAL
1	A	324	MET
1	A	337	ARG
1	A	338	ARG
1	A	341	GLU
1	A	343	ILE
1	A	344	GLU
1	A	345	LYS
1	A	347	SER
1	A	350	LEU
1	A	352	LYS
1	A	358	LEU
1	A	361	LYS
1	A	362	ILE
1	A	365	ARG
1	A	366	GLN
1	A	367	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	66	ASN
1	A	110	GLN
1	A	169	HIS
1	A	180	GLN
1	A	185	GLN
1	A	239	HIS
1	A	256	GLN
1	A	287	GLN
1	A	290	GLN
1	A	329	GLN
1	A	330	GLN
1	A	366	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are 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	DMA	A	401	2	12,13,13	1.69	3 (25%)	15,19,19	1.63	4 (26%)

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	DMA	A	401	2	-	3/13/13/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	DMA	PB-O1B	3.22	1.60	1.50
3	A	401	DMA	PA-O1A	2.85	1.60	1.50
3	A	401	DMA	C5-C3	2.16	1.56	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	DMA	C5-C3-C4	4.19	124.23	114.59
3	A	401	DMA	O2A-PA-O3A	2.41	113.78	107.27
3	A	401	DMA	C5-C3-C2	-2.39	115.47	122.66
3	A	401	DMA	O3A-PA-O1A	-2.03	104.60	110.70

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	DMA	PA-O3A-PB-O3B
3	A	401	DMA	PB-O3A-PA-O1
3	A	401	DMA	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	DMA	2	0

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.