



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:36 AM UTC

PDB ID : 1UBV / pdb_00001ubv
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 ⓘ 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
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

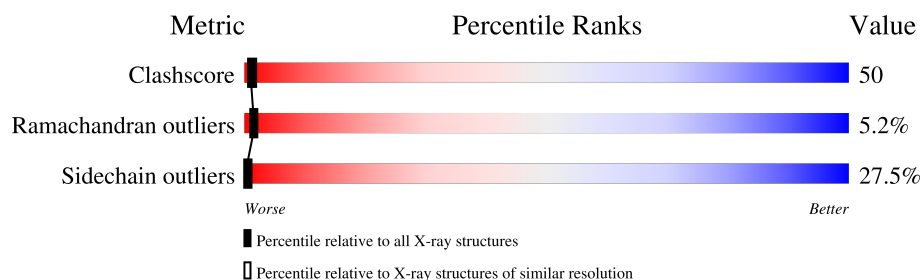
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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

There are 2 unique types of molecules in this entry. The entry contains 2831 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 water.

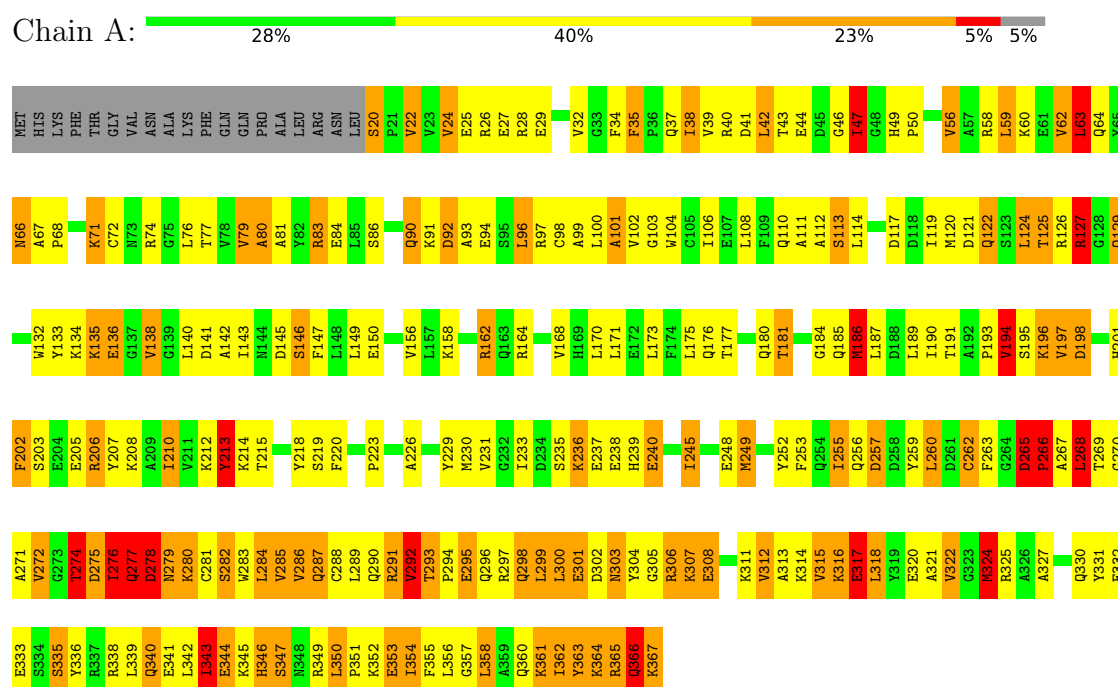
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		

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

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	88.10Å 88.10Å 275.90Å 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}	0.05	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	2831	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.17	3/2855 (0.1%)	1.74	71/3852 (1.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	MET	SD-CE	11.79	2.09	1.79
1	A	343	ILE	CA-CB	-8.84	1.44	1.54
1	A	93	ALA	CA-CB	-5.71	1.44	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	THR	N-CA-C	12.52	124.50	107.73
1	A	317	GLU	N-CA-C	-9.75	100.63	111.07
1	A	343	ILE	CB-CA-C	-9.45	100.00	111.81
1	A	66	ASN	N-CA-C	9.43	125.55	112.45
1	A	190	ILE	CB-CA-C	-9.10	100.47	111.94
1	A	278	ASP	N-CA-C	-8.70	95.12	108.96
1	A	127	ARG	N-CA-C	-8.06	101.93	112.24
1	A	277	GLN	N-CA-C	-7.91	101.96	111.69
1	A	162	ARG	N-CA-C	7.76	120.72	111.33
1	A	38	ILE	N-CA-C	-7.75	102.72	110.62
1	A	305	GLY	N-CA-C	-7.55	103.63	116.01
1	A	346	HIS	N-CA-C	7.23	123.63	114.31
1	A	299	LEU	N-CA-C	-7.04	102.44	111.02
1	A	280	LYS	N-CA-C	6.93	120.15	108.23
1	A	197	VAL	N-CA-C	6.87	123.62	109.34
1	A	210	ILE	N-CA-C	-6.86	103.79	110.72
1	A	146	SER	N-CA-C	-6.86	103.87	111.82
1	A	129	GLN	N-CA-C	-6.84	100.09	110.14
1	A	35	PHE	CA-C-O	6.74	124.83	118.63
1	A	324	MET	N-CA-C	-6.72	104.90	113.23
1	A	213	TYR	N-CA-C	6.56	121.50	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	GLU	N-CA-C	-6.55	104.22	111.36
1	A	354	ILE	CB-CA-C	-6.45	103.45	111.70
1	A	312	VAL	CB-CA-C	-6.36	100.85	111.29
1	A	184	GLY	N-CA-C	-6.34	104.87	113.37
1	A	121	ASP	N-CA-C	-6.33	105.32	114.12
1	A	38	ILE	CB-CA-C	-6.33	103.60	112.14
1	A	43	THR	N-CA-C	6.24	121.77	114.04
1	A	29	GLU	N-CA-C	6.23	120.14	112.54
1	A	27	GLU	N-CA-C	-6.22	104.42	111.07
1	A	42	LEU	N-CA-C	6.09	118.70	111.33
1	A	35	PHE	N-CA-C	6.05	121.12	113.25
1	A	363	TYR	N-CA-C	6.02	123.62	110.80
1	A	80	ALA	N-CA-C	-6.01	104.65	111.14
1	A	265	ASP	N-CA-C	6.01	123.09	109.81
1	A	357	GLY	N-CA-C	-6.01	105.37	112.64
1	A	354	ILE	N-CA-C	5.95	116.42	110.23
1	A	122	GLN	N-CA-C	-5.93	103.22	111.52
1	A	92	ASP	N-CA-C	-5.77	103.31	110.41
1	A	170	LEU	N-CA-C	-5.76	104.69	110.97
1	A	343	ILE	N-CA-C	-5.69	104.78	110.30
1	A	84	GLU	N-CA-C	-5.64	106.44	113.38
1	A	99	ALA	N-CA-C	-5.59	105.09	111.07
1	A	32	VAL	CB-CA-C	-5.55	104.78	111.88
1	A	356	LEU	CB-CA-C	-5.46	102.55	110.96
1	A	229	TYR	CA-C-N	-5.44	111.63	121.14
1	A	229	TYR	C-N-CA	-5.44	111.63	121.14
1	A	325	ARG	N-CA-C	-5.42	104.78	111.33
1	A	293	THR	N-CA-C	-5.39	100.79	109.58
1	A	260	LEU	N-CA-C	-5.38	105.81	112.38
1	A	47	ILE	N-CA-C	5.36	120.50	109.34
1	A	292	VAL	N-CA-C	5.31	120.38	109.34
1	A	201	HIS	CA-C-N	-5.28	114.72	122.06
1	A	201	HIS	C-N-CA	-5.28	114.72	122.06
1	A	43	THR	CB-CA-C	-5.26	99.79	109.15
1	A	257	ASP	N-CA-C	-5.21	105.29	110.97
1	A	83	ARG	CA-C-N	-5.20	113.26	122.26
1	A	83	ARG	C-N-CA	-5.20	113.26	122.26
1	A	315	VAL	CB-CA-C	-5.14	105.30	111.88
1	A	22	VAL	CB-CA-C	-5.14	105.31	112.04
1	A	90	GLN	N-CA-C	5.13	117.81	110.68
1	A	62	VAL	CB-CA-C	-5.11	105.25	112.14
1	A	63	LEU	N-CA-C	-5.08	105.44	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	VAL	N-CA-C	5.08	119.90	109.34
1	A	366	GLN	N-CA-C	-5.07	98.42	107.28
1	A	106	ILE	N-CA-C	-5.05	104.77	111.09
1	A	81	ALA	N-CA-C	5.05	117.17	111.11
1	A	101	ALA	N-CA-C	-5.04	105.47	110.97
1	A	120	MET	CA-C-N	-5.03	114.33	122.23
1	A	120	MET	C-N-CA	-5.03	114.33	122.23
1	A	266	PRO	N-CA-C	5.02	122.81	112.47

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	277	0
2	A	31	0	0	5	0
All	All	2831	0	2782	277	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 50.

All (277) 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	2.09	1.40
1:A:324:MET:HE2	1:A:324:MET:HA	1.34	1.08
1:A:276:ILE:HD12	1:A:316:LYS:HZ3	1.27	1.00
1:A:365:ARG:NE	1:A:367:LYS:H	1.61	0.97
1:A:276:ILE:HG21	1:A:316:LYS:HZ3	1.36	0.90
1:A:306:ARG:NE	1:A:306:ARG:HA	1.84	0.90
1:A:343:ILE:CG2	1:A:352:LYS:HD3	2.03	0.89
1:A:276:ILE:HG21	1:A:316:LYS:NZ	1.88	0.87
1:A:186:MET:HE3	1:A:186:MET:HB2	1.55	0.87
1:A:292:VAL:HG22	1:A:293:THR:H	1.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HE	1:A:367:LYS:H	1.22	0.83
1:A:158:LYS:HG3	1:A:162:ARG:HD2	1.60	0.83
1:A:177:THR:HA	1:A:180:GLN:HE21	1.42	0.82
1:A:126:ARG:O	1:A:129:GLN:HG2	1.78	0.82
1:A:265:ASP:C	1:A:268:LEU:HD23	2.05	0.81
1:A:315:VAL:HB	1:A:316:LYS:HD3	1.62	0.81
1:A:265:ASP:HB3	1:A:266:PRO:HD3	1.63	0.81
1:A:186:MET:CE	1:A:186:MET:HB2	2.11	0.79
1:A:293:THR:HB	1:A:294:PRO:HD2	1.64	0.78
1:A:324:MET:HA	1:A:324:MET:CE	2.13	0.77
1:A:276:ILE:HD12	1:A:316:LYS:NZ	1.99	0.77
1:A:136:GLU:CD	1:A:136:GLU:H	1.93	0.77
1:A:365:ARG:CZ	1:A:367:LYS:H	1.98	0.76
1:A:276:ILE:CG2	1:A:316:LYS:HZ3	1.98	0.76
1:A:318:LEU:O	1:A:322:VAL:HG23	1.86	0.75
1:A:96:LEU:N	1:A:96:LEU:HD23	2.01	0.75
1:A:330:GLN:O	1:A:333:GLU:HG2	1.87	0.74
1:A:342:LEU:HD23	1:A:346:HIS:CD2	2.22	0.74
1:A:238:GLU:HG3	1:A:350:LEU:HD11	1.70	0.73
1:A:274:THR:HG23	1:A:275:ASP:N	2.03	0.73
1:A:268:LEU:HB3	1:A:272:VAL:HB	1.71	0.72
1:A:191:THR:O	1:A:193:PRO:HD3	1.89	0.72
1:A:343:ILE:HG21	1:A:352:LYS:HD3	1.72	0.72
1:A:260:LEU:HD22	1:A:366:GLN:HB3	1.73	0.71
1:A:282:SER:O	1:A:286:VAL:HG23	1.90	0.71
1:A:293:THR:OG1	1:A:295:GLU:HG3	1.91	0.71
1:A:365:ARG:HE	1:A:367:LYS:N	1.88	0.71
1:A:35:PHE:CE2	1:A:39:VAL:HG21	2.26	0.70
1:A:276:ILE:CD1	1:A:316:LYS:HZ3	2.03	0.69
1:A:59:LEU:HD13	1:A:63:LEU:CD2	2.22	0.69
1:A:186:MET:CE	1:A:186:MET:CB	2.70	0.69
1:A:265:ASP:CA	1:A:268:LEU:HD23	2.22	0.69
1:A:290:GLN:NE2	1:A:291:ARG:HH12	1.91	0.69
1:A:318:LEU:O	1:A:321:ALA:HB3	1.93	0.69
1:A:66:ASN:HD21	1:A:132:TRP:HB2	1.57	0.68
1:A:265:ASP:O	1:A:268:LEU:HB2	1.94	0.68
1:A:317:GLU:O	1:A:321:ALA:N	2.20	0.68
1:A:330:GLN:HA	1:A:333:GLU:OE2	1.93	0.68
1:A:245:ILE:C	1:A:245:ILE:HD12	2.19	0.67
1:A:25:GLU:O	1:A:28:ARG:HB2	1.94	0.67
1:A:306:ARG:HD3	1:A:307:LYS:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ARG:HD3	1:A:307:LYS:N	2.10	0.67
1:A:300:LEU:O	1:A:302:ASP:N	2.28	0.67
1:A:364:LYS:O	1:A:365:ARG:HB3	1.95	0.67
1:A:275:ASP:OD1	1:A:278:ASP:HB2	1.93	0.67
1:A:49:HIS:CG	1:A:50:PRO:HD2	2.30	0.67
1:A:306:ARG:HG2	2:A:398:HOH:O	1.94	0.67
1:A:314:LYS:HE3	1:A:317:GLU:OE1	1.95	0.66
1:A:339:LEU:O	1:A:343:ILE:HG12	1.95	0.66
1:A:312:VAL:HG12	1:A:313:ALA:N	2.11	0.66
1:A:114:LEU:N	1:A:114:LEU:HD23	2.06	0.66
1:A:285:VAL:HG21	1:A:304:TYR:CZ	2.31	0.66
1:A:277:GLN:HG3	1:A:278:ASP:N	2.09	0.65
1:A:158:LYS:O	1:A:162:ARG:HB2	1.96	0.65
1:A:196:LYS:NZ	1:A:198:ASP:OD2	2.29	0.65
1:A:288:CYS:SG	1:A:300:LEU:HD11	2.36	0.65
1:A:119:ILE:O	1:A:122:GLN:NE2	2.29	0.65
1:A:191:THR:C	1:A:193:PRO:HD3	2.22	0.65
1:A:255:ILE:HD13	1:A:283:TRP:CD1	2.32	0.65
1:A:340:GLN:N	1:A:340:GLN:OE1	2.31	0.65
1:A:277:GLN:O	1:A:277:GLN:NE2	2.31	0.63
1:A:287:GLN:OE1	1:A:291:ARG:NH1	2.31	0.63
1:A:350:LEU:HB3	1:A:351:PRO:HD2	1.79	0.62
1:A:177:THR:O	1:A:181:THR:HG23	1.99	0.62
1:A:284:LEU:CD2	1:A:324:MET:HG3	2.29	0.62
1:A:358:LEU:HD12	1:A:358:LEU:O	1.98	0.62
1:A:215:THR:HA	1:A:218:TYR:CE1	2.35	0.62
1:A:365:ARG:NE	1:A:367:LYS:N	2.40	0.61
1:A:308:GLU:HB3	1:A:311:LYS:HB2	1.81	0.61
1:A:259:TYR:HE2	1:A:366:GLN:O	1.84	0.61
1:A:365:ARG:HG2	1:A:366:GLN:N	2.16	0.59
1:A:22:VAL:O	1:A:26:ARG:HG3	2.02	0.59
1:A:275:ASP:C	1:A:280:LYS:HD3	2.28	0.59
1:A:20:SER:O	1:A:24:VAL:HB	2.02	0.59
1:A:127:ARG:NH1	2:A:384:HOH:O	2.35	0.59
1:A:290:GLN:HB2	1:A:291:ARG:NH1	2.17	0.59
1:A:42:LEU:HD21	1:A:156:VAL:HG23	1.85	0.59
1:A:46:GLY:C	1:A:56:VAL:HG21	2.28	0.59
1:A:298:GLN:HA	1:A:298:GLN:OE1	2.03	0.58
1:A:358:LEU:HD12	1:A:358:LEU:C	2.27	0.58
1:A:277:GLN:OE1	1:A:307:LYS:HD2	2.04	0.58
1:A:67:ALA:N	1:A:68:PRO:CD	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:N	1:A:68:PRO:HD2	2.18	0.58
1:A:237:GLU:HA	1:A:240:GLU:HG3	1.86	0.57
1:A:191:THR:OG1	1:A:206:ARG:HD2	2.05	0.57
1:A:259:TYR:OH	1:A:367:LYS:HB3	2.04	0.57
1:A:287:GLN:O	1:A:291:ARG:HD2	2.04	0.57
1:A:265:ASP:OD1	1:A:272:VAL:HG11	2.05	0.57
1:A:306:ARG:CZ	1:A:307:LYS:H	2.18	0.57
1:A:35:PHE:CE2	1:A:39:VAL:CG2	2.88	0.57
1:A:293:THR:CB	1:A:295:GLU:HG3	2.35	0.56
1:A:341:GLU:O	1:A:344:GLU:N	2.38	0.56
1:A:122:GLN:HA	1:A:133:TYR:OH	2.06	0.56
1:A:260:LEU:CD2	1:A:366:GLN:HB3	2.35	0.56
1:A:292:VAL:HG22	1:A:296:GLN:HB2	1.87	0.56
1:A:303:ASN:O	1:A:306:ARG:HB2	2.05	0.56
1:A:274:THR:CG2	1:A:275:ASP:N	2.69	0.56
1:A:306:ARG:NH1	1:A:307:LYS:HB2	2.22	0.55
1:A:181:THR:HG22	2:A:396:HOH:O	2.05	0.55
1:A:181:THR:HA	1:A:213:TYR:O	2.06	0.55
1:A:351:PRO:O	1:A:354:ILE:HG13	2.07	0.55
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.72	0.55
1:A:277:GLN:HB2	1:A:307:LYS:HG3	1.88	0.55
1:A:266:PRO:O	1:A:267:ALA:HB3	2.07	0.54
1:A:343:ILE:HG22	1:A:352:LYS:HD3	1.83	0.54
1:A:146:SER:HA	1:A:149:LEU:HD12	1.90	0.54
1:A:58:ARG:HH12	1:A:145:ASP:CG	2.15	0.54
1:A:292:VAL:HG13	1:A:293:THR:N	2.23	0.54
1:A:74:ARG:HE	1:A:219:SER:HB3	1.73	0.54
1:A:147:PHE:O	1:A:150:GLU:HB3	2.08	0.54
1:A:231:VAL:HG23	1:A:233:ILE:HG13	1.89	0.54
1:A:295:GLU:O	1:A:298:GLN:HB2	2.08	0.54
1:A:294:PRO:CD	1:A:295:GLU:H	2.19	0.53
1:A:265:ASP:HB3	1:A:266:PRO:CD	2.37	0.53
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.06	0.53
1:A:272:VAL:HG22	1:A:272:VAL:O	2.09	0.53
1:A:186:MET:CE	1:A:186:MET:CG	2.87	0.53
1:A:207:TYR:HA	1:A:210:ILE:HD12	1.89	0.53
1:A:306:ARG:CD	1:A:307:LYS:H	2.21	0.52
1:A:283:TRP:O	1:A:287:GLN:HB2	2.09	0.52
1:A:34:PHE:CE1	1:A:37:GLN:HG2	2.45	0.52
1:A:274:THR:O	1:A:275:ASP:HB2	2.09	0.52
1:A:71:LYS:O	1:A:72:CYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:NH2	1:A:367:LYS:H	2.07	0.52
1:A:77:THR:CG2	1:A:223:PRO:HB2	2.39	0.52
1:A:58:ARG:O	1:A:62:VAL:HG23	2.10	0.52
1:A:316:LYS:CD	1:A:316:LYS:N	2.73	0.52
1:A:268:LEU:CB	1:A:272:VAL:HB	2.39	0.51
1:A:336:TYR:CZ	1:A:340:GLN:NE2	2.79	0.51
1:A:285:VAL:HG23	2:A:397:HOH:O	2.09	0.51
1:A:285:VAL:HG12	1:A:286:VAL:N	2.25	0.51
1:A:293:THR:CB	1:A:294:PRO:HD2	2.34	0.51
1:A:306:ARG:NH1	1:A:307:LYS:H	2.08	0.51
1:A:74:ARG:HE	1:A:219:SER:CB	2.23	0.51
1:A:110:GLN:O	1:A:113:SER:HB2	2.10	0.51
1:A:332:GLU:OE2	1:A:365:ARG:HB2	2.11	0.51
1:A:361:LYS:C	1:A:362:ILE:HD13	2.36	0.51
1:A:110:GLN:O	1:A:114:LEU:HG	2.11	0.51
1:A:59:LEU:HD13	1:A:63:LEU:HD22	1.92	0.50
1:A:213:TYR:N	1:A:213:TYR:CD1	2.79	0.50
1:A:278:ASP:O	1:A:280:LYS:N	2.44	0.50
1:A:306:ARG:HA	1:A:306:ARG:HE	1.70	0.50
1:A:94:GLU:OE1	1:A:97:ARG:NH1	2.44	0.50
1:A:287:GLN:HB3	1:A:324:MET:SD	2.51	0.50
1:A:98:CYS:O	1:A:102:VAL:HG23	2.12	0.50
1:A:111:ALA:O	1:A:112:ALA:C	2.54	0.50
1:A:226:ALA:O	1:A:230:MET:HG3	2.12	0.50
1:A:344:GLU:OE1	1:A:352:LYS:HE3	2.11	0.49
1:A:46:GLY:HA3	1:A:56:VAL:HG21	1.94	0.49
1:A:195:SER:O	1:A:196:LYS:HB2	2.12	0.49
1:A:236:LYS:O	1:A:240:GLU:HG2	2.12	0.49
1:A:277:GLN:CB	1:A:307:LYS:HG3	2.43	0.49
1:A:173:LEU:O	1:A:177:THR:HG23	2.13	0.49
1:A:79:VAL:HG12	1:A:80:ALA:N	2.27	0.48
1:A:265:ASP:HA	1:A:268:LEU:HD23	1.94	0.48
1:A:278:ASP:O	1:A:280:LYS:HG2	2.13	0.48
1:A:38:ILE:O	1:A:41:ASP:HB2	2.12	0.48
1:A:318:LEU:HA	1:A:321:ALA:HB3	1.95	0.48
1:A:233:ILE:O	1:A:239:HIS:HE1	1.95	0.48
1:A:206:ARG:HG3	1:A:210:ILE:HD11	1.95	0.48
1:A:277:GLN:C	1:A:277:GLN:HE21	2.21	0.48
1:A:352:LYS:O	1:A:353:GLU:C	2.55	0.48
1:A:125:THR:CG2	1:A:126:ARG:N	2.76	0.48
1:A:276:ILE:CD1	1:A:316:LYS:NZ	2.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASP:O	1:A:265:ASP:OD1	2.32	0.48
1:A:367:LYS:HB2	1:A:367:LYS:NZ	2.29	0.48
1:A:342:LEU:HD23	1:A:346:HIS:NE2	2.29	0.48
1:A:215:THR:HA	1:A:218:TYR:HE1	1.78	0.47
1:A:252:TYR:CD1	1:A:252:TYR:C	2.92	0.47
1:A:293:THR:HG23	1:A:296:GLN:OE1	2.14	0.47
1:A:79:VAL:HG21	1:A:100:LEU:HD23	1.97	0.47
1:A:285:VAL:CG2	1:A:304:TYR:CZ	2.96	0.47
1:A:35:PHE:O	1:A:39:VAL:HG23	2.15	0.47
1:A:274:THR:HG23	1:A:275:ASP:H	1.77	0.47
1:A:46:GLY:CA	1:A:56:VAL:HG21	2.45	0.47
1:A:168:VAL:O	1:A:168:VAL:HG12	2.15	0.46
1:A:215:THR:O	1:A:219:SER:OG	2.26	0.46
1:A:101:ALA:O	1:A:103:GLY:N	2.49	0.46
1:A:104:TRP:O	1:A:108:LEU:HG	2.15	0.46
1:A:300:LEU:O	1:A:301:GLU:C	2.57	0.46
1:A:64:GLN:HB3	2:A:375:HOH:O	2.16	0.46
1:A:277:GLN:CG	1:A:307:LYS:HG3	2.45	0.46
1:A:295:GLU:O	1:A:298:GLN:N	2.47	0.46
1:A:203:SER:OG	1:A:206:ARG:HB3	2.15	0.46
1:A:252:TYR:OH	1:A:256:GLN:OE1	2.29	0.46
1:A:260:LEU:HD22	1:A:366:GLN:CB	2.44	0.46
1:A:283:TRP:CZ2	1:A:287:GLN:HG2	2.51	0.46
1:A:285:VAL:CG2	1:A:304:TYR:CE2	2.99	0.46
1:A:60:LYS:O	1:A:64:GLN:HG3	2.16	0.46
1:A:276:ILE:HG13	1:A:304:TYR:CE2	2.50	0.46
1:A:275:ASP:C	1:A:276:ILE:HG22	2.40	0.46
1:A:285:VAL:HG21	1:A:304:TYR:OH	2.16	0.46
1:A:245:ILE:CG2	1:A:346:HIS:HB2	2.47	0.45
1:A:347:SER:HB3	1:A:352:LYS:HG2	1.98	0.45
1:A:275:ASP:CG	1:A:278:ASP:HB2	2.41	0.45
1:A:287:GLN:OE1	1:A:290:GLN:NE2	2.47	0.45
1:A:212:LYS:HE2	1:A:213:TYR:CE1	2.52	0.45
1:A:124:LEU:HD13	1:A:124:LEU:HA	1.63	0.45
1:A:275:ASP:O	1:A:280:LYS:HD3	2.16	0.45
1:A:294:PRO:HD2	1:A:295:GLU:H	1.81	0.45
1:A:101:ALA:C	1:A:103:GLY:N	2.75	0.44
1:A:185:GLN:HE21	1:A:185:GLN:HA	1.81	0.44
1:A:236:LYS:HE3	1:A:240:GLU:OE2	2.17	0.44
1:A:164:ARG:HD3	1:A:164:ARG:HA	1.88	0.44
1:A:202:PHE:N	1:A:202:PHE:HD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:O	1:A:223:PRO:HG2	2.16	0.44
1:A:202:PHE:N	1:A:202:PHE:CD1	2.86	0.44
1:A:260:LEU:CD2	1:A:366:GLN:CB	2.95	0.44
1:A:42:LEU:HD21	1:A:156:VAL:CG2	2.47	0.44
1:A:341:GLU:O	1:A:344:GLU:HB2	2.18	0.44
1:A:277:GLN:NE2	1:A:277:GLN:C	2.76	0.43
1:A:119:ILE:HD11	1:A:142:ALA:HB3	2.00	0.43
1:A:284:LEU:HD23	1:A:324:MET:HG3	1.98	0.43
1:A:249:MET:HB3	1:A:249:MET:HE2	1.38	0.43
1:A:252:TYR:HD2	1:A:335:SER:HG	1.66	0.43
1:A:253:PHE:CD1	1:A:253:PHE:C	2.97	0.43
1:A:276:ILE:CG1	1:A:316:LYS:HZ3	2.32	0.43
1:A:177:THR:HA	1:A:180:GLN:NE2	2.22	0.43
1:A:365:ARG:HG2	1:A:367:LYS:OXT	2.19	0.43
1:A:238:GLU:OE2	1:A:349:ARG:HB3	2.19	0.42
1:A:294:PRO:CG	1:A:295:GLU:N	2.82	0.42
1:A:90:GLN:C	1:A:91:LYS:HG2	2.44	0.42
1:A:141:ASP:C	1:A:143:ILE:N	2.75	0.42
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.79	0.42
1:A:197:VAL:O	1:A:279:ASN:ND2	2.52	0.42
1:A:327:ALA:HA	1:A:330:GLN:HG3	2.01	0.42
1:A:117:ASP:OD1	1:A:117:ASP:O	2.36	0.42
1:A:294:PRO:CD	1:A:295:GLU:N	2.83	0.42
1:A:262:CYS:SG	1:A:263:PHE:N	2.92	0.42
1:A:287:GLN:O	1:A:291:ARG:NH1	2.40	0.42
1:A:34:PHE:O	1:A:37:GLN:HB3	2.19	0.42
1:A:214:LYS:C	1:A:215:THR:HG23	2.44	0.42
1:A:283:TRP:CH2	1:A:287:GLN:HG2	2.55	0.42
1:A:288:CYS:O	1:A:290:GLN:N	2.53	0.42
1:A:363:TYR:O	1:A:364:LYS:C	2.63	0.42
1:A:317:GLU:O	1:A:321:ALA:HB2	2.20	0.41
1:A:343:ILE:O	1:A:347:SER:N	2.44	0.41
1:A:362:ILE:HD12	1:A:362:ILE:HA	1.58	0.41
1:A:74:ARG:O	1:A:77:THR:HB	2.20	0.41
1:A:79:VAL:CG2	1:A:100:LEU:HD23	2.50	0.41
1:A:25:GLU:OE1	1:A:28:ARG:NH1	2.53	0.41
1:A:276:ILE:C	1:A:276:ILE:HD13	2.46	0.41
1:A:312:VAL:O	1:A:313:ALA:C	2.63	0.41
1:A:49:HIS:CD2	1:A:50:PRO:HD2	2.55	0.41
1:A:96:LEU:HD22	1:A:96:LEU:HA	1.77	0.41
1:A:186:MET:HE3	1:A:186:MET:CB	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PRO:O	1:A:267:ALA:CB	2.67	0.41
1:A:293:THR:HB	1:A:295:GLU:HG3	2.00	0.41
1:A:340:GLN:OE1	1:A:340:GLN:CA	2.68	0.41
1:A:339:LEU:HB3	1:A:340:GLN:OE1	2.20	0.41
1:A:268:LEU:HA	1:A:268:LEU:HD13	1.65	0.41
1:A:306:ARG:CD	1:A:307:LYS:N	2.81	0.41
1:A:331:TYR:CD1	1:A:331:TYR:C	2.98	0.41
1:A:345:LYS:HG2	1:A:346:HIS:CE1	2.56	0.41
1:A:59:LEU:O	1:A:63:LEU:HD22	2.21	0.41
1:A:94:GLU:CD	1:A:97:ARG:HH12	2.28	0.41
1:A:268:LEU:O	1:A:270:GLY:N	2.54	0.41
1:A:352:LYS:HA	1:A:355:PHE:HD2	1.86	0.40
1:A:92:ASP:OD1	1:A:92:ASP:N	2.53	0.40
1:A:207:TYR:CE2	1:A:283:TRP:HB2	2.56	0.40
1:A:336:TYR:O	1:A:339:LEU:HB3	2.21	0.40
1:A:47:ILE:N	1:A:56:VAL:HG21	2.36	0.40
1:A:135:LYS:O	1:A:138:VAL:HB	2.21	0.40
1:A:276:ILE:CG1	1:A:316:LYS:NZ	2.84	0.40
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.70	0.40
1:A:276:ILE:CG1	1:A:304:TYR:CE2	3.04	0.40
1:A:300:LEU:C	1:A:302:ASP:N	2.78	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%)	279 (81%)	49 (14%)	18 (5%)	1 1

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	VAL
1	A	198	ASP
1	A	269	THR
1	A	276	ILE
1	A	279	ASN
1	A	301	GLU
1	A	265	ASP
1	A	281	CYS
1	A	289	LEU
1	A	300	LEU
1	A	364	LYS
1	A	113	SER
1	A	196	LYS
1	A	266	PRO
1	A	268	LEU
1	A	275	ASP
1	A	271	ALA
1	A	138	VAL

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	298/314 (95%)	216 (72%)	82 (28%)	0 1

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	24	VAL
1	A	40	ARG
1	A	44	GLU
1	A	47	ILE
1	A	56	VAL
1	A	59	LEU
1	A	63	LEU
1	A	71	LYS

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Mol	Chain	Res	Type
1	A	79	VAL
1	A	83	ARG
1	A	86	SER
1	A	96	LEU
1	A	124	LEU
1	A	125	THR
1	A	127	ARG
1	A	134	LYS
1	A	135	LYS
1	A	136	GLU
1	A	140	LEU
1	A	171	LEU
1	A	175	LEU
1	A	176	GLN
1	A	181	THR
1	A	186	MET
1	A	189	LEU
1	A	194	VAL
1	A	202	PHE
1	A	205	GLU
1	A	206	ARG
1	A	208	LYS
1	A	213	TYR
1	A	235	SER
1	A	236	LYS
1	A	240	GLU
1	A	245	ILE
1	A	248	GLU
1	A	249	MET
1	A	255	ILE
1	A	257	ASP
1	A	262	CYS
1	A	268	LEU
1	A	272	VAL
1	A	274	THR
1	A	276	ILE
1	A	277	GLN
1	A	278	ASP
1	A	282	SER
1	A	284	LEU
1	A	285	VAL
1	A	286	VAL

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Mol	Chain	Res	Type
1	A	287	GLN
1	A	291	ARG
1	A	292	VAL
1	A	295	GLU
1	A	297	ARG
1	A	298	GLN
1	A	299	LEU
1	A	303	ASN
1	A	306	ARG
1	A	307	LYS
1	A	308	GLU
1	A	316	LYS
1	A	317	GLU
1	A	318	LEU
1	A	322	VAL
1	A	324	MET
1	A	335	SER
1	A	338	ARG
1	A	340	GLN
1	A	343	ILE
1	A	344	GLU
1	A	347	SER
1	A	350	LEU
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	366	GLN
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	180	GLN
1	A	185	GLN
1	A	239	HIS
1	A	254	GLN
1	A	290	GLN

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Mol	Chain	Res	Type
1	A	360	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.