Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:35 PM GMT

PDB ID	:	1UBV
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

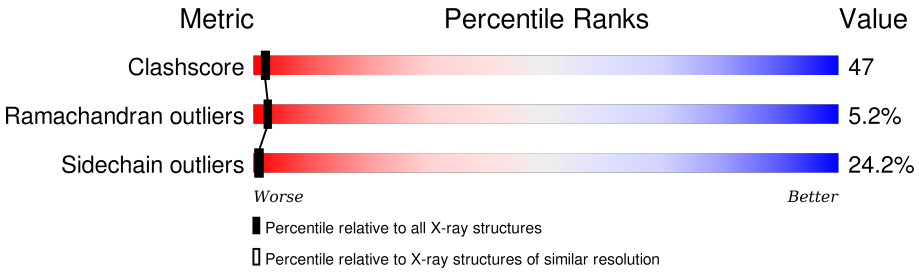
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	367	36% 37% 20% • 5%

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		

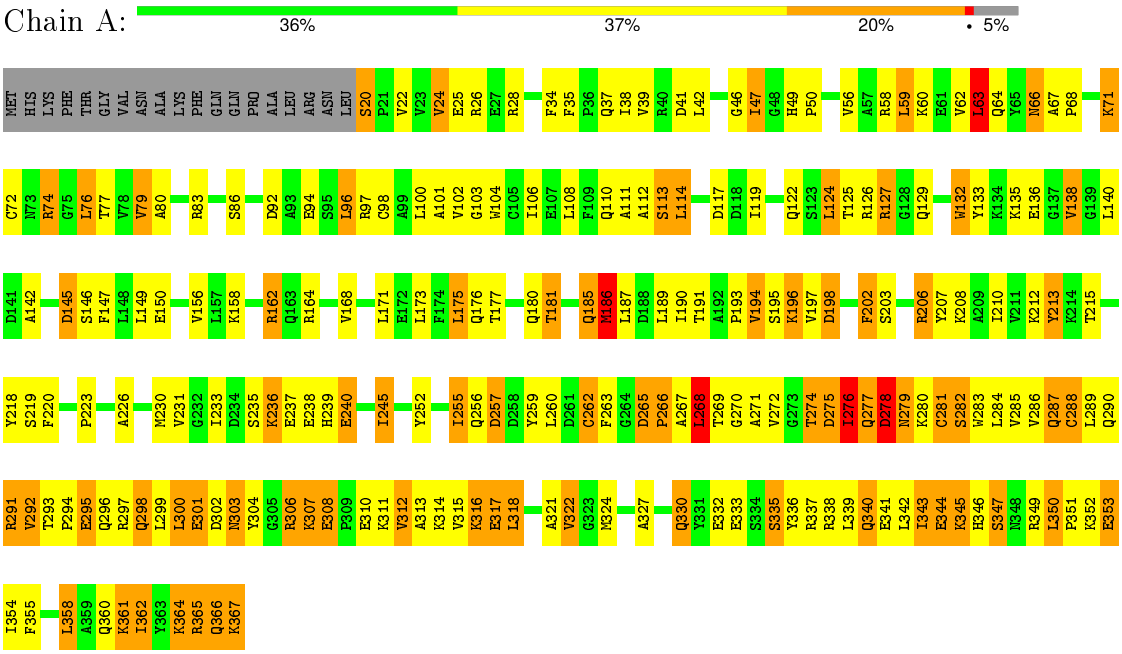
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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 (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 V. 5-E	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	0.94	2/2855 (0.1%)	1.30	19/3852 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	MET	SD-CE	5.57	2.09	1.77
1	A	132	TRP	CE3-CZ3	5.00	1.47	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	LEU	CA-CB-CG	7.80	133.23	115.30
1	A	175	LEU	CB-CG-CD1	7.78	124.23	111.00
1	A	63	LEU	CA-CB-CG	6.59	130.46	115.30
1	A	162	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	288	CYS	CA-CB-SG	6.18	125.12	114.00
1	A	278	ASP	N-CA-C	-5.88	95.12	111.00
1	A	145	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	343	ILE	CB-CA-C	-5.80	100.00	111.60
1	A	114	LEU	CA-CB-CG	-5.79	102.00	115.30
1	A	145	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	257	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	190	ILE	CB-CA-C	-5.56	100.47	111.60
1	A	312	VAL	CB-CA-C	-5.55	100.85	111.40
1	A	66	ASN	N-CA-C	5.39	125.55	111.00
1	A	106	ILE	CG1-CB-CG2	-5.35	99.62	111.40
1	A	76	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	A	74	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	268	LEU	CA-CB-CG	-5.24	103.25	115.30
1	A	343	ILE	CG1-CB-CG2	5.06	122.53	111.40

There are no chirality outliers.

There are no planarity outliers.

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	2800	0	2782	262	0
2	A	31	0	0	5	0
All	All	2831	0	2782	262	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 (262) 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:276:ILE:HD12	1:A:316:LYS:HZ1	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:HZ1	1.36	0.90
1:A:306:ARG:HA	1:A:306:ARG:NE	1.84	0.90
1:A:343:ILE:CG2	1:A:352:LYS:HD3	2.03	0.89
1:A:186:MET:HE3	1:A:186:MET:HB2	1.53	0.88
1:A:276:ILE:HG21	1:A:316:LYS:NZ	1.88	0.87
1:A:292:VAL:HG22	1:A:293:THR:H	1.41	0.83
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: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:HB2	1:A:186:MET:CE	2.11	0.79
1:A:293:THR:HB	1:A:294:PRO:HD2	1.64	0.78
1:A:324:MET:CE	1:A:324:MET:HA	2.13	0.77
1:A:276:ILE:HD12	1:A:316:LYS:NZ	1.99	0.77
1:A:265:ASP:C	1:A:268:LEU:HD23	2.05	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:HZ1	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:324:MET:HA	1:A:324:MET:HE2	1.66	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:282:SER:O	1:A:286:VAL:HG23	1.90	0.71
1:A:260:LEU:HD22	1:A:366:GLN:HB3	1.73	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:136:GLU:H	1:A:136:GLU:CD	1.93	0.70
1:A:35:PHE:CE2	1:A:39:VAL:HG21	2.26	0.70
1:A:276:ILE:CD1	1:A:316:LYS:HZ1	2.03	0.69
1:A:59:LEU:HD13	1:A:63:LEU:CD2	2.22	0.69
1:A:186:MET:CB	1:A:186:MET:CE	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: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
1:A:306:ARG:HD3	1:A:307:LYS:N	2.10	0.67
1:A:364:LYS:O	1:A:365:ARG:HB3	1.95	0.67
1:A:300:LEU:O	1:A:302:ASP:N	2.28	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:HD23	1:A:114:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:340:GLN:N	1:A:340:GLN:OE1	2.31	0.65
1:A:255:ILE:HD13	1:A:283:TRP:CD1	2.32	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:245:ILE:C	1:A:245:ILE:HD12	2.19	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:O	1:A:358:LEU:HD12	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:365:ARG:HG2	1:A:366:GLN:N	2.16	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:22:VAL:O	1:A:26:ARG:HG3	2.02	0.59
1:A:290:GLN:HB2	1:A:291:ARG:NH1	2.17	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:191:THR:C	1:A:193:PRO:HD3	2.22	0.59
1:A:42:LEU:HD21	1:A:156:VAL:HG23	1.85	0.59
1:A:298:GLN:OE1	1:A:298:GLN:HA	2.03	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
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:259:TYR:OH	1:A:367:LYS:HB3	2.04	0.57
1:A:191:THR:OG1	1:A:206:ARG:HD2	2.05	0.57
1:A:287:GLN:O	1:A:291:ARG:HD2	2.04	0.57
1:A:306:ARG:CZ	1:A:307:LYS:H	2.18	0.57
1:A:265:ASP:OD1	1:A:272:VAL:HG11	2.05	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: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:122:GLN:HA	1:A:133:TYR:OH	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:MET:HE3	1:A:186:MET:CB	2.31	0.55
1:A:306:ARG:NH1	1:A:307:LYS:HB2	2.22	0.55
1:A:181:THR:HA	1:A:213:TYR:O	2.06	0.55
1:A:181:THR:HG22	2:A:396:HOH:O	2.05	0.55
1:A:275:ASP:C	1:A:280:LYS:HD3	2.28	0.55
1:A:351:PRO:O	1:A:354:ILE:HG13	2.07	0.55
1:A:277:GLN:HB2	1:A:307:LYS:HG3	1.88	0.55
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.72	0.55
1:A:343:ILE:HG22	1:A:352:LYS:HD3	1.83	0.54
1:A:266:PRO:O	1:A:267:ALA:HB3	2.07	0.54
1:A:146:SER:HA	1:A:149:LEU:HD12	1.90	0.54
1:A:46:GLY:C	1:A:56:VAL:HG21	2.28	0.54
1:A:292:VAL:HG13	1:A:293:THR:N	2.23	0.54
1:A:358:LEU:HD12	1:A:358:LEU:C	2.27	0.54
1:A:74:ARG:HE	1:A:219:SER:HB3	1.73	0.54
1:A:295:GLU:O	1:A:298:GLN:HB2	2.08	0.54
1:A:231:VAL:HG23	1:A:233:ILE:HG13	1.89	0.54
1:A:147:PHE:O	1:A:150:GLU:HB3	2.08	0.54
1:A:294:PRO:CD	1:A:295:GLU:H	2.19	0.53
1:A:344:GLU:HA	1:A:344:GLU:OE1	2.06	0.53
1:A:265:ASP:HB3	1:A:266:PRO:CD	2.37	0.53
1:A:272:VAL:HG22	1:A:272:VAL:O	2.09	0.53
1:A:186:MET:CG	1:A:186:MET:CE	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:365:ARG:NH2	1:A:367:LYS:H	2.07	0.52
1:A:71:LYS:O	1:A:72:CYS:HB2	2.09	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:336:TYR:CZ	1:A:340:GLN:NE2	2.79	0.51
1:A:268:LEU:CB	1:A:272:VAL:HB	2.39	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:332:GLU:OE2	1:A:365:ARG:HB2	2.11	0.51
1:A:110:GLN:O	1:A:113:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:HE	1:A:219:SER:CB	2.23	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:278:ASP:O	1:A:280:LYS:N	2.44	0.50
1:A:306:ARG:HE	1:A:306:ARG:HA	1.70	0.50
1:A:213:TYR:CD1	1:A:213:TYR:N	2.79	0.50
1:A:287:GLN:HB3	1:A:324:MET:SD	2.51	0.50
1:A:94:GLU:OE1	1:A:97:ARG:NH1	2.44	0.50
1:A:98:CYS:O	1:A:102:VAL:HG23	2.12	0.50
1:A:226:ALA:O	1:A:230:MET:HG3	2.12	0.50
1:A:58:ARG:HH12	1:A:145:ASP:CG	2.15	0.49
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:278:ASP:O	1:A:280:LYS:HG2	2.13	0.48
1:A:265:ASP:HA	1:A:268:LEU:HD23	1.94	0.48
1:A:79:VAL:HG12	1:A:80:ALA:N	2.27	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:252:TYR:HD2	1:A:335:SER:HG	1.61	0.48
1:A:276:ILE:CD1	1:A:316:LYS:NZ	2.69	0.48
1:A:125:THR:CG2	1:A:126:ARG:N	2.76	0.48
1:A:367:LYS:HB2	1:A:367:LYS:NZ	2.29	0.48
1:A:265:ASP:OD1	1:A:265:ASP:O	2.32	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: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:274:THR:HG23	1:A:275:ASP:H	1.77	0.47
1:A:35:PHE:O	1:A:39:VAL:HG23	2.15	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: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:277:GLN:CG	1:A:307:LYS:HG3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLU:O	1:A:298:GLN:N	2.47	0.46
1:A:64:GLN:HB3	2:A:375:HOH:O	2.16	0.46
1:A:260:LEU:HD22	1:A:366:GLN:CB	2.44	0.46
1:A:203:SER:OG	1:A:206:ARG:HB3	2.15	0.46
1:A:361:LYS:C	1:A:362:ILE:HD13	2.36	0.46
1:A:285:VAL:CG2	1:A:304:TYR:CE2	2.99	0.46
1:A:283:TRP:CZ2	1:A:287:GLN:HG2	2.51	0.46
1:A:276:ILE:HG13	1:A:304:TYR:CE2	2.50	0.46
1:A:60:LYS:O	1:A:64:GLN:HG3	2.16	0.46
1:A:285:VAL:HG21	1:A:304:TYR:OH	2.16	0.46
1:A:347:SER:HB3	1:A:352:LYS:HG2	1.98	0.45
1:A:245:ILE:CG2	1:A:346:HIS:HB2	2.47	0.45
1:A:287:GLN:OE1	1:A:290:GLN:NE2	2.47	0.45
1:A:252:TYR:OH	1:A:256:GLN:OE1	2.29	0.45
1:A:212:LYS:HE2	1:A:213:TYR:CE1	2.52	0.45
1:A:111:ALA:O	1:A:112:ALA:C	2.54	0.45
1:A:275:ASP:O	1:A:280:LYS:HD3	2.16	0.45
1:A:124:LEU:HD13	1:A:124:LEU:HA	1.63	0.45
1:A:294:PRO:HD2	1:A:295:GLU:H	1.81	0.45
1:A:236:LYS:HE3	1:A:240:GLU:OE2	2.17	0.44
1:A:185:GLN:HA	1:A:185:GLN:HE21	1.81	0.44
1:A:220:PHE:O	1:A:223:PRO:HG2	2.16	0.44
1:A:164:ARG:HA	1:A:164:ARG:HD3	1.88	0.44
1:A:202:PHE:N	1:A:202:PHE:HD1	2.16	0.44
1:A:260:LEU:CD2	1:A:366:GLN:CB	2.95	0.44
1:A:202:PHE:N	1:A:202:PHE:CD1	2.86	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:284:LEU:HD23	1:A:324:MET:HG3	1.98	0.43
1:A:119:ILE:HD11	1:A:142:ALA:HB3	2.00	0.43
1:A:352:LYS:O	1:A:353:GLU:C	2.55	0.43
1:A:276:ILE:CG1	1:A:316:LYS:HZ1	2.32	0.43
1:A:277:GLN:C	1:A:277:GLN:HE21	2.21	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:294:PRO:CG	1:A:295:GLU:N	2.82	0.42
1:A:238:GLU:OE2	1:A:349:ARG:HB3	2.19	0.42
1:A:252:TYR:CD1	1:A:252:TYR:C	2.92	0.42
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.79	0.42
1:A:327:ALA:HA	1:A:330:GLN:HG3	2.01	0.42
1:A:197:VAL:O	1:A:279:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:CD	1:A:295:GLU:N	2.83	0.42
1:A:117:ASP:OD1	1:A:117:ASP:O	2.36	0.42
1:A:287:GLN:O	1:A:291:ARG:NH1	2.40	0.42
1:A:262:CYS:SG	1:A:263:PHE:N	2.92	0.42
1:A:34:PHE:O	1:A:37:GLN:HB3	2.19	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:300:LEU:O	1:A:301:GLU:C	2.57	0.41
1:A:317:GLU:O	1:A:321:ALA:HB2	2.20	0.41
1:A:275:ASP:C	1:A:276:ILE:HG22	2.40	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:96:LEU:HA	1:A:96:LEU:HD22	1.77	0.41
1:A:49:HIS:CD2	1:A:50:PRO:HD2	2.55	0.41
1:A:340:GLN:OE1	1:A:340:GLN:CA	2.68	0.41
1:A:293:THR:HB	1:A:295:GLU:HG3	2.00	0.41
1:A:266:PRO:O	1:A:267:ALA:CB	2.67	0.41
1:A:339:LEU:HB3	1:A:340:GLN:OE1	2.20	0.41
1:A:306:ARG:CD	1:A:307:LYS:N	2.81	0.41
1:A:268:LEU:HA	1:A:268:LEU:HD13	1.65	0.41
1:A:345:LYS:HG2	1:A:346:HIS:CE1	2.56	0.41
1:A:268:LEU:O	1:A:270:GLY:N	2.54	0.41
1:A:59:LEU:O	1:A:63:LEU:HD22	2.21	0.41
1:A:352:LYS:HA	1:A:355:PHE:HD2	1.86	0.40
1:A:336:TYR:O	1:A:339:LEU:HB3	2.21	0.40
1:A:207:TYR:CE2	1:A:283:TRP:HB2	2.56	0.40
1:A:92:ASP:OD1	1:A:92:ASP:N	2.53	0.40
1:A:47:ILE:N	1:A:56:VAL:HG21	2.36	0.40
1:A:276:ILE:CG1	1:A:316:LYS:NZ	2.84	0.40
1:A:135:LYS:O	1:A:138:VAL:HB	2.21	0.40
1:A:276:ILE:CG1	1:A:304:TYR:CE2	3.04	0.40
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.70	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%)	279 (81%)	49 (14%)	18 (5%)	2 2

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%)	226 (76%)	72 (24%)	1 1

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	24	VAL
1	A	47	ILE
1	A	59	LEU
1	A	63	LEU
1	A	71	LYS
1	A	79	VAL
1	A	83	ARG
1	A	86	SER
1	A	96	LEU
1	A	124	LEU
1	A	127	ARG
1	A	140	LEU
1	A	171	LEU
1	A	175	LEU
1	A	176	GLN
1	A	181	THR
1	A	185	GLN
1	A	186	MET
1	A	189	LEU
1	A	194	VAL
1	A	202	PHE
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	255	ILE
1	A	257	ASP
1	A	262	CYS
1	A	268	LEU
1	A	274	THR
1	A	276	ILE
1	A	277	GLN
1	A	278	ASP
1	A	281	CYS

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Mol	Chain	Res	Type
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	298	GLN
1	A	299	LEU
1	A	303	ASN
1	A	306	ARG
1	A	307	LYS
1	A	308	GLU
1	A	310	GLU
1	A	316	LYS
1	A	317	GLU
1	A	318	LEU
1	A	322	VAL
1	A	330	GLN
1	A	335	SER
1	A	337	ARG
1	A	338	ARG
1	A	340	GLN
1	A	344	GLU
1	A	345	LYS
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	180	GLN
1	A	185	GLN
1	A	239	HIS

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Mol	Chain	Res	Type
1	A	254	GLN
1	A	290	GLN
1	A	360	GLN
1	A	366	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.