Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:35 PM GMT

PDB ID	:	1UBW
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:

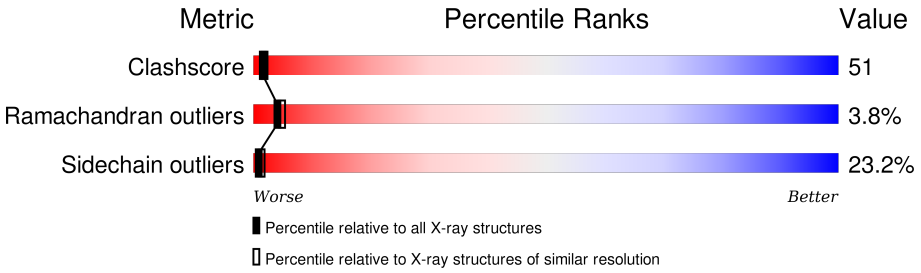
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	34% 40% 18% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2902 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			

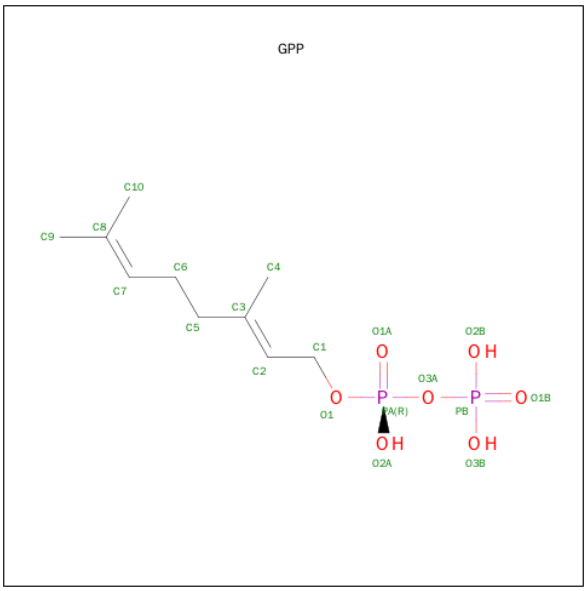
There are 3 discrepancies between the modelled and reference sequences:

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

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

- Molecule 3 is GERANYL DIPHOSPHATE (three-letter code: GPP) (formula: $C_{10}H_{20}O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			19	10	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		

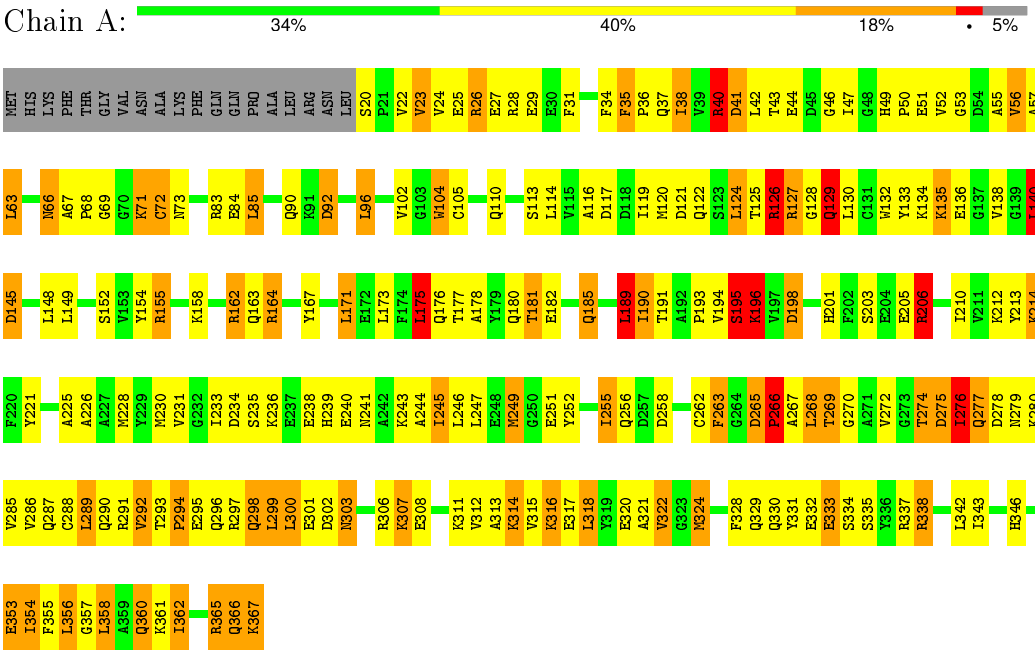
3 Residue-property plots (i)

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	88.70Å 88.70Å 274.90Å 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}	0.07	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	2902	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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, GPP

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	0.97	1/2855 (0.0%)	1.37	23/3852 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	TRP	CB-CG	-5.97	1.39	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	LEU	CB-CG-CD1	8.51	125.47	111.00
1	A	171	LEU	CA-CB-CG	8.24	134.25	115.30
1	A	40	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	92	ASP	CB-CG-OD1	-7.55	111.50	118.30
1	A	189	LEU	CA-CB-CG	-6.55	100.24	115.30
1	A	85	LEU	CA-CB-CG	6.46	130.16	115.30
1	A	362	ILE	CG1-CB-CG2	-6.29	97.56	111.40
1	A	69	GLY	N-CA-C	6.28	128.81	113.10
1	A	124	LEU	CB-CG-CD1	-6.25	100.37	111.00
1	A	66	ASN	N-CA-C	6.14	127.57	111.00
1	A	190	ILE	CB-CA-C	-5.60	100.39	111.60
1	A	206	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	58	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	244	ALA	C-N-CA	-5.57	107.77	121.70
1	A	140	LEU	CA-CB-CG	-5.57	102.49	115.30
1	A	117	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	96	LEU	CA-CB-CG	-5.50	102.65	115.30
1	A	276	ILE	N-CA-C	-5.42	96.37	111.00
1	A	129	GLN	N-CA-C	-5.38	96.47	111.00
1	A	41	ASP	CB-CG-OD1	5.17	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	PHE	C-N-CD	-5.14	109.30	120.60
1	A	126	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	145	ASP	CB-CG-OD2	-5.04	113.77	118.30

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	285	0
2	A	2	0	0	0	0
3	A	19	0	17	4	0
4	A	81	0	0	13	0
All	All	2902	0	2799	285	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 51.

All (285) 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:292:VAL:HG22	1:A:296:GLN:HB2	1.36	1.07
1:A:59:LEU:HD22	1:A:63:LEU:HD22	1.29	1.07
1:A:40:ARG:HG3	1:A:40:ARG:HH11	1.21	1.05
1:A:276:ILE:HG13	1:A:316:LYS:HE2	1.49	0.92
1:A:277:GLN:NE2	1:A:307:LYS:HD2	1.84	0.92
1:A:329:GLN:NE2	1:A:365:ARG:HG3	1.84	0.92
1:A:316:LYS:HD2	1:A:316:LYS:N	1.86	0.91
1:A:185:GLN:HE21	1:A:185:GLN:HA	1.33	0.91
1:A:276:ILE:HD11	1:A:315:VAL:HG11	1.51	0.90
1:A:49:HIS:ND1	1:A:50:PRO:HD2	1.88	0.88
1:A:306:ARG:HA	1:A:306:ARG:NE	1.87	0.86
1:A:276:ILE:HG13	1:A:316:LYS:CE	2.05	0.86
1:A:292:VAL:CG1	1:A:297:ARG:HB2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:HB3	1:A:68:PRO:HD3	1.60	0.83
1:A:316:LYS:H	1:A:316:LYS:HD2	1.42	0.82
1:A:262:CYS:HB3	1:A:263:PHE:CD1	2.14	0.82
1:A:287:GLN:HB2	1:A:324:MET:HE3	1.62	0.81
1:A:274:THR:HG23	1:A:276:ILE:HG22	1.62	0.80
1:A:292:VAL:HG11	1:A:297:ARG:HB2	1.64	0.79
1:A:265:ASP:OD1	1:A:272:VAL:HG11	1.83	0.79
1:A:292:VAL:CG2	1:A:296:GLN:HB2	2.13	0.78
1:A:366:GLN:C	1:A:367:LYS:HE2	2.04	0.78
1:A:276:ILE:HG13	1:A:316:LYS:HZ3	1.45	0.78
1:A:329:GLN:HE22	1:A:365:ARG:HG3	1.48	0.77
1:A:318:LEU:O	1:A:321:ALA:HB3	1.83	0.76
1:A:365:ARG:HG2	1:A:366:GLN:N	1.99	0.76
1:A:287:GLN:HB2	1:A:324:MET:CE	2.15	0.75
1:A:276:ILE:HG13	1:A:316:LYS:NZ	2.01	0.75
1:A:46:GLY:HA3	1:A:56:VAL:HG11	1.69	0.74
1:A:59:LEU:CD2	1:A:63:LEU:HD22	2.15	0.74
1:A:96:LEU:N	1:A:96:LEU:HD23	2.03	0.74
1:A:177:THR:O	1:A:181:THR:HG23	1.88	0.74
1:A:126:ARG:HG3	1:A:127:ARG:HG2	1.70	0.73
1:A:284:LEU:HD22	1:A:324:MET:HG3	1.70	0.73
1:A:49:HIS:CE1	1:A:51:GLU:HB2	2.24	0.73
1:A:275:ASP:OD1	1:A:278:ASP:HB2	1.89	0.72
1:A:298:GLN:OE1	1:A:301:GLU:HB3	1.91	0.71
1:A:300:LEU:HG	1:A:318:LEU:HD13	1.73	0.70
1:A:350:LEU:HB3	1:A:351:PRO:HD2	1.74	0.70
1:A:311:LYS:O	1:A:315:VAL:HG23	1.91	0.70
1:A:293:THR:N	1:A:296:GLN:OE1	2.25	0.70
1:A:300:LEU:HG	1:A:318:LEU:CD1	2.22	0.69
1:A:365:ARG:HG2	1:A:366:GLN:H	1.57	0.69
1:A:263:PHE:HE1	1:A:284:LEU:HD13	1.56	0.69
1:A:358:LEU:O	1:A:358:LEU:HD12	1.91	0.69
1:A:274:THR:CG2	1:A:276:ILE:HG22	2.22	0.69
1:A:185:GLN:HA	1:A:185:GLN:NE2	2.08	0.68
1:A:126:ARG:O	1:A:129:GLN:NE2	2.26	0.68
1:A:354:ILE:HG22	1:A:355:PHE:N	2.09	0.68
1:A:246:LEU:HA	1:A:249:MET:HG3	1.76	0.68
1:A:314:LYS:O	1:A:317:GLU:HB3	1.94	0.67
1:A:40:ARG:NH1	1:A:40:ARG:HG3	1.95	0.67
1:A:173:LEU:O	1:A:177:THR:HG23	1.94	0.67
1:A:302:ASP:HB3	4:A:435:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ASN:O	1:A:306:ARG:HB2	1.96	0.66
1:A:358:LEU:HD12	1:A:362:ILE:HD13	1.77	0.66
1:A:303:ASN:OD1	1:A:303:ASN:N	2.27	0.66
1:A:90:GLN:HG3	4:A:488:HOH:O	1.95	0.66
1:A:35:PHE:HB3	1:A:36:PRO:HD3	1.78	0.66
1:A:49:HIS:CG	1:A:50:PRO:HD2	2.31	0.66
1:A:295:GLU:OE1	1:A:295:GLU:N	2.29	0.66
1:A:330:GLN:O	1:A:333:GLU:HG2	1.96	0.66
1:A:178:ALA:O	1:A:182:GLU:HG3	1.97	0.65
1:A:228:MET:HE2	1:A:239:HIS:CE1	2.32	0.64
1:A:276:ILE:CD1	1:A:315:VAL:HG11	2.26	0.64
1:A:164:ARG:HE	1:A:164:ARG:HA	1.62	0.64
1:A:297:ARG:O	1:A:301:GLU:HB2	1.97	0.64
1:A:276:ILE:HD13	1:A:276:ILE:O	1.97	0.64
1:A:176:GLN:O	1:A:180:GLN:HG3	1.97	0.64
1:A:293:THR:O	1:A:295:GLU:N	2.31	0.63
1:A:92:ASP:O	1:A:96:LEU:HG	1.99	0.63
1:A:251:GLU:O	1:A:255:ILE:HD13	1.99	0.63
1:A:46:GLY:CA	1:A:56:VAL:HG11	2.28	0.63
1:A:276:ILE:HG21	1:A:316:LYS:HE2	1.81	0.62
1:A:282:SER:HB3	1:A:285:VAL:HG23	1.81	0.62
1:A:357:GLY:O	1:A:361:LYS:HG2	2.00	0.61
1:A:124:LEU:HD13	1:A:134:LYS:CE	2.31	0.61
1:A:276:ILE:C	1:A:276:ILE:HD13	2.21	0.61
1:A:278:ASP:O	1:A:280:LYS:N	2.34	0.61
1:A:284:LEU:CD2	1:A:324:MET:HG3	2.30	0.61
1:A:163:GLN:HB3	4:A:423:HOH:O	2.01	0.60
1:A:366:GLN:O	1:A:367:LYS:HB2	2.02	0.60
1:A:92:ASP:OD1	1:A:92:ASP:N	2.31	0.60
1:A:22:VAL:O	1:A:26:ARG:HD2	2.01	0.60
1:A:34:PHE:O	1:A:37:GLN:HB3	2.03	0.59
1:A:126:ARG:HG3	1:A:127:ARG:CG	2.33	0.59
1:A:124:LEU:HD13	1:A:134:LYS:HE2	1.85	0.58
1:A:278:ASP:O	1:A:280:LYS:HB2	2.03	0.58
1:A:282:SER:O	1:A:286:VAL:HG23	2.03	0.58
1:A:59:LEU:HD22	1:A:63:LEU:CD2	2.20	0.58
1:A:226:ALA:O	1:A:230:MET:HG3	2.04	0.58
1:A:66:ASN:HD21	1:A:132:TRP:HB2	1.69	0.58
1:A:154:TYR:CZ	1:A:175:LEU:HD13	2.39	0.57
1:A:25:GLU:OE2	1:A:28:ARG:NH1	2.35	0.57
1:A:37:GLN:O	1:A:40:ARG:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:O	1:A:72:CYS:HB2	2.05	0.56
1:A:354:ILE:HG22	1:A:355:PHE:CG	2.40	0.56
1:A:306:ARG:HG2	4:A:475:HOH:O	2.06	0.56
1:A:49:HIS:CE1	1:A:50:PRO:HD2	2.39	0.56
1:A:274:THR:HG23	1:A:276:ILE:H	1.71	0.56
1:A:265:ASP:HB3	1:A:266:PRO:HD3	1.88	0.56
1:A:162:ARG:HG2	1:A:167:TYR:CZ	2.41	0.56
1:A:25:GLU:O	1:A:29:GLU:N	2.34	0.56
1:A:144:ASN:O	1:A:148:LEU:HD12	2.05	0.56
1:A:358:LEU:CD1	1:A:362:ILE:HD13	2.36	0.55
1:A:263:PHE:CD1	1:A:263:PHE:N	2.74	0.55
1:A:293:THR:O	1:A:296:GLN:N	2.40	0.55
1:A:191:THR:OG1	1:A:206:ARG:HD2	2.06	0.55
1:A:366:GLN:O	1:A:367:LYS:HE2	2.07	0.55
1:A:194:VAL:HG23	1:A:194:VAL:O	2.07	0.55
1:A:365:ARG:NH1	1:A:367:LYS:H	2.04	0.55
1:A:277:GLN:C	1:A:277:GLN:CD	2.66	0.55
1:A:214:LYS:HG2	1:A:215:THR:HG23	1.90	0.54
1:A:283:TRP:O	1:A:287:GLN:HG2	2.07	0.54
1:A:190:ILE:HG22	1:A:191:THR:N	2.21	0.54
1:A:280:LYS:NZ	3:A:401:GPP:O3B	2.33	0.54
1:A:25:GLU:HA	1:A:28:ARG:CB	2.36	0.54
1:A:155:ARG:NH1	4:A:409:HOH:O	2.31	0.54
1:A:318:LEU:O	1:A:322:VAL:HG23	2.08	0.54
1:A:177:THR:HA	1:A:180:GLN:HE21	1.73	0.54
1:A:265:ASP:HA	1:A:268:LEU:HG	1.90	0.53
1:A:350:LEU:HD12	4:A:506:HOH:O	2.07	0.53
1:A:43:THR:O	1:A:47:ILE:HG12	2.07	0.53
1:A:59:LEU:O	1:A:59:LEU:HD22	2.09	0.53
1:A:296:GLN:HB3	1:A:318:LEU:HD21	1.90	0.53
1:A:47:ILE:N	1:A:56:VAL:HG21	2.23	0.53
1:A:243:LYS:O	1:A:247:LEU:HG	2.09	0.53
1:A:297:ARG:HG3	1:A:297:ARG:O	2.08	0.53
1:A:276:ILE:CG1	1:A:316:LYS:HZ3	2.19	0.53
1:A:316:LYS:CD	1:A:316:LYS:N	2.68	0.53
1:A:241:ASN:HB3	1:A:346:HIS:O	2.10	0.52
1:A:303:ASN:HB3	1:A:311:LYS:HD2	1.92	0.52
1:A:255:ILE:CD1	1:A:255:ILE:N	2.73	0.52
1:A:294:PRO:HG2	1:A:295:GLU:OE1	2.10	0.52
1:A:25:GLU:HA	1:A:28:ARG:HB3	1.92	0.52
1:A:285:VAL:HG22	4:A:431:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:TYR:CD1	1:A:213:TYR:N	2.75	0.51
1:A:358:LEU:HD12	1:A:358:LEU:C	2.29	0.51
1:A:35:PHE:CZ	1:A:67:ALA:HB3	2.45	0.51
1:A:206:ARG:O	1:A:210:ILE:HG13	2.11	0.51
1:A:289:LEU:O	1:A:291:ARG:N	2.44	0.51
1:A:122:GLN:HA	1:A:133:TYR:OH	2.10	0.51
1:A:298:GLN:OE1	1:A:298:GLN:HA	2.11	0.51
1:A:158:LYS:HB2	4:A:422:HOH:O	2.10	0.51
1:A:52:VAL:O	1:A:55:ALA:N	2.44	0.51
1:A:276:ILE:HG21	1:A:316:LYS:CE	2.41	0.51
1:A:20:SER:C	1:A:22:VAL:H	2.14	0.51
1:A:343:ILE:HG22	1:A:352:LYS:HG2	1.93	0.51
1:A:284:LEU:HD22	1:A:324:MET:CG	2.40	0.51
1:A:35:PHE:HB3	1:A:36:PRO:CD	2.41	0.50
1:A:236:LYS:HG2	1:A:240:GLU:OE2	2.12	0.50
1:A:36:PRO:CB	1:A:40:ARG:HH12	2.24	0.50
1:A:102:VAL:O	1:A:105:CYS:HB2	2.11	0.50
1:A:47:ILE:N	1:A:56:VAL:CG2	2.75	0.50
1:A:71:LYS:HB3	1:A:73:ASN:OD1	2.12	0.49
1:A:126:ARG:O	1:A:127:ARG:C	2.51	0.49
1:A:23:VAL:CG1	1:A:24:VAL:N	2.75	0.49
1:A:291:ARG:O	1:A:291:ARG:HG2	2.13	0.49
1:A:43:THR:HG21	1:A:60:LYS:HB2	1.95	0.49
1:A:22:VAL:HG12	1:A:26:ARG:HD2	1.94	0.49
1:A:276:ILE:CG1	1:A:315:VAL:HG11	2.43	0.49
1:A:292:VAL:HG13	1:A:297:ARG:HB2	1.91	0.48
1:A:268:LEU:HD22	1:A:268:LEU:HA	1.58	0.48
1:A:121:ASP:O	1:A:122:GLN:HB2	2.12	0.48
1:A:277:GLN:HE21	1:A:307:LYS:HD2	1.75	0.48
1:A:182:GLU:HG2	3:A:401:GPP:C10	2.44	0.48
1:A:214:LYS:HD2	3:A:401:GPP:C2	2.43	0.48
1:A:266:PRO:O	1:A:267:ALA:HB3	2.14	0.48
1:A:57:ALA:O	1:A:60:LYS:HB3	2.13	0.48
1:A:274:THR:HG23	1:A:275:ASP:N	2.29	0.47
1:A:276:ILE:CG1	1:A:316:LYS:HE2	2.31	0.47
1:A:49:HIS:HA	1:A:50:PRO:HD3	1.68	0.47
1:A:124:LEU:O	1:A:130:LEU:HD12	2.14	0.47
1:A:84:GLU:OE2	1:A:353:GLU:HB2	2.15	0.47
1:A:312:VAL:O	1:A:316:LYS:HD2	2.15	0.47
1:A:268:LEU:CD2	1:A:366:GLN:HE22	2.27	0.47
1:A:263:PHE:CE1	1:A:284:LEU:HD13	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:O	1:A:143:ILE:HD12	2.14	0.47
1:A:185:GLN:HE21	1:A:185:GLN:CA	2.05	0.47
1:A:306:ARG:CZ	1:A:307:LYS:H	2.27	0.47
1:A:262:CYS:SG	1:A:263:PHE:CE1	3.08	0.47
1:A:289:LEU:HA	1:A:289:LEU:HD23	1.44	0.47
1:A:293:THR:OG1	1:A:296:GLN:OE1	2.28	0.47
1:A:36:PRO:HB2	1:A:40:ARG:HH12	1.80	0.47
1:A:252:TYR:CD1	1:A:252:TYR:C	2.89	0.47
1:A:135:LYS:HE3	1:A:135:LYS:HB3	1.42	0.47
1:A:312:VAL:HG12	1:A:313:ALA:N	2.30	0.46
1:A:201:HIS:O	1:A:203:SER:N	2.49	0.46
1:A:295:GLU:H	1:A:295:GLU:CD	2.17	0.46
1:A:269:THR:HG23	1:A:269:THR:O	2.16	0.46
1:A:180:GLN:NE2	4:A:496:HOH:O	2.46	0.46
1:A:35:PHE:CE2	1:A:68:PRO:HG3	2.50	0.46
1:A:24:VAL:O	1:A:28:ARG:N	2.39	0.46
1:A:328:PHE:O	1:A:331:TYR:N	2.48	0.46
1:A:315:VAL:HG12	1:A:316:LYS:NZ	2.31	0.46
1:A:365:ARG:CZ	1:A:367:LYS:H	2.28	0.46
1:A:276:ILE:C	1:A:276:ILE:CD1	2.84	0.46
1:A:24:VAL:O	1:A:27:GLU:HB2	2.16	0.46
1:A:293:THR:C	1:A:295:GLU:N	2.67	0.45
1:A:277:GLN:OE1	1:A:278:ASP:N	2.49	0.45
1:A:136:GLU:HA	4:A:466:HOH:O	2.14	0.45
1:A:59:LEU:O	1:A:63:LEU:HB2	2.16	0.45
1:A:256:GLN:HB3	4:A:499:HOH:O	2.16	0.45
1:A:96:LEU:HA	1:A:96:LEU:HD22	1.79	0.45
1:A:354:ILE:HG22	1:A:355:PHE:CD1	2.51	0.45
1:A:228:MET:CE	1:A:239:HIS:CE1	2.99	0.45
1:A:294:PRO:HA	1:A:297:ARG:HB3	1.99	0.45
1:A:46:GLY:O	1:A:53:GLY:HA2	2.17	0.45
1:A:360:GLN:HG3	1:A:360:GLN:O	2.17	0.45
1:A:182:GLU:HA	3:A:401:GPP:H102	1.98	0.45
1:A:212:LYS:HB3	1:A:213:TYR:CD1	2.51	0.45
1:A:215:THR:HA	1:A:218:TYR:CE1	2.52	0.45
1:A:365:ARG:CG	1:A:366:GLN:N	2.76	0.45
1:A:25:GLU:HA	1:A:28:ARG:HB2	1.98	0.45
1:A:127:ARG:HB2	1:A:129:GLN:NE2	2.32	0.45
1:A:155:ARG:NH1	1:A:155:ARG:HG2	2.32	0.45
1:A:31:PHE:CE2	1:A:104:TRP:CE2	3.04	0.45
1:A:342:LEU:O	1:A:346:HIS:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ALA:HB1	1:A:120:MET:CE	2.47	0.44
1:A:215:THR:HA	1:A:218:TYR:CD1	2.53	0.44
1:A:335:SER:N	1:A:338:ARG:HH21	2.15	0.44
1:A:58:ARG:NH1	1:A:145:ASP:OD2	2.50	0.44
1:A:274:THR:CG2	1:A:275:ASP:N	2.80	0.44
1:A:49:HIS:HE1	1:A:51:GLU:HB2	1.77	0.44
1:A:195:SER:O	1:A:196:LYS:HG2	2.18	0.44
1:A:287:GLN:CB	1:A:324:MET:CE	2.91	0.44
1:A:308:GLU:OE1	1:A:311:LYS:HE2	2.17	0.44
1:A:333:GLU:CG	1:A:334:SER:N	2.81	0.44
1:A:47:ILE:HA	1:A:56:VAL:HG22	1.99	0.44
1:A:351:PRO:O	1:A:354:ILE:HB	2.18	0.44
1:A:124:LEU:HD13	1:A:134:LYS:HE3	1.98	0.44
1:A:296:GLN:O	1:A:298:GLN:N	2.51	0.43
1:A:234:ASP:HB3	4:A:498:HOH:O	2.18	0.43
1:A:268:LEU:O	1:A:270:GLY:N	2.51	0.43
1:A:287:GLN:CB	1:A:324:MET:HE1	2.48	0.43
1:A:206:ARG:HE	1:A:206:ARG:HA	1.82	0.43
1:A:276:ILE:HD11	1:A:315:VAL:HG21	1.98	0.43
1:A:245:ILE:HD12	1:A:245:ILE:HG21	1.79	0.43
1:A:25:GLU:O	1:A:29:GLU:HG3	2.18	0.43
1:A:119:ILE:HD11	1:A:142:ALA:HB3	1.99	0.43
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.66	0.43
1:A:180:GLN:O	1:A:213:TYR:HB3	2.19	0.43
1:A:85:LEU:HB3	1:A:231:VAL:HG21	2.01	0.43
1:A:287:GLN:HB2	1:A:324:MET:HE1	1.99	0.42
1:A:221:TYR:HA	1:A:246:LEU:HD13	2.01	0.42
1:A:189:LEU:CD1	1:A:189:LEU:N	2.76	0.42
1:A:299:LEU:HD23	1:A:303:ASN:HD21	1.83	0.42
1:A:49:HIS:CG	1:A:50:PRO:CD	3.01	0.42
1:A:318:LEU:O	1:A:322:VAL:N	2.44	0.42
1:A:185:GLN:HG3	1:A:189:LEU:HD22	2.01	0.42
1:A:140:LEU:HA	1:A:140:LEU:HD12	1.31	0.42
1:A:303:ASN:HB3	1:A:311:LYS:CD	2.49	0.42
1:A:356:LEU:O	1:A:360:GLN:N	2.35	0.42
1:A:245:ILE:HD11	1:A:355:PHE:CD1	2.54	0.42
1:A:38:ILE:HG22	1:A:42:LEU:HD12	2.01	0.42
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.42	0.42
1:A:221:TYR:CE1	1:A:225:ALA:HB2	2.54	0.42
1:A:23:VAL:HG12	1:A:24:VAL:N	2.34	0.42
1:A:312:VAL:O	1:A:315:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:THR:C	1:A:295:GLU:H	2.24	0.41
1:A:296:GLN:C	1:A:298:GLN:H	2.22	0.41
1:A:311:LYS:O	1:A:314:LYS:HB3	2.20	0.41
1:A:245:ILE:HD11	1:A:355:PHE:CG	2.56	0.41
1:A:243:LYS:HE2	1:A:243:LYS:HB2	1.82	0.41
1:A:182:GLU:O	1:A:185:GLN:HB3	2.19	0.41
1:A:277:GLN:O	1:A:277:GLN:NE2	2.53	0.41
1:A:24:VAL:O	1:A:28:ARG:HB2	2.20	0.41
1:A:110:GLN:O	1:A:113:SER:HB2	2.20	0.41
1:A:296:GLN:C	1:A:298:GLN:N	2.73	0.41
1:A:149:LEU:O	1:A:152:SER:HB2	2.21	0.41
1:A:329:GLN:O	1:A:333:GLU:HB3	2.21	0.41
1:A:155:ARG:CG	4:A:493:HOH:O	2.68	0.41
1:A:40:ARG:HG2	1:A:44:GLU:OE1	2.21	0.41
1:A:277:GLN:OE1	1:A:278:ASP:HB2	2.21	0.41
1:A:275:ASP:OD1	1:A:278:ASP:CB	2.66	0.41
1:A:285:VAL:HG23	1:A:285:VAL:H	1.57	0.41
1:A:288:CYS:O	1:A:289:LEU:O	2.39	0.41
1:A:191:THR:C	1:A:193:PRO:HD3	2.41	0.41
1:A:203:SER:OG	1:A:206:ARG:HB3	2.21	0.40
1:A:252:TYR:HE2	1:A:332:GLU:HA	1.86	0.40
1:A:255:ILE:O	1:A:258:ASP:HB2	2.21	0.40
1:A:126:ARG:HG3	1:A:127:ARG:N	2.35	0.40
1:A:38:ILE:HA	1:A:41:ASP:OD2	2.20	0.40
1:A:189:LEU:N	1:A:189:LEU:HD13	2.35	0.40
1:A:110:GLN:O	1:A:114:LEU:HG	2.21	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%)	285 (82%)	48 (14%)	13 (4%)	4 5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	A	198	ASP
1	A	269	THR
1	A	289	LEU
1	A	290	GLN
1	A	196	LYS
1	A	265	ASP
1	A	128	GLY
1	A	266	PRO
1	A	263	PHE
1	A	279	ASN
1	A	294	PRO
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%)	229 (77%)	69 (23%)	1 1

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	26	ARG
1	A	38	ILE
1	A	40	ARG
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	72	CYS
1	A	83	ARG
1	A	125	THR
1	A	126	ARG
1	A	127	ARG
1	A	129	GLN
1	A	135	LYS
1	A	140	LEU
1	A	155	ARG
1	A	162	ARG
1	A	164	ARG
1	A	171	LEU
1	A	175	LEU
1	A	181	THR
1	A	185	GLN
1	A	189	LEU
1	A	195	SER
1	A	196	LYS
1	A	198	ASP
1	A	205	GLU
1	A	206	ARG
1	A	214	LYS
1	A	218	TYR
1	A	219	SER
1	A	233	ILE
1	A	235	SER
1	A	238	GLU
1	A	245	ILE
1	A	249	MET
1	A	255	ILE
1	A	266	PRO
1	A	268	LEU
1	A	274	THR
1	A	275	ASP
1	A	276	ILE
1	A	277	GLN
1	A	292	VAL
1	A	298	GLN
1	A	299	LEU
1	A	300	LEU
1	A	303	ASN
1	A	307	LYS

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Mol	Chain	Res	Type
1	A	314	LYS
1	A	316	LYS
1	A	318	LEU
1	A	320	GLU
1	A	322	VAL
1	A	324	MET
1	A	333	GLU
1	A	337	ARG
1	A	338	ARG
1	A	349	ARG
1	A	350	LEU
1	A	353	GLU
1	A	354	ILE
1	A	356	LEU
1	A	358	LEU
1	A	360	GLN
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	66	ASN
1	A	129	GLN
1	A	180	GLN
1	A	185	GLN
1	A	329	GLN
1	A	360	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 carbohydrates 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	GPP	A	401	2	16,18,18	1.54	2 (12%)	21,25,25	2.87	11 (52%)

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	GPP	A	401	2	-	0/19/19/19	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	GPP	PB-O1B	3.13	1.61	1.51
3	A	401	GPP	PA-O1A	3.83	1.65	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	GPP	O3B-PB-O1B	-4.97	94.57	110.58
3	A	401	GPP	O2B-PB-O1B	-3.79	98.38	110.58
3	A	401	GPP	C4-C3-C2	-3.70	116.24	123.50
3	A	401	GPP	O2B-PB-O3A	-3.40	89.69	105.09
3	A	401	GPP	PA-O3A-PB	-2.79	123.31	132.67
3	A	401	GPP	C6-C7-C8	-2.52	118.04	127.73
3	A	401	GPP	C9-C8-C7	-2.32	115.13	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	GPP	C10-C8-C7	-2.26	115.34	122.61
3	A	401	GPP	C6-C5-C3	3.59	124.40	112.71
3	A	401	GPP	C4-C3-C5	5.23	123.40	115.41
3	A	401	GPP	C10-C8-C9	6.06	129.53	114.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GPP	4	0

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 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.