



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:48 PM GMT

PDB ID : 2E8X
Title : S. cerevisiae geranylgeranyl pyrophosphate synthase in complex with magnesium and GPP
Authors : Guo, R.T.; Ko, T.P.; Chen, C.K.-M.; Jeng, W.Y.; Chang, T.H.; Liang, P.H.; Oldfield, E.; Wang, A.H.-J.
Deposited on : 2007-01-24
Resolution : 2.04 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

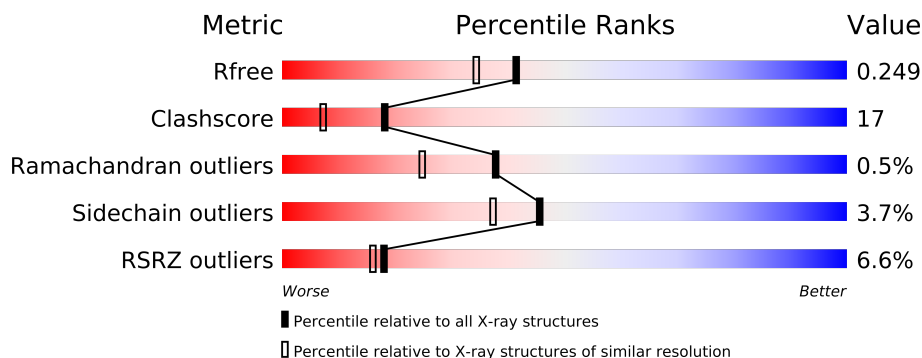
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.04 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))
R_{free}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	340	
1	B	340	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	1302	-	X
3	GPP	B	1002	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5401 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Geranylgeranyl pyrophosphate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2417	1552	409	446	10			
1	B	317	Total	C	N	O	S	0	0	0
			2592	1665	437	480	10			

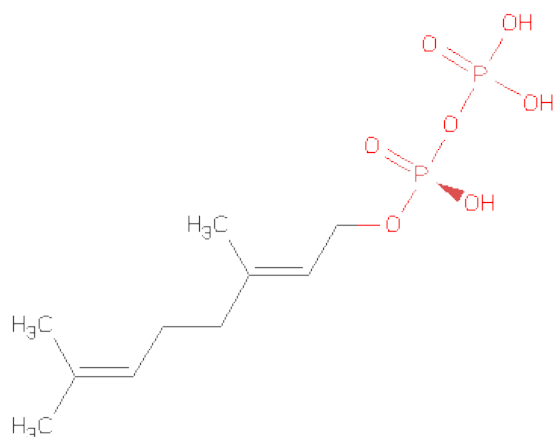
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q12051
A	2	THR	-	CLONING ARTIFACT	UNP Q12051
A	3	LYS	-	CLONING ARTIFACT	UNP Q12051
A	4	ASN	-	CLONING ARTIFACT	UNP Q12051
A	5	LYS	-	CLONING ARTIFACT	UNP Q12051
B	1	MET	-	CLONING ARTIFACT	UNP Q12051
B	2	THR	-	CLONING ARTIFACT	UNP Q12051
B	3	LYS	-	CLONING ARTIFACT	UNP Q12051
B	4	ASN	-	CLONING ARTIFACT	UNP Q12051
B	5	LYS	-	CLONING ARTIFACT	UNP Q12051

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is GERANYL DIPHOSPHATE (three-letter code: GPP) (formula: C₁₀H₂₀O₇P₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	157	Total	O	0	0
			157	157		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.09Å 116.60Å 128.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.40 – 2.04 28.43 – 2.04	Depositor EDS
% Data completeness (in resolution range)	94.6 (28.40-2.04) 94.5 (28.43-2.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.04Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.249 0.204 , 0.249	Depositor DCC
R_{free} test set	2170 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43423 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5401	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.80	1/2459 (0.0%)	0.83	2/3326 (0.1%)
1	B	0.75	0/2639	0.78	1/3570 (0.0%)
All	All	0.77	1/5098 (0.0%)	0.81	3/6896 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	MET	SD-CE	-5.50	1.47	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	LEU	CA-CB-CG	-7.43	98.22	115.30
1	A	269	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	269	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2417	0	2476	88	0
1	B	2592	0	2637	97	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	19	0	17	3	0
3	B	19	0	17	2	0
4	A	193	0	0	8	1
4	B	157	0	0	5	1
All	All	5401	0	5147	173	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (173) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:THR:H	1:A:166:MET:HE3	1.04	1.14
1:A:251:LYS:HG2	4:A:732:HOH:O	1.57	1.04
1:A:258:GLN:HE21	1:A:258:GLN:H	0.97	0.95
1:A:223:GLN:HE21	1:A:281:GLN:HE22	1.08	0.93
1:A:38:LYS:HE2	1:A:89:ARG:HB3	1.52	0.90
1:A:163:THR:N	1:A:166:MET:HE3	1.88	0.87
1:A:225:SER:HB3	1:A:228:LYS:HB2	1.56	0.86
1:A:225:SER:HG	1:A:228:LYS:N	1.77	0.82
1:A:258:GLN:N	1:A:258:GLN:HE21	1.78	0.81
1:A:163:THR:H	1:A:166:MET:CE	1.91	0.80
1:B:258:GLN:HG2	1:B:286:ASP:OD2	1.83	0.78
1:A:223:GLN:HE21	1:A:281:GLN:NE2	1.81	0.77
1:A:38:LYS:HD3	1:A:89:ARG:HG3	1.66	0.77
1:B:52:ASN:HD21	1:B:57:LEU:H	1.32	0.76
1:A:52:ASN:HD21	1:A:57:LEU:H	1.32	0.76
1:A:38:LYS:HE2	1:A:89:ARG:CB	2.19	0.72
1:B:52:ASN:ND2	1:B:57:LEU:H	1.88	0.72
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.36	0.72
1:A:163:THR:HG23	1:A:166:MET:CE	2.21	0.71
1:B:55:MET:CE	1:B:187:GLU:HA	2.23	0.69
1:A:38:LYS:HE3	1:A:89:ARG:O	1.93	0.68
1:B:128:LEU:O	1:B:132:LEU:HG	1.94	0.68
1:A:293:THR:O	1:A:297:ILE:HG13	1.93	0.68
1:A:140:LEU:O	1:A:144:HIS:HD2	1.77	0.68
1:B:55:MET:HE2	1:B:187:GLU:HA	1.75	0.68
1:A:38:LYS:CE	1:A:89:ARG:O	2.42	0.68
1:A:225:SER:HB3	1:A:228:LYS:CB	2.25	0.67
1:B:260:ASN:O	1:B:264:ARG:HG3	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:329:GLU:N	4:B:462:HOH:O	2.28	0.66
1:B:96:HIS:HD2	4:B:686:HOH:O	1.77	0.66
1:A:30:LYS:HB2	1:A:31:PRO:HD3	1.77	0.66
1:A:223:GLN:NE2	1:A:281:GLN:HE22	1.89	0.66
1:A:123:THR:HG21	1:A:128:LEU:HD23	1.77	0.66
1:A:163:THR:HG23	1:A:166:MET:HE2	1.77	0.66
1:B:330:LEU:HD12	1:B:330:LEU:N	2.10	0.65
1:A:159:GLU:OE2	4:A:691:HOH:O	2.15	0.65
1:A:44:ARG:O	1:A:48:ILE:HG13	1.96	0.65
1:B:143:LEU:HD11	3:B:1002:GPP:H52	1.78	0.64
1:B:336:HIS:O	1:B:339:GLU:HG2	1.98	0.64
1:A:240:SER:OG	1:A:242:PRO:HD2	1.98	0.62
1:B:38:LYS:HG3	1:B:90:ARG:HG2	1.82	0.61
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.65	0.60
1:B:330:LEU:HD12	1:B:330:LEU:H	1.67	0.60
4:A:683:HOH:O	1:B:144:HIS:HE1	1.85	0.60
1:A:198:SER:N	4:A:719:HOH:O	2.34	0.60
1:B:50:GLN:CD	1:B:329:GLU:HG2	2.22	0.60
1:B:213:ARG:HD3	4:B:703:HOH:O	2.01	0.60
1:A:281:GLN:HA	1:A:281:GLN:NE2	2.17	0.59
1:A:258:GLN:NE2	1:A:258:GLN:H	1.83	0.58
1:A:52:ASN:ND2	1:A:57:LEU:H	2.01	0.58
1:A:139:GLU:HB2	1:A:181:LEU:HD22	1.84	0.58
1:A:281:GLN:HE21	1:A:281:GLN:HA	1.67	0.58
1:A:38:LYS:HB3	1:A:90:ARG:HG3	1.86	0.58
1:A:224:MET:HE2	1:A:228:LYS:NZ	2.20	0.57
1:B:47:LEU:HD13	1:B:333:ILE:HD13	1.86	0.57
1:B:273:LYS:HE3	1:B:277:LEU:HD11	1.86	0.57
1:A:56:ASN:HD22	1:A:192:SER:HB2	1.71	0.56
1:A:96:HIS:HE1	4:A:675:HOH:O	1.88	0.56
1:B:58:PRO:HG2	1:B:61:GLN:HB2	1.87	0.55
1:A:180:ARG:HH11	1:A:204:ASN:ND2	2.02	0.55
1:A:139:GLU:HB2	1:A:181:LEU:CD2	2.36	0.55
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.54	0.54
1:A:157:LEU:HD12	1:A:158:PRO:HA	1.90	0.54
1:A:20:TRP:CH2	1:A:24:ASN:HB3	2.43	0.54
1:A:246:ALA:HB2	1:A:283:LEU:HD22	1.90	0.53
1:A:145:ARG:HB3	1:B:20:TRP:CZ3	2.42	0.53
1:B:337:LEU:HD12	1:B:340:LEU:HD11	1.91	0.53
1:A:225:SER:OG	1:A:228:LYS:N	2.40	0.53
1:B:331:LEU:C	1:B:331:LEU:HD23	2.29	0.53
1:A:44:ARG:HG3	1:A:44:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:52:ASN:HD21	1:B:57:LEU:N	2.03	0.52
1:B:241:PHE:HB3	1:B:242:PRO:HD3	1.92	0.51
1:B:304:ILE:HG21	1:B:334:ILE:CD1	2.40	0.51
1:B:116:MET:O	1:B:119:VAL:HB	2.11	0.51
1:B:273:LYS:O	1:B:277:LEU:HG	2.10	0.51
1:B:38:LYS:HG3	1:B:90:ARG:CG	2.41	0.51
1:B:143:LEU:HD11	3:B:1002:GPP:C5	2.41	0.51
1:B:21:SER:H	1:B:24:ASN:HD22	1.59	0.51
1:A:35:ILE:HG13	1:A:38:LYS:HD2	1.91	0.51
1:A:273:LYS:HG2	4:A:639:HOH:O	2.11	0.51
1:A:52:ASN:HD21	1:A:57:LEU:N	2.07	0.50
1:A:224:MET:CE	1:A:228:LYS:NZ	2.74	0.50
1:A:225:SER:CB	1:A:228:LYS:HG3	2.41	0.50
1:B:54:VAL:HG12	1:B:195:HIS:HB2	1.94	0.50
1:B:48:ILE:HG22	1:B:62:LEU:HD11	1.92	0.50
1:A:117:GLN:N	1:B:137:ASN:HD21	2.09	0.50
1:B:32:TYR:O	1:B:35:ILE:HG22	2.10	0.50
1:A:303:MET:HG2	1:B:7:GLU:OE1	2.12	0.49
1:B:244:VAL:O	1:B:248:ASN:ND2	2.45	0.49
1:B:278:LYS:O	1:B:281:GLN:HG2	2.12	0.49
1:A:85:ASN:ND2	4:A:675:HOH:O	2.46	0.49
1:B:119:VAL:HG11	1:B:133:ILE:HD13	1.93	0.48
1:A:11:ASP:OD1	1:B:311:LYS:NZ	2.46	0.48
1:A:52:ASN:HD22	1:A:55:MET:HB2	1.79	0.48
1:A:224:MET:CE	1:A:228:LYS:HZ2	2.27	0.48
1:B:304:ILE:HG21	1:B:334:ILE:HD11	1.96	0.48
1:A:200:VAL:HB	1:A:201:PRO:HD3	1.95	0.48
1:B:243:ILE:HG21	1:B:266:LEU:HD11	1.96	0.47
1:A:225:SER:HB3	1:A:228:LYS:CG	2.45	0.47
1:A:302:ASN:HB3	1:A:306:ASN:ND2	2.29	0.47
4:A:683:HOH:O	1:B:144:HIS:CE1	2.64	0.47
1:B:120:SER:HA	1:B:129:TYR:CE1	2.50	0.47
1:B:55:MET:HE1	1:B:187:GLU:HA	1.96	0.46
1:B:21:SER:HB2	1:B:23:GLN:OE1	2.14	0.46
1:A:6:MET:HE1	1:B:299:GLN:CB	2.45	0.46
1:B:203:ILE:HA	1:B:203:ILE:HD12	1.73	0.46
1:B:50:GLN:HG3	1:B:329:GLU:HG2	1.98	0.46
1:B:35:ILE:O	1:B:38:LYS:HB3	2.16	0.46
1:A:6:MET:HE1	1:B:299:GLN:HB2	1.97	0.46
1:B:55:MET:O	1:B:191:PRO:HD2	2.15	0.46
1:A:302:ASN:O	1:A:306:ASN:HB2	2.16	0.46
1:A:203:ILE:HA	1:A:203:ILE:HD12	1.76	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:130:HIS:HD2	1:B:129:TYR:CD2	2.34	0.45
1:A:224:MET:HE2	1:A:228:LYS:HZ3	1.79	0.45
1:B:282:ILE:O	1:B:286:ASP:HB3	2.15	0.45
1:B:183:LEU:HD22	1:B:203:ILE:HB	1.98	0.45
1:B:330:LEU:CD1	1:B:330:LEU:H	2.28	0.45
1:A:228:LYS:HB3	1:A:228:LYS:HE2	1.75	0.45
1:B:55:MET:CE	1:B:190:SER:HB2	2.47	0.45
1:A:48:ILE:HG22	1:A:62:LEU:HD11	1.99	0.45
1:B:147:GLN:NE2	4:B:707:HOH:O	2.44	0.45
1:B:34:HIS:HE1	1:B:93:THR:O	2.00	0.45
1:A:123:THR:CG2	1:A:128:LEU:HD23	2.44	0.45
1:B:140:LEU:O	1:B:144:HIS:HD2	1.99	0.44
1:B:21:SER:H	1:B:24:ASN:ND2	2.14	0.44
1:B:28:ILE:HD13	1:B:28:ILE:N	2.31	0.44
1:A:38:LYS:CD	1:A:89:ARG:HG3	2.42	0.44
1:A:117:GLN:CA	1:B:137:ASN:HD21	2.31	0.44
1:A:300:LEU:CD2	1:B:10:ILE:HG13	2.48	0.44
1:A:179:PHE:HB3	1:A:203:ILE:HG13	1.98	0.44
1:B:157:LEU:HG	1:B:158:PRO:HA	2.00	0.44
1:B:126:GLU:HB2	1:B:127:PRO:HD3	2.00	0.44
1:B:122:LEU:HD13	1:B:189:LEU:HD11	2.00	0.44
1:B:330:LEU:CD1	1:B:330:LEU:N	2.79	0.43
1:A:130:HIS:CD2	1:B:129:TYR:CD2	3.06	0.43
1:B:79:ILE:HD11	1:B:108:ALA:HB3	2.00	0.43
1:B:258:GLN:O	1:B:262:ILE:HG13	2.17	0.43
1:B:120:SER:HA	1:B:129:TYR:HE1	1.83	0.43
1:B:309:GLU:O	1:B:310:ASN:C	2.57	0.43
1:B:249:PHE:CD2	1:B:287:THR:HG22	2.52	0.43
1:B:222:PHE:CE2	1:B:277:LEU:HD23	2.53	0.43
1:A:105:ILE:HD11	1:B:105:ILE:HD11	2.00	0.43
1:A:38:LYS:HE3	1:A:92:GLN:HB3	2.00	0.43
1:B:50:GLN:CG	1:B:329:GLU:HG2	2.49	0.43
1:B:58:PRO:O	1:B:61:GLN:N	2.51	0.43
1:B:183:LEU:HD21	1:B:199:LEU:C	2.40	0.43
1:B:62:LEU:CD1	1:B:186:MET:HE3	2.48	0.42
3:A:1001:GPP:H62	3:A:1001:GPP:H2	1.74	0.42
1:B:43:PHE:CG	1:B:339:GLU:HG3	2.55	0.42
1:B:224:MET:O	1:B:225:SER:HB2	2.19	0.42
1:A:38:LYS:HE2	1:A:89:ARG:O	2.17	0.42
1:B:204:ASN:HA	1:B:204:ASN:HD22	1.55	0.42
1:B:96:HIS:HE1	4:B:684:HOH:O	2.02	0.42
1:A:300:LEU:HD21	1:B:10:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:222:PHE:HE2	1:B:277:LEU:HD23	1.84	0.42
1:B:58:PRO:O	1:B:60:ASP:N	2.52	0.42
1:B:52:ASN:HA	1:B:52:ASN:HD22	1.61	0.41
1:A:183:LEU:HD21	1:A:199:LEU:HB2	2.01	0.41
1:B:114:ARG:HD2	1:B:114:ARG:HA	1.88	0.41
1:B:147:GLN:HA	1:B:147:GLN:HE21	1.84	0.41
1:A:143:LEU:CD2	3:A:1001:GPP:H93	2.49	0.41
1:A:5:LYS:O	1:A:9:LYS:HG3	2.21	0.41
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.85	0.41
1:A:207:GLY:O	1:A:210:TYR:HB3	2.21	0.41
1:A:143:LEU:HD23	3:A:1001:GPP:H93	2.02	0.41
1:B:55:MET:HE1	1:B:187:GLU:HG2	2.03	0.41
1:B:58:PRO:O	1:B:59:LYS:C	2.59	0.41
1:B:239:LEU:N	1:B:239:LEU:HD22	2.36	0.41
1:A:200:VAL:O	1:A:203:ILE:HG22	2.21	0.40
1:A:281:GLN:HE21	1:A:281:GLN:CA	2.31	0.40
1:B:52:ASN:CG	1:B:57:LEU:H	2.25	0.40
1:A:18:PRO:HG2	1:B:180:ARG:NH2	2.36	0.40
1:A:101:VAL:N	1:A:102:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:530:HOH:O	4:B:633:HOH:O[4_455]	2.19	0.01

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	291/340 (86%)	287 (99%)	4 (1%)	0	100	100
1	B	309/340 (91%)	296 (96%)	10 (3%)	3 (1%)	22	9
All	All	600/680 (88%)	583 (97%)	14 (2%)	3 (0%)	38	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	LYS
1	B	310	ASN
1	B	102	PRO

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	277/317 (87%)	268 (97%)	9 (3%)	51	44
1	B	297/317 (94%)	285 (96%)	12 (4%)	42	33
All	All	574/634 (90%)	553 (96%)	21 (4%)	45	37

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	41	LYS
1	A	76	SER
1	A	123	THR
1	A	141	ILE
1	A	178	LEU
1	A	181	LEU
1	A	258	GLN
1	A	273	LYS
1	B	28	ILE
1	B	52	ASN
1	B	60	ASP
1	B	70	GLU
1	B	90	ARG
1	B	102	PRO
1	B	120	SER
1	B	147	GLN
1	B	181	LEU
1	B	251	LYS
1	B	257	GLU
1	B	281	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	56	ASN
1	A	61	GLN
1	A	85	ASN
1	A	96	HIS
1	A	130	HIS
1	A	144	HIS
1	A	164	GLN
1	A	204	ASN
1	A	258	GLN
1	A	260	ASN
1	A	281	GLN
1	A	298	ASN
1	A	306	ASN
1	B	4	ASN
1	B	24	ASN
1	B	34	HIS
1	B	52	ASN
1	B	96	HIS
1	B	137	ASN
1	B	144	HIS
1	B	147	GLN
1	B	197	HIS
1	B	204	ASN
1	B	281	GLN
1	B	288	ASN
1	B	298	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	1001	2	18,18,18	1.99	6 (33%)	25,25,25	1.26	3 (12%)
3	GPP	B	1002	2	18,18,18	1.95	6 (33%)	25,25,25	1.31	4 (16%)

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	1001	2	-	0/19/19/19	0/0/0/0
3	GPP	B	1002	2	-	0/19/19/19	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	GPP	C6-C7	-3.93	1.39	1.50
3	B	1002	GPP	C6-C7	-3.78	1.39	1.50
3	B	1002	GPP	C2-C3	3.35	1.39	1.32
3	A	1001	GPP	C2-C3	3.15	1.39	1.32
3	A	1001	GPP	PB-O1B	3.07	1.61	1.51
3	B	1002	GPP	PB-O1B	3.02	1.61	1.51
3	B	1002	GPP	C1-C2	-2.86	1.39	1.49
3	A	1001	GPP	PA-O1A	2.83	1.62	1.51
3	A	1001	GPP	C1-C2	-2.72	1.39	1.49
3	B	1002	GPP	PA-O1A	2.60	1.61	1.51
3	A	1001	GPP	C7-C8	2.42	1.40	1.32
3	B	1002	GPP	C7-C8	2.20	1.39	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	GPP	C4-C3-C5	3.14	120.17	115.39
3	A	1001	GPP	C4-C3-C5	2.95	119.88	115.39
3	A	1001	GPP	O3B-PB-O3A	2.46	116.81	105.14
3	B	1002	GPP	PA-O3A-PB	-2.42	124.60	131.68
3	B	1002	GPP	C10-C8-C9	2.21	120.25	114.62
3	A	1001	GPP	PA-O3A-PB	-2.16	125.34	131.68
3	B	1002	GPP	C1-C2-C3	2.01	129.75	126.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/340 (87%)	0.21	21 (7%) 16 14	26, 40, 78, 94	0
1	B	317/340 (93%)	0.32	20 (6%) 19 18	26, 45, 88, 106	0
All	All	614/680 (90%)	0.27	41 (6%) 18 15	26, 43, 84, 106	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	332	TYR	5.1
1	B	196	GLY	4.6
1	A	306	ASN	4.4
1	B	42	ASN	4.4
1	A	191	PRO	4.4
1	A	42	ASN	4.2
1	B	230	PHE	4.2
1	A	40	GLY	4.1
1	A	230	PHE	3.9
1	B	90	ARG	3.7
1	A	39	PRO	3.7
1	A	229	GLY	3.6
1	A	46	ASN	3.5
1	A	224	MET	3.3
1	A	38	LYS	3.2
1	B	39	PRO	3.2
1	A	54	VAL	3.2
1	B	339	GLU	2.9
1	A	90	ARG	2.9
1	B	309	GLU	2.9
1	A	305	LYS	2.8
1	A	53	ARG	2.8
1	B	221	ASP	2.8
1	B	340	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	179	PHE	2.7
1	B	336	HIS	2.6
1	B	225	SER	2.6
1	A	171	VAL	2.6
1	A	41	LYS	2.5
1	A	43	PHE	2.5
1	B	40	GLY	2.5
1	A	307	ASP	2.4
1	B	192	SER	2.3
1	B	4	ASN	2.3
1	B	195	HIS	2.2
1	A	4	ASN	2.2
1	B	308	ASN	2.2
1	B	157	LEU	2.1
1	A	124	THR	2.1
1	B	331	LEU	2.0
1	A	56	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	A	1302	1/1	0.19	4.93	33,33,33,33	0
3	GPP	B	1002	19/19	0.21	2.01	45,54,59,64	0
2	MG	A	1301	1/1	0.19	0.95	30,30,30,30	0
2	MG	B	1303	1/1	0.11	0.87	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GPP	A	1001	19/19	0.14	0.17	39,46,53,54	0
2	MG	B	1304	1/1	0.13	0.14	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.