



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:43 PM UTC

PDB ID : 2E8U / pdb_00002e8u
Title : S. cerevisiae geranylgeranyl pyrophosphate synthase in complex with magnesium and IPP (P21)
Authors : Guo, R.T.; Chen, C.K.-M.; Ko, T.P.; Jeng, W.Y.; Chang, T.H.; Liang, P.H.; Oldfield, E.; Wang, A.H.-J.
Deposited on : 2007-01-23
Resolution : 2.08 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

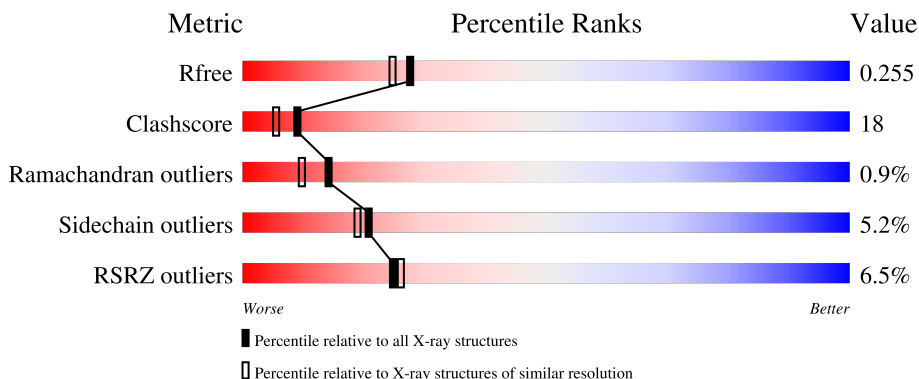
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	340	5% 57% 22% 5% 15%
1	B	340	6% 58% 27% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5284 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 Geranylgeranyl pyrophosphate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2348	1510	395	433	10			
1	B	301	Total	C	N	O	S	0	0	0
			2460	1583	414	455	8			

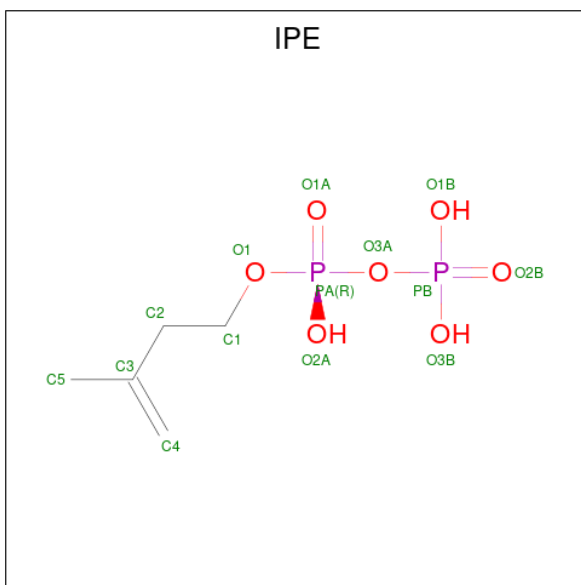
There are 10 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (CCD ID: IPE) (formula: C₅H₁₂O₇P₂).



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

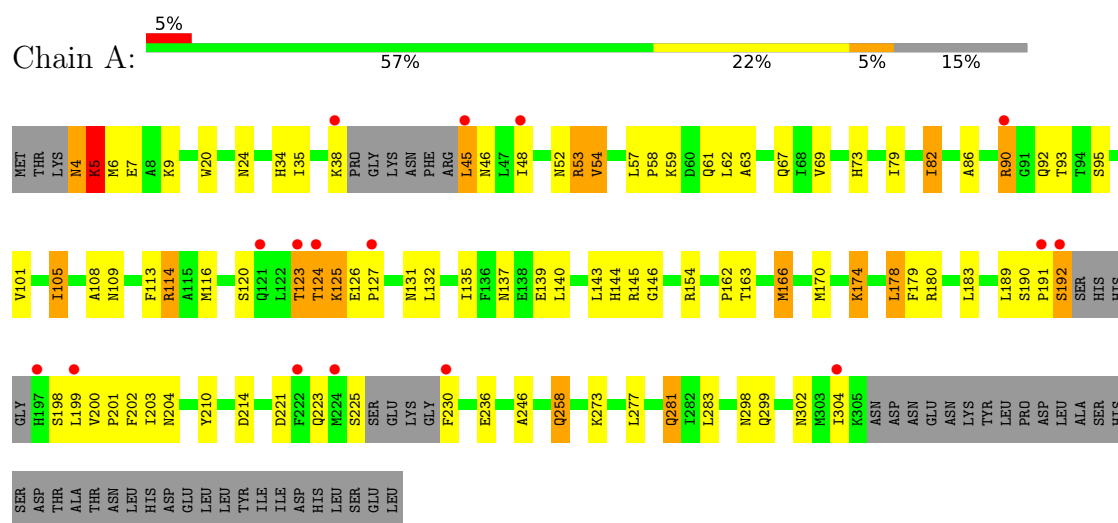
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	217	Total	O	0	0
			217	217		
4	B	199	Total	O	0	0
			199	199		

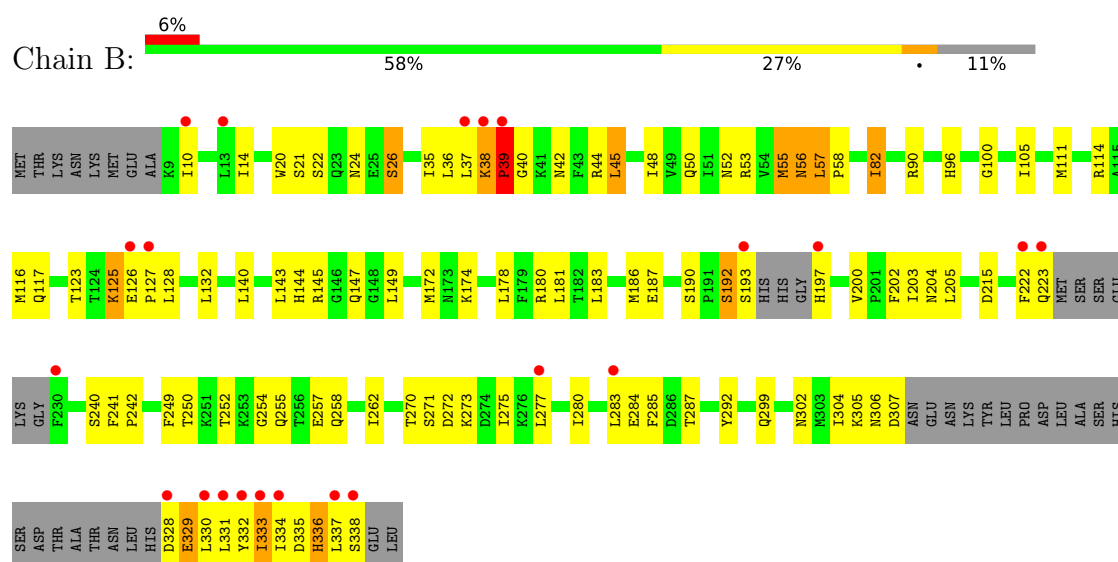
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

• Molecule 1: Geranylgeranyl pyrophosphate synthetase



• Molecule 1: Geranylgeranyl pyrophosphate synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.24Å 47.71Å 91.83Å 90.00° 110.71° 90.00°	Depositor
Resolution (Å)	40.54 – 2.08 40.54 – 2.08	Depositor EDS
% Data completeness (in resolution range)	97.1 (40.54-2.08) 97.1 (40.54-2.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.56 (at 2.08Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.257 0.197 , 0.255	Depositor DCC
R_{free} test set	1972 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.762	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5284	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IPE

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	1.15	3/2388 (0.1%)	1.17	12/3231 (0.4%)
1	B	1.14	6/2504 (0.2%)	1.22	15/3391 (0.4%)
All	All	1.14	9/4892 (0.2%)	1.20	27/6622 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	VAL	CA-CB	14.70	1.62	1.54
1	A	166	MET	SD-CE	-11.06	1.51	1.79
1	B	55	MET	SD-CE	-9.99	1.54	1.79
1	B	186	MET	SD-CE	7.36	1.98	1.79
1	A	170	MET	SD-CE	6.80	1.96	1.79
1	B	111	MET	SD-CE	6.31	1.95	1.79
1	B	35	ILE	CA-CB	5.92	1.62	1.54
1	B	100	GLY	CA-C	5.25	1.57	1.51
1	B	82	ILE	CA-C	5.14	1.59	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	GLY	N-CA-C	-10.43	96.10	110.80
1	A	59	LYS	N-CA-C	8.78	120.46	111.07
1	B	174	LYS	N-CA-C	7.78	119.39	111.07
1	A	174	LYS	N-CA-C	7.41	119.00	111.07
1	B	329	GLU	N-CA-C	-7.22	103.41	111.28
1	A	124	THR	N-CA-C	-7.21	105.40	114.56
1	A	82	ILE	N-CA-C	-6.66	104.27	110.53
1	B	38	LYS	CA-C-N	6.62	128.12	119.84
1	B	38	LYS	C-N-CA	6.62	128.12	119.84
1	A	5	LYS	N-CA-C	-6.41	104.34	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	THR	N-CA-C	6.41	119.05	108.99
1	A	114	ARG	N-CA-C	-6.40	104.39	111.36
1	B	285	PHE	N-CA-C	6.32	120.99	113.28
1	B	287	THR	N-CA-C	-6.13	105.96	113.50
1	A	95	SER	N-CA-C	5.85	117.66	111.28
1	B	114	ARG	N-CA-C	-5.80	104.92	112.23
1	B	270	THR	N-CA-C	5.71	119.23	110.20
1	B	262	ILE	N-CA-C	-5.67	104.98	110.42
1	A	105	ILE	CB-CA-C	-5.58	104.83	111.97
1	A	54	VAL	CB-CA-C	-5.42	105.41	111.80
1	B	257	GLU	N-CA-C	5.41	117.18	111.28
1	A	86	ALA	N-CA-C	5.39	116.44	109.65
1	B	10	ILE	N-CA-C	-5.24	105.60	110.53
1	A	214	ASP	N-CA-C	-5.18	105.53	111.07
1	B	58	PRO	N-CA-C	-5.07	103.32	111.38
1	A	190	SER	N-CA-C	5.06	116.20	109.93
1	B	56	ASN	N-CA-C	5.03	118.38	111.54

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	2348	0	2405	105	0
1	B	2460	0	2508	89	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	28	0	18	5	0
3	B	28	0	18	3	0
4	A	217	0	0	8	0
4	B	199	0	0	4	0
All	All	5284	0	4949	181	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 18.

All (181) 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:163:THR:H	1:A:166:MET:HE3	1.05	1.17
1:A:38:LYS:HD2	1:A:90:ARG:CG	1.84	1.05
1:A:38:LYS:CD	1:A:90:ARG:HG3	1.85	1.05
1:A:223:GLN:HE21	1:A:281:GLN:HE22	1.02	0.98
1:A:258:GLN:HE21	1:A:258:GLN:H	1.18	0.92
1:B:37:LEU:HG	4:B:783:HOH:O	1.70	0.90
1:A:163:THR:N	1:A:166:MET:HE3	1.86	0.90
1:A:125:LYS:HB3	1:A:125:LYS:NZ	1.87	0.89
1:A:163:THR:H	1:A:166:MET:CE	1.84	0.89
1:A:52:ASN:HD21	1:A:57:LEU:H	1.19	0.89
1:B:255:GLN:HB3	1:B:258:GLN:OE1	1.73	0.88
1:B:202:PHE:CE1	1:B:334:ILE:HD11	2.10	0.87
1:A:126:GLU:HB3	1:B:126:GLU:HB3	1.54	0.87
1:B:202:PHE:HE1	1:B:334:ILE:HD11	1.37	0.87
1:B:52:ASN:HD21	1:B:57:LEU:H	1.23	0.86
1:A:5:LYS:HZ3	1:A:5:LYS:HB2	1.45	0.82
1:A:143:LEU:HD11	3:A:1102:IPE:H53	1.63	0.80
1:A:230:PHE:HE1	4:A:645:HOH:O	1.64	0.79
1:B:302:ASN:O	1:B:306:ASN:HB3	1.84	0.77
1:A:73:HIS:HE1	3:A:1101:IPE:O3B	1.66	0.77
1:A:281:GLN:HA	1:A:281:GLN:HE21	1.49	0.77
1:A:223:GLN:NE2	1:A:281:GLN:HE22	1.81	0.77
1:B:56:ASN:ND2	1:B:192:SER:OG	2.17	0.76
1:A:191:PRO:O	1:A:192:SER:HB2	1.87	0.75
1:B:125:LYS:C	1:B:127:PRO:HD2	2.12	0.73
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.35	0.72
1:A:281:GLN:HA	1:A:281:GLN:NE2	2.07	0.70
1:B:180:ARG:HH11	1:B:204:ASN:ND2	1.90	0.69
1:A:163:THR:HG23	1:A:166:MET:HE2	1.73	0.69
1:B:39:PRO:O	1:B:90:ARG:HD3	1.93	0.69
1:B:223:GLN:HE22	1:B:284:GLU:HG3	1.58	0.68
1:A:123:THR:HG22	1:A:124:THR:H	1.58	0.68
1:A:163:THR:HG23	1:A:166:MET:CE	2.22	0.68
1:B:55:MET:HE3	1:B:190:SER:HB2	1.75	0.68
1:A:180:ARG:HH11	1:A:204:ASN:ND2	1.92	0.68
1:A:223:GLN:HE21	1:A:281:GLN:NE2	1.85	0.68
1:A:125:LYS:HB3	1:A:125:LYS:HZ3	1.59	0.67
1:A:126:GLU:HB3	1:B:126:GLU:CB	2.25	0.67
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.43	0.66
1:A:210:TYR:O	4:A:730:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:HD3	4:A:741:HOH:O	1.95	0.66
1:A:210:TYR:CE2	4:A:731:HOH:O	2.49	0.65
1:B:223:GLN:HB2	1:B:280:ILE:HG21	1.79	0.65
1:A:230:PHE:HB2	4:A:677:HOH:O	1.97	0.63
1:A:125:LYS:NZ	1:A:125:LYS:CB	2.62	0.62
1:A:126:GLU:CB	1:B:126:GLU:HB3	2.27	0.62
1:B:197:HIS:HB3	4:B:581:HOH:O	1.99	0.62
1:B:328:ASP:N	4:B:613:HOH:O	2.33	0.61
1:A:48:ILE:HG22	1:A:62:LEU:HD11	1.81	0.61
1:B:50:GLN:OE1	1:B:329:GLU:HG2	2.00	0.61
1:A:90:ARG:NH2	3:A:1101:IPE:O2B	2.33	0.60
1:A:116:MET:HE2	1:B:116:MET:SD	2.42	0.60
1:A:6:MET:HE1	1:B:299:GLN:OE1	2.01	0.59
1:A:131:ASN:O	1:A:135:ILE:HG13	2.02	0.59
1:A:140:LEU:O	1:A:144:HIS:HD2	1.86	0.58
1:B:143:LEU:HD11	3:B:1104:IPE:C5	2.33	0.58
1:B:39:PRO:O	1:B:90:ARG:CD	2.52	0.57
1:B:39:PRO:O	1:B:90:ARG:NE	2.37	0.57
1:B:333:ILE:O	1:B:336:HIS:HB3	2.05	0.57
1:A:113:PHE:CE2	1:B:140:LEU:HD13	2.40	0.57
1:A:281:GLN:HE21	1:A:281:GLN:CA	2.17	0.57
1:B:304:ILE:HG21	1:B:334:ILE:CD1	2.35	0.57
1:B:44:ARG:NH1	3:B:1103:IPE:H52	2.19	0.56
1:B:140:LEU:O	1:B:144:HIS:HD2	1.88	0.56
1:A:125:LYS:HB3	1:A:125:LYS:HZ2	1.67	0.56
1:A:4:ASN:ND2	4:A:709:HOH:O	2.38	0.56
1:A:183:LEU:HD21	1:A:199:LEU:HB2	1.86	0.56
1:B:21:SER:H	1:B:24:ASN:ND2	2.04	0.56
1:A:79:ILE:HD11	1:A:108:ALA:HB3	1.88	0.55
1:A:45:LEU:O	1:A:48:ILE:N	2.40	0.55
1:A:52:ASN:ND2	1:A:57:LEU:H	1.96	0.55
1:A:180:ARG:HD3	1:A:204:ASN:HD21	1.72	0.54
1:B:55:MET:CE	1:B:190:SER:HB2	2.37	0.54
1:B:205:LEU:HD23	1:B:304:ILE:CG1	2.37	0.54
1:A:58:PRO:HD2	1:A:61:GLN:HE21	1.72	0.54
1:A:163:THR:CG2	1:A:166:MET:HE2	2.38	0.53
1:B:50:GLN:OE1	1:B:53:ARG:NH1	2.42	0.53
1:A:246:ALA:HB2	1:A:283:LEU:HD22	1.90	0.52
1:B:22:SER:O	1:B:26:SER:OG	2.27	0.52
1:B:222:PHE:CZ	1:B:273:LYS:HD2	2.45	0.52
1:A:63:ALA:O	1:A:67:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD11	1:A:189:LEU:HD21	1.92	0.52
1:A:162:PRO:HA	1:A:166:MET:CE	2.40	0.52
1:B:336:HIS:ND1	1:B:336:HIS:C	2.68	0.52
1:B:127:PRO:HG2	1:B:128:LEU:H	1.75	0.51
1:B:304:ILE:CD1	1:B:334:ILE:HD13	2.40	0.51
1:A:125:LYS:CB	1:A:125:LYS:HZ2	2.20	0.51
3:A:1101:IPE:C4	3:A:1102:IPE:H41	2.41	0.51
1:B:273:LYS:O	1:B:277:LEU:HG	2.11	0.51
1:A:20:TRP:CH2	1:A:24:ASN:HB3	2.45	0.51
1:A:38:LYS:HD2	1:A:90:ARG:HG3	0.88	0.51
1:B:223:GLN:NE2	1:B:284:GLU:CG	2.74	0.51
1:A:5:LYS:H	1:A:5:LYS:HD3	1.76	0.50
1:A:139:GLU:HA	1:A:139:GLU:OE2	2.11	0.50
1:B:273:LYS:HE3	1:B:277:LEU:HD11	1.93	0.50
1:A:109:ASN:HB3	1:B:144:HIS:CE1	2.46	0.50
1:B:42:ASN:OD1	1:B:45:LEU:HD22	2.11	0.50
1:B:96:HIS:HE1	4:B:779:HOH:O	1.95	0.50
1:A:105:ILE:HD11	1:B:105:ILE:HD11	1.91	0.50
1:B:272:ASP:OD2	1:B:275:ILE:HG13	2.11	0.50
1:A:5:LYS:HB2	1:A:5:LYS:NZ	2.21	0.50
1:A:163:THR:N	1:A:166:MET:CE	2.60	0.50
1:A:179:PHE:HB3	1:A:203:ILE:HG13	1.94	0.50
1:B:126:GLU:N	1:B:127:PRO:HD2	2.27	0.49
1:B:223:GLN:NE2	1:B:284:GLU:CD	2.70	0.49
1:B:180:ARG:HD3	1:B:204:ASN:HD21	1.77	0.49
1:A:162:PRO:HA	1:A:166:MET:HE3	1.93	0.49
1:A:4:ASN:HA	1:A:7:GLU:HB2	1.95	0.49
1:A:5:LYS:O	1:A:9:LYS:HG3	2.12	0.49
1:A:126:GLU:HB3	1:B:126:GLU:CG	2.43	0.49
1:B:223:GLN:NE2	1:B:284:GLU:HG3	2.26	0.48
1:B:258:GLN:CD	1:B:258:GLN:H	2.21	0.48
1:B:21:SER:H	1:B:24:ASN:HD22	1.62	0.48
1:A:82:ILE:HD13	1:A:105:ILE:HG13	1.95	0.48
1:B:55:MET:CE	1:B:187:GLU:HA	2.44	0.48
1:B:143:LEU:HD11	3:B:1104:IPE:H52	1.94	0.48
1:B:126:GLU:N	1:B:127:PRO:CD	2.77	0.47
1:B:334:ILE:O	1:B:337:LEU:N	2.44	0.47
1:A:299:GLN:O	1:A:302:ASN:HB2	2.14	0.47
1:A:137:ASN:HD21	1:B:117:GLN:N	2.12	0.47
1:A:126:GLU:O	1:B:126:GLU:OE2	2.33	0.47
1:A:210:TYR:HE2	4:A:731:HOH:O	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:HG22	1:A:125:LYS:H	1.80	0.46
1:A:45:LEU:O	1:A:46:ASN:C	2.58	0.46
1:A:38:LYS:HB2	1:A:90:ARG:CB	2.45	0.46
1:A:45:LEU:C	1:A:45:LEU:HD12	2.40	0.46
1:B:55:MET:HE3	1:B:190:SER:CB	2.44	0.46
1:B:38:LYS:O	1:B:90:ARG:HD3	2.15	0.46
1:A:58:PRO:HD2	1:A:61:GLN:NE2	2.31	0.46
1:A:154:ARG:HD2	1:A:236:GLU:HG2	1.98	0.45
1:A:198:SER:OG	1:A:200:VAL:HG23	2.16	0.45
1:B:241:PHE:HB3	1:B:242:PRO:HD3	1.98	0.45
1:B:55:MET:HE2	1:B:187:GLU:HA	1.98	0.45
1:B:306:ASN:O	1:B:306:ASN:OD1	2.33	0.45
1:A:5:LYS:HD3	1:A:5:LYS:N	2.32	0.45
1:A:48:ILE:CG2	1:A:62:LEU:HD11	2.44	0.45
1:A:202:PHE:HE1	1:A:304:ILE:HD13	1.82	0.44
1:A:221:ASP:O	1:A:225:SER:O	2.36	0.44
1:A:52:ASN:O	1:A:54:VAL:N	2.50	0.44
1:B:82:ILE:HD13	1:B:105:ILE:HG13	1.99	0.44
1:B:304:ILE:HD13	1:B:334:ILE:HD13	2.00	0.44
1:A:20:TRP:CD2	1:B:145:ARG:HD3	2.52	0.44
1:A:45:LEU:HG	1:A:46:ASN:N	2.33	0.44
1:B:190:SER:OG	1:B:192:SER:HB2	2.17	0.44
1:B:223:GLN:NE2	1:B:284:GLU:OE1	2.51	0.44
1:A:69:VAL:HG13	1:A:178:LEU:HD22	2.00	0.44
1:B:307:ASP:O	1:B:307:ASP:CG	2.61	0.44
1:A:34:HIS:HE1	1:A:93:THR:O	2.01	0.44
1:B:202:PHE:CZ	1:B:334:ILE:HD11	2.53	0.44
1:B:331:LEU:HD12	1:B:331:LEU:HA	1.85	0.43
1:A:52:ASN:HD21	1:A:57:LEU:N	2.01	0.43
1:B:305:LYS:HA	1:B:331:LEU:HD11	1.99	0.43
1:A:38:LYS:HB2	1:A:90:ARG:HB3	2.00	0.43
1:B:39:PRO:O	1:B:90:ARG:CZ	2.66	0.43
1:A:92:GLN:HG3	1:A:93:THR:N	2.33	0.43
1:A:114:ARG:HA	1:A:114:ARG:HD2	1.86	0.43
1:A:35:ILE:O	1:A:38:LYS:HG2	2.18	0.43
1:B:172:MET:HE3	1:B:172:MET:HB3	1.97	0.43
1:A:73:HIS:CE1	3:A:1101:IPE:O3B	2.58	0.42
1:B:292:TYR:CD1	1:B:292:TYR:C	2.97	0.42
1:A:52:ASN:C	1:A:54:VAL:N	2.75	0.42
1:A:52:ASN:O	1:A:53:ARG:C	2.61	0.42
1:A:191:PRO:O	1:A:192:SER:CB	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:HD22	1:A:298:ASN:HA	1.67	0.42
1:B:50:GLN:CD	1:B:329:GLU:HG2	2.44	0.42
1:B:249:PHE:O	1:B:250:THR:C	2.62	0.42
1:B:255:GLN:CB	1:B:258:GLN:OE1	2.57	0.42
1:B:128:LEU:O	1:B:132:LEU:HG	2.20	0.42
1:A:126:GLU:O	1:A:127:PRO:C	2.62	0.42
1:A:277:LEU:HD12	1:A:277:LEU:HA	1.92	0.42
1:A:201:PRO:HA	1:B:14:ILE:O	2.20	0.41
1:B:332:TYR:O	1:B:333:ILE:C	2.64	0.41
1:B:183:LEU:HD21	1:B:200:VAL:N	2.36	0.41
1:A:145:ARG:HB3	1:B:20:TRP:CZ3	2.56	0.41
1:B:38:LYS:N	1:B:39:PRO:CD	2.84	0.41
1:A:120:SER:HB3	4:A:654:HOH:O	2.21	0.41
1:A:69:VAL:HG13	1:A:178:LEU:CD2	2.51	0.41
1:B:44:ARG:O	1:B:48:ILE:HG13	2.20	0.41
1:B:215:ASP:HB3	1:B:240:SER:HB2	2.03	0.40
1:A:146:GLY:HA3	1:A:174:LYS:HB2	2.04	0.40
1:B:222:PHE:HZ	1:B:273:LYS:HD2	1.86	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	280/340 (82%)	276 (99%)	3 (1%)	1 (0%)	30	28
1	B	293/340 (86%)	280 (96%)	9 (3%)	4 (1%)	9	5
All	All	573/680 (84%)	556 (97%)	12 (2%)	5 (1%)	14	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	PRO
1	A	53	ARG
1	B	125	LYS
1	B	254	GLY
1	B	333	ILE

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	270/317 (85%)	260 (96%)	10 (4%)	30	31
1	B	283/317 (89%)	264 (93%)	19 (7%)	15	11
All	All	553/634 (87%)	524 (95%)	29 (5%)	21	19

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	5	LYS
1	A	45	LEU
1	A	90	ARG
1	A	123	THR
1	A	125	LYS
1	A	178	LEU
1	A	192	SER
1	A	258	GLN
1	A	281	GLN
1	B	26	SER
1	B	36	LEU
1	B	39	PRO
1	B	45	LEU
1	B	57	LEU
1	B	147	GLN
1	B	149	LEU
1	B	178	LEU
1	B	181	LEU

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Mol	Chain	Res	Type
1	B	192	SER
1	B	193	SER
1	B	203	ILE
1	B	252	THR
1	B	271	SER
1	B	283	LEU
1	B	330	LEU
1	B	335	ASP
1	B	336	HIS
1	B	338	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	52	ASN
1	A	61	GLN
1	A	73	HIS
1	A	85	ASN
1	A	96	HIS
1	A	109	ASN
1	A	117	GLN
1	A	130	HIS
1	A	137	ASN
1	A	144	HIS
1	A	147	GLN
1	A	204	ASN
1	A	255	GLN
1	A	258	GLN
1	A	260	ASN
1	A	281	GLN
1	A	295	ASN
1	A	298	ASN
1	A	299	GLN
1	B	23	GLN
1	B	24	ASN
1	B	34	HIS
1	B	52	ASN
1	B	56	ASN
1	B	92	GLN
1	B	96	HIS
1	B	109	ASN

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Mol	Chain	Res	Type
1	B	137	ASN
1	B	144	HIS
1	B	204	ASN
1	B	223	GLN
1	B	281	GLN
1	B	288	ASN
1	B	298	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	IPE	B	1103	-	12,13,13	2.81	5 (41%)	16,19,19	1.24	2 (12%)
3	IPE	B	1104	2	12,13,13	2.80	5 (41%)	16,19,19	1.28	2 (12%)
3	IPE	A	1101	-	12,13,13	2.81	5 (41%)	16,19,19	1.22	2 (12%)
3	IPE	A	1102	2	12,13,13	2.78	4 (33%)	16,19,19	1.10	1 (6%)

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	IPE	B	1103	-	-	3/13/13/13	-
3	IPE	B	1104	2	-	0/13/13/13	-
3	IPE	A	1101	-	-	6/13/13/13	-
3	IPE	A	1102	2	-	3/13/13/13	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	IPE	C4-C3	7.16	1.53	1.33
3	A	1101	IPE	C4-C3	7.11	1.53	1.33
3	B	1104	IPE	C4-C3	7.11	1.53	1.33
3	B	1103	IPE	C4-C3	7.08	1.53	1.33
3	B	1103	IPE	PB-O2B	3.71	1.62	1.50
3	A	1102	IPE	PB-O2B	3.55	1.61	1.50
3	A	1101	IPE	PB-O2B	3.54	1.61	1.50
3	B	1104	IPE	PB-O2B	3.43	1.61	1.50
3	A	1101	IPE	PA-O1A	3.14	1.61	1.50
3	A	1102	IPE	PA-O1A	3.14	1.61	1.50
3	B	1103	IPE	PA-O1A	3.04	1.61	1.50
3	B	1104	IPE	PA-O1A	2.96	1.61	1.50
3	B	1104	IPE	C5-C3	-2.47	1.39	1.48
3	A	1102	IPE	C5-C3	-2.37	1.39	1.48
3	A	1101	IPE	C5-C3	-2.34	1.39	1.48
3	B	1103	IPE	C5-C3	-2.34	1.39	1.48
3	B	1104	IPE	PA-O3A	2.32	1.62	1.59
3	A	1101	IPE	PA-O3A	2.24	1.61	1.59
3	B	1103	IPE	PA-O3A	2.13	1.61	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1103	IPE	O2A-PA-O3A	3.10	115.66	107.27
3	A	1102	IPE	O2A-PA-O3A	2.82	114.89	107.27
3	B	1104	IPE	O2A-PA-O3A	2.41	113.79	107.27
3	A	1101	IPE	O2A-PA-O3A	2.40	113.75	107.27
3	A	1101	IPE	O3B-PB-O3A	2.39	112.65	104.64
3	B	1103	IPE	O3B-PB-O3A	2.27	112.25	104.64
3	B	1104	IPE	O3B-PB-O3A	2.14	111.82	104.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	IPE	C1-O1-PA-O1A
3	A	1101	IPE	C1-O1-PA-O2A
3	B	1103	IPE	C1-C2-C3-C4
3	B	1103	IPE	C1-C2-C3-C5
3	A	1101	IPE	PA-O3A-PB-O1B
3	B	1103	IPE	PA-O3A-PB-O1B
3	A	1101	IPE	C1-C2-C3-C4
3	A	1101	IPE	C1-O1-PA-O3A
3	A	1102	IPE	C1-O1-PA-O1A
3	A	1102	IPE	C1-O1-PA-O2A
3	A	1102	IPE	C1-O1-PA-O3A
3	A	1101	IPE	C1-C2-C3-C5

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1103	IPE	1	0
3	B	1104	IPE	2	0
3	A	1101	IPE	4	0
3	A	1102	IPE	2	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

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	288/340 (84%)	0.32	16 (5%) 30 31	18, 37, 69, 81	0
1	B	301/340 (88%)	0.38	22 (7%) 21 22	19, 35, 69, 96	0
All	All	589/680 (86%)	0.35	38 (6%) 25 26	18, 36, 70, 96	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	ILE	6.0
1	B	332	TYR	4.1
1	A	123	THR	4.1
1	B	37	LEU	4.0
1	B	330	LEU	4.0
1	B	193	SER	3.6
1	A	224	MET	3.3
1	B	328	ASP	3.3
1	A	124	THR	3.3
1	B	222	PHE	3.2
1	B	230	PHE	3.1
1	A	222	PHE	3.0
1	A	230	PHE	3.0
1	B	337	LEU	2.9
1	B	338	SER	2.8
1	B	10	ILE	2.8
1	A	90	ARG	2.8
1	A	199	LEU	2.8
1	A	191	PRO	2.7
1	B	333	ILE	2.7
1	A	192	SER	2.7
1	B	197	HIS	2.6
1	B	127	PRO	2.5
1	A	45	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	38	LYS	2.4
1	A	197	HIS	2.4
1	B	126	GLU	2.3
1	A	127	PRO	2.3
1	B	38	LYS	2.3
1	A	304	ILE	2.2
1	A	121	GLN	2.2
1	B	39	PRO	2.2
1	B	331	LEU	2.1
1	B	13	LEU	2.1
1	A	48	ILE	2.1
1	B	283	LEU	2.0
1	B	223	GLN	2.0
1	B	277	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IPE	A	1101	14/14	0.86	0.16	71,73,77,77	0
3	IPE	A	1102	14/14	0.96	0.09	29,34,50,50	0
3	IPE	B	1103	14/14	0.96	0.10	35,38,41,41	0
2	MG	A	1301	1/1	0.98	0.04	26,26,26,26	0
3	IPE	B	1104	14/14	0.98	0.07	26,32,38,38	0
2	MG	A	1302	1/1	0.99	0.07	20,20,20,20	0
2	MG	B	1303	1/1	1.00	0.03	23,23,23,23	0
2	MG	B	1304	1/1	1.00	0.04	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.