



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:56 AM UTC

PDB ID : 2DH4 / pdb_00002dh4
Title : Geranylgeranyl pyrophosphate synthase
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Deposited on : 2006-03-22
Resolution : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	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

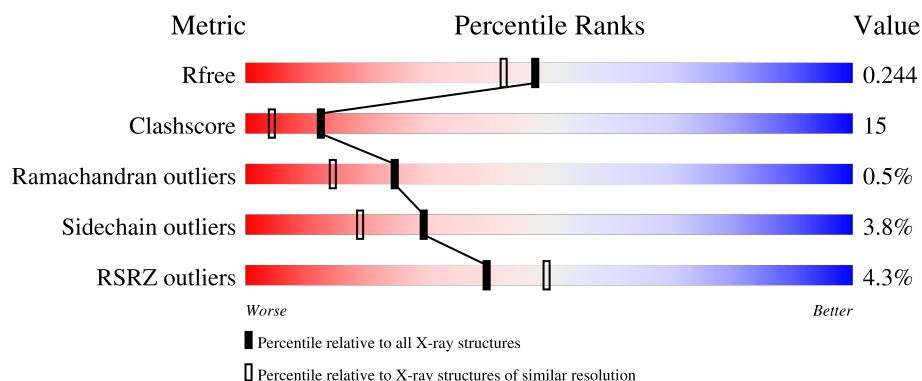
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	3% 68% 24% ...
1	B	340	5% 71% 21% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5900 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 YPL069C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2660	1704	450	496	10			
1	B	326	Total	C	N	O	S	0	0	0
			2660	1704	450	496	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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	297	Total	O	0	0
			297	297		

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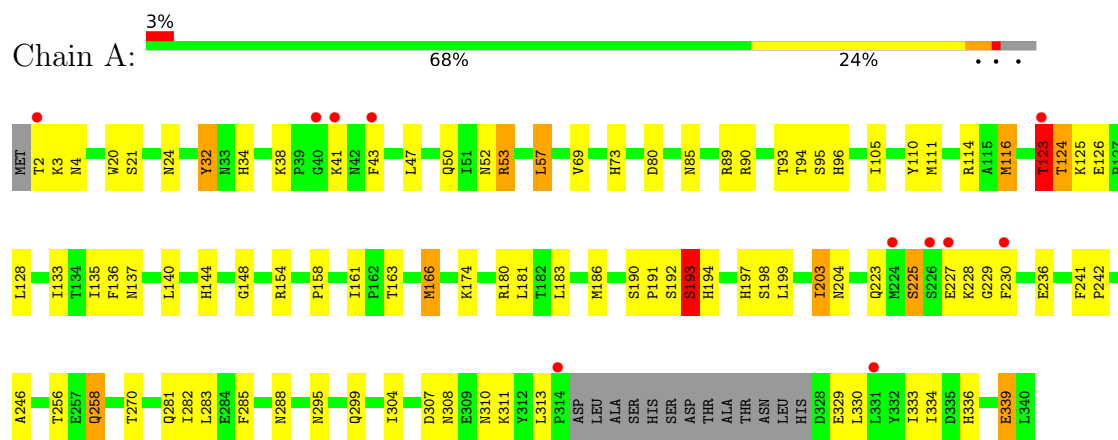
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	281	Total 281	O 281	0	0

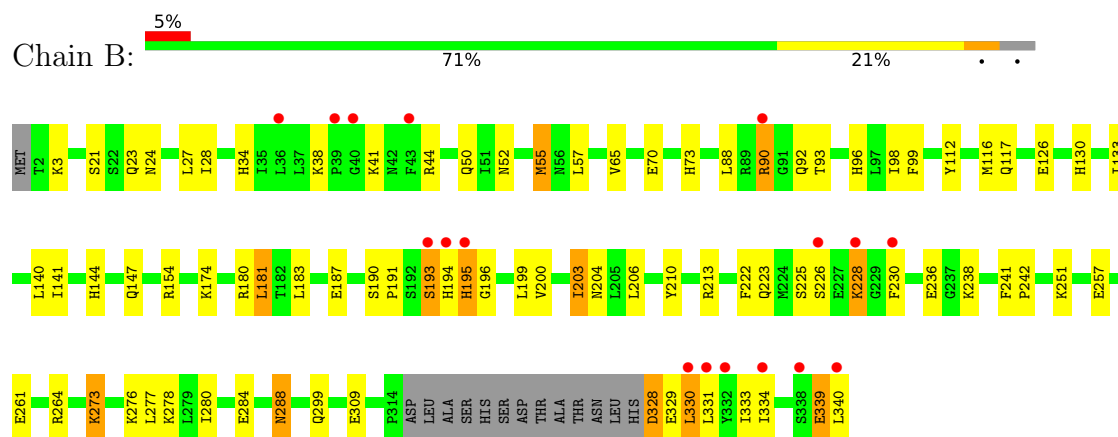
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: YPL069C



• Molecule 1: YPL069C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.75Å 116.33Å 129.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.98 50.00 – 1.98	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-1.98) 90.5 (50.00-1.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.243 0.189 , 0.244	Depositor DCC
R_{free} test set	2381 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.2	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	0.96	EDS
Total number of atoms	5900	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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

5.1 Standard geometry

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

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	0.99	3/2710 (0.1%)	1.11	14/3667 (0.4%)
1	B	0.97	2/2710 (0.1%)	1.07	8/3667 (0.2%)
All	All	0.98	5/5420 (0.1%)	1.09	22/7334 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	MET	SD-CE	-10.68	1.52	1.79
1	A	186	MET	SD-CE	8.47	2.00	1.79
1	B	200	VAL	CA-CB	8.14	1.58	1.54
1	A	116	MET	SD-CE	8.02	1.99	1.79
1	B	55	MET	SD-CE	-7.64	1.60	1.79

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ILE	N-CA-C	-7.75	103.25	110.53
1	A	161	ILE	N-CA-C	-7.12	99.98	107.60
1	A	285	PHE	N-CA-C	6.95	121.89	113.41
1	A	124	THR	N-CA-C	-6.53	105.05	114.12
1	B	191	PRO	N-CA-C	-6.36	105.24	113.57
1	A	174	LYS	N-CA-C	6.29	117.83	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	VAL	N-CA-C	-6.16	104.34	110.62
1	B	174	LYS	N-CA-C	6.11	117.63	110.97
1	A	123	THR	CB-CA-C	-6.03	99.35	111.17
1	A	105	ILE	CB-CA-C	-5.84	104.50	111.97
1	B	228	LYS	N-CA-C	-5.78	104.42	112.45
1	A	191	PRO	N-CA-C	-5.64	106.34	114.18
1	A	114	ARG	N-CA-C	-5.47	105.40	111.36
1	B	112	TYR	N-CA-C	-5.38	105.41	111.28
1	A	95	SER	N-CA-C	5.37	117.83	111.33
1	B	98	ILE	CB-CA-C	-5.33	105.42	111.55
1	B	140	LEU	N-CA-C	-5.33	105.55	111.36
1	B	238	LYS	N-CA-C	5.24	117.83	110.23
1	A	57	LEU	N-CA-C	-5.24	103.43	109.93
1	A	270	THR	N-CA-C	5.23	118.63	110.32
1	A	53	ARG	N-CA-C	-5.10	106.32	112.54
1	A	256	THR	N-CA-C	5.04	116.47	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	TYR	Sidechain

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	2660	0	2702	93	0
1	B	2660	0	2702	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	297	0	0	15	0
3	B	281	0	0	16	0
All	All	5900	0	5404	165	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 15.

All (165) 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:223:GLN:HE21	1:A:281:GLN:HE22	1.06	1.00
1:A:258:GLN:HE21	1:A:258:GLN:H	1.09	0.98
1:A:52:ASN:HD21	1:A:57:LEU:H	1.06	0.98
1:A:41:LYS:HE2	3:A:357:HOH:O	1.66	0.96
1:B:226:SER:HB3	1:B:273:LYS:NZ	1.81	0.95
1:B:330:LEU:HG	1:B:331:LEU:N	1.80	0.95
1:A:163:THR:H	1:A:166:MET:HE3	1.33	0.94
1:A:123:THR:HG22	1:A:125:LYS:H	1.32	0.92
1:B:23:GLN:HG2	3:B:376:HOH:O	1.66	0.92
1:B:52:ASN:HD21	1:B:57:LEU:H	1.10	0.91
1:A:94:THR:HG21	1:A:96:HIS:CD2	2.07	0.90
1:B:273:LYS:HE3	1:B:277:LEU:HD11	1.56	0.85
1:A:307:ASP:HA	3:A:544:HOH:O	1.82	0.80
1:B:226:SER:HB3	1:B:273:LYS:HZ3	1.47	0.79
1:B:34:HIS:HD2	3:B:484:HOH:O	1.65	0.78
1:A:34:HIS:HD2	3:A:423:HOH:O	1.67	0.77
1:A:223:GLN:HE21	1:A:281:GLN:NE2	1.82	0.77
1:A:94:THR:CG2	1:A:96:HIS:CD2	2.67	0.76
1:A:38:LYS:HE2	1:A:89:ARG:O	1.86	0.75
1:A:80:ASP:OD1	3:A:368:HOH:O	2.05	0.75
1:B:226:SER:HB3	1:B:273:LYS:HZ2	1.50	0.75
1:A:116:MET:HE2	1:B:116:MET:SD	2.28	0.74
1:A:38:LYS:HD2	1:A:89:ARG:HG3	1.69	0.73
1:A:52:ASN:ND2	1:A:57:LEU:H	1.86	0.73
1:A:163:THR:N	1:A:166:MET:HE3	2.03	0.72
1:B:340:LEU:OXT	3:B:584:HOH:O	2.06	0.72
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.38	0.72
1:A:299:GLN:HE21	1:B:3:LYS:HD3	1.55	0.72
1:A:53:ARG:HH11	1:A:53:ARG:HG2	1.55	0.71
1:A:154:ARG:HD2	1:A:236:GLU:O	1.92	0.70
1:A:336:HIS:O	1:A:339:GLU:HG2	1.92	0.69
1:A:163:THR:HG23	1:A:166:MET:CE	2.23	0.68
1:A:123:THR:HG23	3:A:511:HOH:O	1.94	0.66
1:B:38:LYS:CG	1:B:90:ARG:HG2	2.26	0.66
1:A:223:GLN:NE2	1:A:281:GLN:HE22	1.87	0.65
1:A:3:LYS:HG3	1:B:299:GLN:HE21	1.61	0.65
1:A:183:LEU:HD21	1:A:199:LEU:HB2	1.79	0.65
1:A:34:HIS:HE1	1:A:93:THR:O	1.79	0.64
1:A:135:ILE:HG22	1:A:181:LEU:HD12	1.80	0.64
1:B:180:ARG:HH11	1:B:204:ASN:ND2	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:THR:HG21	1:A:96:HIS:NE2	2.13	0.63
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.45	0.62
1:B:96:HIS:HE1	3:B:516:HOH:O	1.81	0.62
1:A:136:PHE:HA	1:A:181:LEU:HD11	1.81	0.61
1:B:55:MET:HE3	1:B:55:MET:HA	1.80	0.61
1:A:166:MET:HE1	3:A:439:HOH:O	2.00	0.61
1:B:52:ASN:ND2	1:B:57:LEU:H	1.91	0.61
1:A:140:LEU:O	1:A:144:HIS:HD2	1.84	0.60
1:B:55:MET:CE	1:B:190:SER:HB2	2.32	0.60
1:A:38:LYS:HE2	1:A:89:ARG:HB3	1.82	0.60
1:A:38:LYS:CE	1:A:89:ARG:O	2.49	0.60
1:A:180:ARG:HH11	1:A:204:ASN:ND2	1.99	0.60
1:B:38:LYS:HG3	1:B:90:ARG:HG2	1.84	0.59
1:A:330:LEU:HD11	1:A:334:ILE:HD11	1.84	0.59
1:B:55:MET:HE2	1:B:187:GLU:HA	1.83	0.59
1:A:50:GLN:CD	1:A:329:GLU:HG2	2.28	0.59
1:B:154:ARG:HD2	1:B:236:GLU:HG2	1.85	0.59
1:B:90:ARG:HG3	1:B:90:ARG:NH1	2.17	0.59
1:A:258:GLN:HE21	1:A:258:GLN:N	1.90	0.58
1:B:241:PHE:HB3	1:B:242:PRO:HD3	1.86	0.58
1:A:38:LYS:HD3	1:A:90:ARG:HB2	1.85	0.58
1:A:110:TYR:HE1	1:B:141:ILE:HG23	1.68	0.57
1:A:288:ASN:ND2	3:A:558:HOH:O	2.32	0.57
1:A:225:SER:HB2	1:A:228:LYS:HD3	1.87	0.57
1:A:24:ASN:OD1	3:A:346:HOH:O	2.17	0.57
1:B:328:ASP:N	1:B:328:ASP:OD1	2.38	0.57
1:A:246:ALA:HB2	1:A:283:LEU:HD22	1.87	0.56
1:A:53:ARG:HG2	1:A:53:ARG:NH1	2.16	0.56
1:A:123:THR:HG22	1:A:124:THR:H	1.70	0.56
1:B:257:GLU:OE1	1:B:264:ARG:NH1	2.38	0.56
1:A:183:LEU:CD2	1:A:203:ILE:HB	2.36	0.56
1:A:38:LYS:CD	1:A:89:ARG:HG3	2.34	0.55
1:A:96:HIS:HE1	3:A:473:HOH:O	1.89	0.55
1:A:123:THR:HG22	1:A:124:THR:N	2.22	0.55
1:B:38:LYS:HE3	1:B:90:ARG:HD3	1.89	0.55
1:B:41:LYS:HG3	1:B:70:GLU:OE2	2.06	0.55
1:A:135:ILE:HG22	1:A:181:LEU:CD1	2.37	0.54
1:A:133:ILE:HG23	1:B:116:MET:CE	2.38	0.54
1:B:38:LYS:NZ	3:B:501:HOH:O	2.40	0.54
1:A:34:HIS:CE1	1:A:93:THR:O	2.59	0.53
1:A:50:GLN:HG3	1:A:329:GLU:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PHE:HB3	1:A:242:PRO:HD3	1.90	0.53
3:A:512:HOH:O	1:B:130:HIS:HE1	1.91	0.53
1:A:180:ARG:HD3	1:A:204:ASN:HD21	1.75	0.51
1:A:197:HIS:HD2	1:A:198:SER:O	1.94	0.51
1:A:313:LEU:HD21	1:A:330:LEU:HD22	1.92	0.51
1:B:144:HIS:HE1	3:B:358:HOH:O	1.93	0.51
1:B:55:MET:HE3	1:B:190:SER:HB2	1.92	0.51
1:B:126:GLU:OE2	1:B:126:GLU:HA	2.11	0.51
1:A:21:SER:H	1:A:24:ASN:HD22	1.59	0.50
1:A:90:ARG:NH2	3:A:465:HOH:O	2.44	0.50
1:A:144:HIS:HE1	3:B:352:HOH:O	1.94	0.49
1:A:47:LEU:HD13	1:A:333:ILE:HD13	1.93	0.49
1:B:225:SER:HB3	1:B:228:LYS:HB2	1.94	0.49
1:B:21:SER:H	1:B:24:ASN:HD22	1.60	0.49
1:B:99:PHE:HB3	3:B:555:HOH:O	2.13	0.49
1:B:21:SER:H	1:B:24:ASN:ND2	2.11	0.48
1:B:50:GLN:HG3	1:B:333:ILE:HD11	1.93	0.48
1:A:3:LYS:HE3	1:B:299:GLN:NE2	2.29	0.48
1:A:288:ASN:HB2	3:A:542:HOH:O	2.14	0.48
1:A:94:THR:HG22	1:A:96:HIS:CD2	2.49	0.48
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.77	0.48
1:B:180:ARG:HD3	1:B:204:ASN:HD21	1.79	0.48
1:B:50:GLN:CD	1:B:329:GLU:HG2	2.38	0.48
1:A:123:THR:HG21	1:A:128:LEU:HD23	1.95	0.48
1:B:225:SER:CB	1:B:228:LYS:HG3	2.43	0.48
1:A:225:SER:HB3	1:A:228:LYS:HB2	1.94	0.48
1:A:295:ASN:HD21	1:B:3:LYS:NZ	2.11	0.48
1:A:38:LYS:HE2	1:A:89:ARG:CB	2.44	0.47
1:A:50:GLN:CG	1:A:329:GLU:HG2	2.44	0.47
1:B:226:SER:CB	1:B:273:LYS:HZ3	2.22	0.47
1:B:330:LEU:HA	3:B:565:HOH:O	2.13	0.47
1:B:144:HIS:CE1	3:B:358:HOH:O	2.67	0.47
1:B:210:TYR:CD2	1:B:210:TYR:C	2.92	0.47
1:A:20:TRP:CH2	1:A:24:ASN:HB3	2.50	0.47
1:A:148:GLY:HA3	1:B:28:ILE:HD12	1.96	0.47
1:B:73:HIS:HE1	3:B:472:HOH:O	1.97	0.47
1:A:163:THR:HG23	1:A:166:MET:HE3	1.94	0.46
1:B:55:MET:HE1	1:B:195:HIS:CE1	2.51	0.46
1:B:193:SER:OG	1:B:194:HIS:N	2.48	0.46
1:A:43:PHE:CE2	1:A:339:GLU:HG3	2.51	0.46
1:A:41:LYS:HE3	1:A:41:LYS:HB2	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HD21	1:B:199:LEU:HB2	1.98	0.45
1:A:229:GLY:HA3	3:A:393:HOH:O	2.16	0.45
1:A:126:GLU:HB3	1:B:126:GLU:HB3	1.99	0.45
1:B:38:LYS:HG2	1:B:90:ARG:HG2	1.97	0.45
1:A:73:HIS:HE1	3:A:460:HOH:O	1.99	0.44
1:A:126:GLU:OE2	1:A:126:GLU:HA	2.18	0.44
1:A:137:ASN:HD21	1:B:117:GLN:N	2.14	0.44
1:B:181:LEU:O	1:B:181:LEU:HD12	2.17	0.44
1:A:304:ILE:HG22	1:A:330:LEU:HD21	2.00	0.44
1:A:2:THR:HG22	1:A:4:ASN:H	1.83	0.44
1:B:223:GLN:HE22	1:B:284:GLU:HG2	1.81	0.44
1:A:299:GLN:NE2	1:B:3:LYS:HD3	2.29	0.43
1:A:190:SER:OG	1:A:192:SER:HB3	2.18	0.43
1:B:27:LEU:HD12	3:B:373:HOH:O	2.18	0.43
1:A:32:TYR:CD1	1:A:111:MET:HG3	2.54	0.43
1:B:213:ARG:NH1	1:B:334:ILE:O	2.51	0.43
1:B:230:PHE:O	1:B:276:LYS:NZ	2.48	0.43
1:B:339:GLU:H	1:B:339:GLU:HG2	1.70	0.43
1:B:44:ARG:NH1	3:B:622:HOH:O	2.40	0.43
1:A:183:LEU:HD23	1:A:203:ILE:HB	1.99	0.43
1:A:47:LEU:HD13	1:A:333:ILE:HG21	1.99	0.42
1:B:34:HIS:CD2	3:B:484:HOH:O	2.53	0.42
1:B:194:HIS:C	1:B:196:GLY:H	2.27	0.42
1:B:34:HIS:HE1	1:B:93:THR:O	2.02	0.42
1:B:133:ILE:HD12	1:B:133:ILE:HG23	1.70	0.42
1:B:88:LEU:HD11	3:B:519:HOH:O	2.19	0.42
1:A:308:ASN:C	1:A:310:ASN:H	2.28	0.42
1:B:228:LYS:HE2	1:B:228:LYS:HB3	1.87	0.42
1:B:225:SER:HB3	1:B:228:LYS:CG	2.50	0.42
1:A:304:ILE:HG21	1:A:330:LEU:HD11	2.01	0.41
1:B:27:LEU:CD1	3:B:373:HOH:O	2.69	0.41
1:B:44:ARG:NH1	1:B:73:HIS:CE1	2.88	0.41
1:B:222:PHE:HD2	1:B:280:ILE:CD1	2.33	0.41
1:B:38:LYS:HG3	1:B:90:ARG:CG	2.49	0.41
1:B:183:LEU:HD22	1:B:203:ILE:HB	2.02	0.41
1:B:288:ASN:HD22	1:B:288:ASN:HA	1.66	0.41
1:B:206:LEU:HD12	1:B:206:LEU:HA	1.96	0.41
1:A:193:SER:HB2	1:A:194:HIS:H	1.70	0.41
1:B:90:ARG:HH11	1:B:90:ARG:CG	2.34	0.41
1:B:261:GLU:OE2	1:B:278:LYS:NZ	2.54	0.41
1:B:38:LYS:HG3	1:B:90:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASN:ND2	3:A:473:HOH:O	2.52	0.40
1:A:133:ILE:HG23	1:A:133:ILE:HD12	1.71	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	322/340 (95%)	315 (98%)	6 (2%)	1 (0%)	36	27
1	B	322/340 (95%)	314 (98%)	6 (2%)	2 (1%)	21	12
All	All	644/680 (95%)	629 (98%)	12 (2%)	3 (0%)	24	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	SER
1	B	193	SER
1	B	195	HIS

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	305/317 (96%)	294 (96%)	11 (4%)	31	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	305/317 (96%)	293 (96%)	12 (4%)	28	17
All	All	610/634 (96%)	587 (96%)	23 (4%)	29	19

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	VAL
1	A	123	THR
1	A	158	PRO
1	A	193	SER
1	A	203	ILE
1	A	225	SER
1	A	227	GLU
1	A	230	PHE
1	A	258	GLN
1	A	311	LYS
1	A	339	GLU
1	B	90	ARG
1	B	92	GLN
1	B	147	GLN
1	B	181	LEU
1	B	203	ILE
1	B	251	LYS
1	B	273	LYS
1	B	288	ASN
1	B	309	GLU
1	B	328	ASP
1	B	330	LEU
1	B	339	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	34	HIS
1	A	52	ASN
1	A	56	ASN
1	A	61	GLN
1	A	85	ASN
1	A	96	HIS
1	A	106	ASN

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Mol	Chain	Res	Type
1	A	109	ASN
1	A	130	HIS
1	A	137	ASN
1	A	144	HIS
1	A	197	HIS
1	A	204	ASN
1	A	258	GLN
1	A	260	ASN
1	A	281	GLN
1	A	288	ASN
1	A	295	ASN
1	A	298	ASN
1	A	299	GLN
1	A	336	HIS
1	B	24	ASN
1	B	34	HIS
1	B	50	GLN
1	B	52	ASN
1	B	92	GLN
1	B	96	HIS
1	B	109	ASN
1	B	117	GLN
1	B	121	GLN
1	B	137	ASN
1	B	144	HIS
1	B	147	GLN
1	B	197	HIS
1	B	204	ASN
1	B	288	ASN
1	B	298	ASN
1	B	299	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	326/340 (95%)	-0.06	11 (3%) 48 58	21, 33, 71, 83	0
1	B	326/340 (95%)	0.08	17 (5%) 33 42	19, 35, 73, 87	0
All	All	652/680 (95%)	0.01	28 (4%) 40 49	19, 34, 72, 87	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	LEU	3.9
1	B	226	SER	3.1
1	B	194	HIS	3.1
1	A	331	LEU	3.0
1	B	40	GLY	3.0
1	B	332	TYR	2.9
1	A	2	THR	2.9
1	B	39	PRO	2.9
1	A	230	PHE	2.8
1	B	334	ILE	2.7
1	A	43	PHE	2.6
1	A	40	GLY	2.6
1	B	43	PHE	2.6
1	B	230	PHE	2.6
1	A	41	LYS	2.5
1	A	226	SER	2.3
1	A	123	THR	2.3
1	A	224	MET	2.3
1	B	331	LEU	2.3
1	A	314	PRO	2.2
1	B	193	SER	2.2
1	B	195	HIS	2.2
1	B	90	ARG	2.2
1	B	228	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	227	GLU	2.1
1	B	340	LEU	2.1
1	B	338	SER	2.1
1	B	36	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
2	MG	B	341	1/1	0.95	0.09	29,29,29,29	0
2	MG	A	341	1/1	0.96	0.10	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.