W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 09:18 pm GMT

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PDB ID	:	2E94
Title	:	S. cerevisiae geranylgeranyl pyrophosphate synthase in complex with magnesium and BPH-364
Authors	:	Guo, R.T.; Ko, T.P.; Cao, R.; 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	:	2.18 Å(reported)

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 2.18 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.
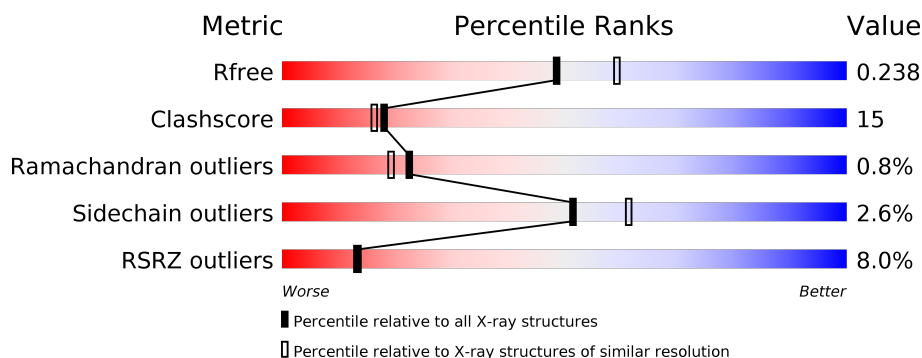
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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.

Mol	Chain	Length	Quality of chain
1	A	340	7% 68% 19% • 11%
1	B	340	7% 67% 21% • 10%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5670 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	303	Total 2460	C 1577	N 418	O 455	S 10	0	0	0
1	B	306	Total 2494	C 1600	N 423	O 461	S 10	0	0	0

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	A	1	Total 1	Mg 1	0	0

- Molecule 3 is 3-BIPHENYL-3-YL-1-(2-HYDROXY-2,2-DIPHOSPHONOETHYL)PYRIDINIUM (three-letter code: 364) (formula: $C_{19}H_{20}NO_7P_2$).
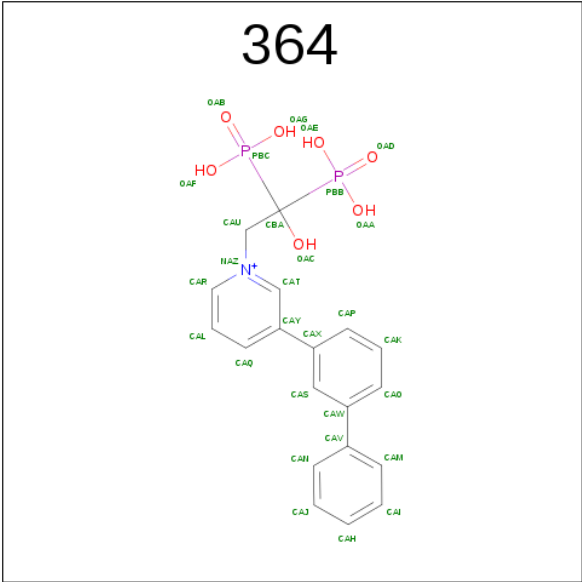
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
3	B	1	Total	C	N	O	P	0	0
			29	19	1	7	2		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	354	Total	O	0	0
			354	354		
4	B	303	Total	O	0	0
			303	303		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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

Chain A:

• Molecule 1: Geranylgeranyl pyrophosphate synthetase

Chain B:
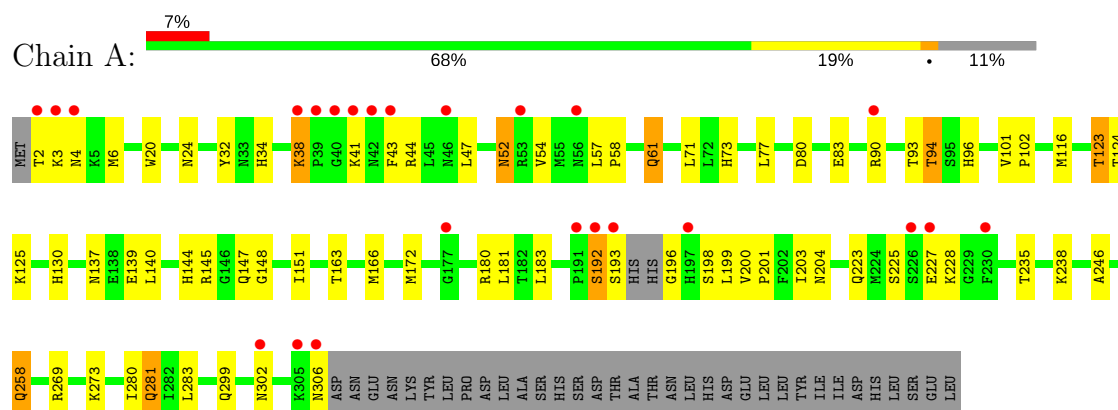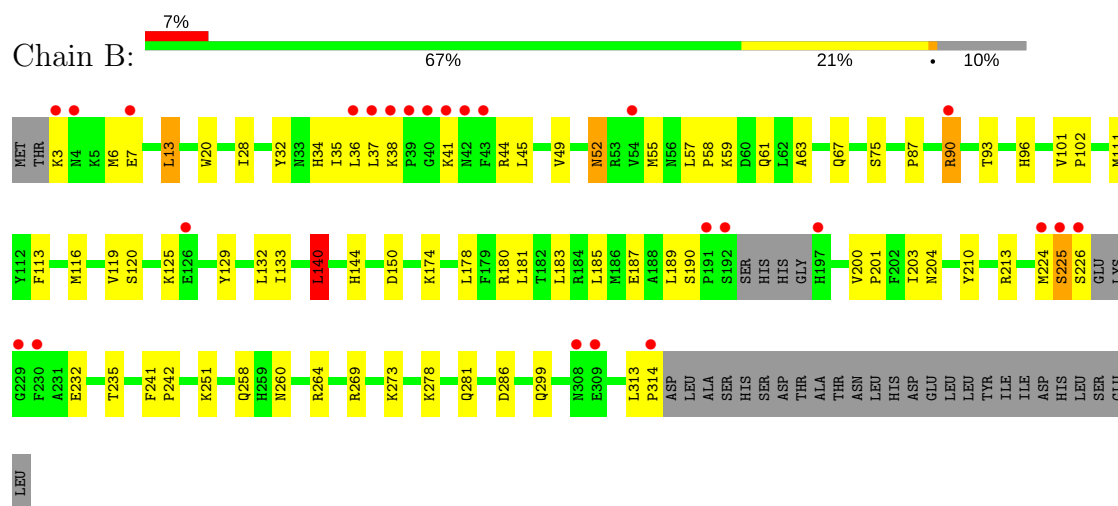
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.57Å 116.39Å 128.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.50 – 2.18 31.53 – 2.18	Depositor EDS
% Data completeness (in resolution range)	94.2 (31.50-2.18) 94.2 (31.53-2.18)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.66 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.236 0.181 , 0.238	Depositor DCC
R_{free} test set	1744 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5670	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 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, 364

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	0.70	0/2504	0.74	0/3387
1	B	0.68	0/2539	0.72	2/3435 (0.1%)
All	All	0.69	0/5043	0.73	2/6822 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	140	LEU	CA-CB-CG	-7.29	98.52	115.30
1	B	150	ASP	CB-CG-OD1	5.12	122.91	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	210	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	2460	0	2519	91	0
1	B	2494	0	2546	77	0
2	A	1	0	0	0	0
3	A	29	0	16	3	0
3	B	29	0	16	4	0
4	A	354	0	0	11	0
4	B	303	0	0	9	0
All	All	5670	0	5097	153	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 (153) 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	1.01	1.13
1:B:213:ARG:HD3	4:B:857:HOH:O	1.57	1.03
1:A:258:GLN:HE21	1:A:258:GLN:H	1.10	0.99
1:A:223:GLN:HE21	1:A:281:GLN:HE22	1.02	0.96
1:A:299:GLN:HE21	1:B:3:LYS:HG3	1.31	0.94
1:A:52:ASN:HD21	1:A:57:LEU:H	1.14	0.93
1:A:80:ASP:HB2	4:A:503:HOH:O	1.68	0.93
1:A:163:THR:N	1:A:166:MET:HE3	1.84	0.91
1:A:38:LYS:HD2	1:A:90:ARG:HG3	1.51	0.91
1:B:52:ASN:HD21	1:B:57:LEU:H	1.23	0.87
1:B:55:MET:HE2	1:B:187:GLU:HA	1.58	0.84
1:A:196:GLY:N	4:A:956:HOH:O	2.09	0.84
1:A:2:THR:HG22	1:A:4:ASN:H	1.43	0.83
1:A:94:THR:CG2	1:A:96:HIS:CD2	2.65	0.78
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.30	0.78
1:A:163:THR:H	1:A:166:MET:CE	1.93	0.76
1:A:223:GLN:NE2	1:A:281:GLN:HE22	1.81	0.76
1:B:55:MET:HE3	1:B:190:SER:HB2	1.68	0.76
1:B:55:MET:CE	1:B:187:GLU:HA	2.15	0.74
1:A:38:LYS:HD2	1:A:90:ARG:CG	2.16	0.74
1:A:223:GLN:HE21	1:A:281:GLN:NE2	1.82	0.74
1:A:94:THR:HG21	1:A:96:HIS:NE2	2.01	0.74
1:A:52:ASN:ND2	1:A:57:LEU:H	1.87	0.72
1:B:140:LEU:O	1:B:144:HIS:HD2	1.73	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:CD	1:A:90:ARG:HG3	2.20	0.71
1:A:94:THR:HG21	1:A:96:HIS:CD2	2.25	0.70
1:A:163:THR:HG23	1:A:166:MET:CE	2.21	0.70
3:A:1101:364:OAD	4:A:401:HOH:O	2.09	0.69
1:A:34:HIS:HE1	1:A:93:THR:O	1.75	0.69
1:A:299:GLN:NE2	1:B:3:LYS:HG3	2.08	0.67
1:A:123:THR:HG22	1:A:125:LYS:H	1.60	0.67
1:A:180:ARG:HH11	1:A:204:ASN:ND2	1.93	0.66
1:B:36:LEU:C	1:B:38:LYS:H	1.98	0.66
1:A:281:GLN:HA	1:A:281:GLN:NE2	2.12	0.64
1:A:281:GLN:HE21	1:A:281:GLN:HA	1.62	0.64
1:B:224:MET:O	1:B:225:SER:HB2	1.98	0.62
1:A:273:LYS:HD3	4:A:1015:HOH:O	1.99	0.62
1:A:38:LYS:HG2	4:A:455:HOH:O	1.99	0.61
1:B:241:PHE:HB3	1:B:242:PRO:HD3	1.82	0.61
1:B:55:MET:CE	1:B:190:SER:HB2	2.29	0.61
1:A:183:LEU:HD21	1:A:199:LEU:HB2	1.81	0.60
1:A:225:SER:HB3	1:A:228:LYS:HD3	1.84	0.60
1:A:225:SER:HB3	1:A:228:LYS:CG	2.32	0.59
1:A:52:ASN:HD21	1:A:57:LEU:N	1.94	0.59
1:B:286:ASP:HB2	4:B:900:HOH:O	2.01	0.59
1:A:44:ARG:NH2	4:A:1017:HOH:O	2.35	0.58
1:B:258:GLN:HG2	1:B:286:ASP:OD2	2.04	0.58
3:A:1101:364:OAB	4:A:401:HOH:O	2.17	0.57
1:A:258:GLN:N	1:A:258:GLN:HE21	1.92	0.57
1:A:299:GLN:HG2	1:B:3:LYS:HD3	1.85	0.57
1:A:299:GLN:HG2	1:B:3:LYS:CD	2.34	0.57
1:B:96:HIS:HD2	4:B:467:HOH:O	1.86	0.57
1:A:200:VAL:HB	1:A:201:PRO:HD3	1.86	0.56
1:B:55:MET:HE3	1:B:190:SER:CB	2.35	0.56
1:B:52:ASN:HD22	1:B:55:MET:HB2	1.70	0.56
1:B:3:LYS:O	1:B:7:GLU:HG3	2.05	0.56
1:B:41:LYS:HB2	4:B:1004:HOH:O	2.05	0.56
1:A:299:GLN:HG2	1:B:3:LYS:NZ	2.22	0.55
1:A:302:ASN:HB3	1:A:306:ASN:ND2	2.22	0.55
1:A:246:ALA:HB2	1:A:283:LEU:HD22	1.88	0.55
4:A:545:HOH:O	1:B:144:HIS:HE1	1.89	0.55
1:B:178:LEU:HB3	3:B:1102:364:CAJ	2.37	0.54
1:B:178:LEU:HB3	3:B:1102:364:HAJ	1.89	0.54
1:B:180:ARG:HH11	1:B:204:ASN:ND2	2.04	0.54
1:B:38:LYS:HG3	1:B:90:ARG:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:SER:CB	1:B:273:LYS:NZ	2.72	0.53
1:A:148:GLY:HA3	1:B:28:ILE:HD12	1.91	0.52
1:A:58:PRO:HG2	1:A:61:GLN:HB2	1.90	0.52
1:A:225:SER:HB3	1:A:228:LYS:HB2	1.91	0.52
1:B:45:LEU:O	1:B:49:VAL:HG23	2.10	0.52
1:B:232:GLU:HB2	4:B:606:HOH:O	2.09	0.52
1:A:196:GLY:CA	4:A:956:HOH:O	2.55	0.51
1:A:225:SER:HB3	1:A:228:LYS:CD	2.40	0.51
1:B:34:HIS:HE1	1:B:93:THR:O	1.94	0.51
1:B:278:LYS:O	1:B:281:GLN:HG2	2.11	0.50
1:A:123:THR:HG22	1:A:124:THR:H	1.75	0.50
1:A:140:LEU:O	1:A:144:HIS:HD2	1.94	0.50
1:B:180:ARG:HD3	1:B:204:ASN:HD21	1.77	0.50
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.60	0.49
3:B:1102:364:OAD	4:B:1057:HOH:O	2.19	0.49
1:A:148:GLY:C	1:B:28:ILE:HD11	2.34	0.48
1:B:226:SER:HB3	1:B:273:LYS:NZ	2.28	0.48
1:A:144:HIS:HE1	4:B:504:HOH:O	1.96	0.48
1:A:198:SER:OG	1:A:200:VAL:HG23	2.12	0.48
1:A:137:ASN:ND2	1:B:116:MET:HG2	2.29	0.48
1:A:41:LYS:HA	1:A:44:ARG:NH2	2.28	0.48
1:B:38:LYS:CG	1:B:90:ARG:HG2	2.44	0.47
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.75	0.47
1:B:226:SER:CB	1:B:273:LYS:HZ2	2.28	0.47
1:B:226:SER:HB2	1:B:273:LYS:HE3	1.96	0.47
1:B:119:VAL:HG11	1:B:133:ILE:HD13	1.97	0.47
1:B:52:ASN:ND2	1:B:57:LEU:H	2.03	0.47
1:B:200:VAL:N	1:B:201:PRO:CD	2.78	0.46
1:A:145:ARG:HG2	1:B:20:TRP:CZ2	2.51	0.46
1:B:75:SER:OG	1:B:111:MET:HB2	2.15	0.46
1:A:43:PHE:O	1:A:47:LEU:N	2.49	0.46
1:B:63:ALA:O	1:B:67:GLN:HG3	2.16	0.46
1:A:192:SER:O	1:A:193:SER:HB2	2.16	0.46
1:A:235:THR:O	1:A:269:ARG:HA	2.16	0.46
1:A:148:GLY:HA3	1:B:28:ILE:CD1	2.45	0.46
1:A:238:LYS:HE2	4:A:508:HOH:O	2.15	0.45
1:B:260:ASN:O	1:B:264:ARG:HG3	2.16	0.45
1:A:6:MET:HE3	1:B:299:GLN:CD	2.37	0.45
1:A:281:GLN:HE21	1:A:281:GLN:CA	2.26	0.45
1:B:32:TYR:O	1:B:35:ILE:HG22	2.17	0.45
1:A:41:LYS:HB2	1:A:41:LYS:HE3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASN:C	1:A:54:VAL:H	2.20	0.45
1:A:20:TRP:CH2	1:A:24:ASN:HB3	2.52	0.45
1:B:174:LYS:HE3	3:B:1102:364:OAG	2.17	0.45
1:B:36:LEU:C	1:B:38:LYS:N	2.66	0.45
1:B:38:LYS:HB3	1:B:38:LYS:NZ	2.32	0.44
1:A:192:SER:O	1:A:193:SER:CB	2.65	0.44
1:B:140:LEU:O	1:B:144:HIS:CD2	2.62	0.44
1:A:101:VAL:HB	1:A:102:PRO:HD3	1.98	0.44
1:B:87:PRO:HD2	4:B:607:HOH:O	2.18	0.44
1:B:181:LEU:HD12	1:B:185:LEU:HG	1.99	0.44
1:A:302:ASN:HB3	1:A:306:ASN:HD22	1.83	0.44
1:B:251:LYS:HE3	4:B:907:HOH:O	2.18	0.44
1:A:43:PHE:CD1	1:A:43:PHE:N	2.85	0.43
1:B:36:LEU:O	1:B:38:LYS:N	2.51	0.43
1:A:80:ASP:OD2	3:A:1101:364:OAA	2.36	0.43
1:B:183:LEU:HD22	1:B:203:ILE:HB	2.00	0.43
1:B:235:THR:O	1:B:269:ARG:HA	2.18	0.43
1:A:6:MET:HE3	1:B:299:GLN:HB3	2.00	0.43
1:A:172:MET:HG3	1:B:13:LEU:HD12	2.01	0.43
1:A:193:SER:O	4:A:1022:HOH:O	2.20	0.43
1:A:83:GLU:HG2	1:B:102:PRO:HA	2.01	0.43
1:A:147:GLN:HG3	1:A:151:ILE:HD12	2.00	0.43
1:A:223:GLN:HB2	1:A:280:ILE:HG21	2.01	0.43
1:A:6:MET:HE3	1:B:299:GLN:CB	2.49	0.42
1:A:183:LEU:HD21	1:A:199:LEU:CB	2.48	0.42
1:A:32:TYR:CZ	1:A:71:LEU:HD23	2.53	0.42
1:B:132:LEU:HD11	1:B:189:LEU:HD21	2.01	0.42
1:B:313:LEU:HB3	1:B:314:PRO:HD2	2.02	0.42
1:A:123:THR:HG22	1:A:124:THR:N	2.33	0.42
1:A:246:ALA:CB	1:A:283:LEU:HD22	2.49	0.42
1:B:44:ARG:NH1	1:B:44:ARG:HB2	2.34	0.42
1:A:34:HIS:CE1	1:A:93:THR:O	2.63	0.42
1:B:58:PRO:HG2	1:B:61:GLN:HB2	2.02	0.42
1:A:130:HIS:CD2	1:B:129:TYR:CE2	3.08	0.41
1:A:140:LEU:HD13	1:B:113:PHE:CZ	2.54	0.41
1:B:101:VAL:HB	1:B:102:PRO:HD3	2.02	0.41
1:A:225:SER:HB3	1:A:228:LYS:CB	2.49	0.41
1:A:44:ARG:HD3	1:A:73:HIS:CD2	2.55	0.41
1:A:203:ILE:HD12	1:A:203:ILE:HA	1.87	0.41
1:A:73:HIS:O	1:A:77:LEU:HG	2.20	0.41
1:B:224:MET:O	1:B:225:SER:CB	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:HG23	1:A:166:MET:HE1	1.98	0.41
1:A:139:GLU:HB2	1:A:181:LEU:HD12	2.03	0.41
1:B:55:MET:HE2	1:B:187:GLU:CA	2.41	0.41
1:A:116:MET:CE	1:B:116:MET:SD	3.09	0.40
1:B:133:ILE:HD13	1:B:133:ILE:HA	1.87	0.40
1:B:41:LYS:HA	1:B:44:ARG:NH2	2.36	0.40

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/340 (88%)	292 (98%)	5 (2%)	2 (1%)	25	22
1	B	300/340 (88%)	293 (98%)	4 (1%)	3 (1%)	18	14
All	All	599/680 (88%)	585 (98%)	9 (2%)	5 (1%)	22	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	SER
1	B	59	LYS
1	B	225	SER
1	B	37	LEU
1	A	3	LYS

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	282/317 (89%)	274 (97%)	8 (3%)	49	58
1	B	286/317 (90%)	279 (98%)	7 (2%)	54	65
All	All	568/634 (90%)	553 (97%)	15 (3%)	51	61

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	52	ASN
1	A	61	GLN
1	A	94	THR
1	A	123	THR
1	A	227	GLU
1	A	258	GLN
1	A	281	GLN
1	B	6	MET
1	B	13	LEU
1	B	52	ASN
1	B	90	ARG
1	B	120	SER
1	B	125	LYS
1	B	140	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) 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	130	HIS
1	A	137	ASN
1	A	144	HIS
1	A	204	ASN
1	A	258	GLN

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Mol	Chain	Res	Type
1	A	260	ASN
1	A	281	GLN
1	A	298	ASN
1	A	299	GLN
1	A	306	ASN
1	B	24	ASN
1	B	52	ASN
1	B	96	HIS
1	B	109	ASN
1	B	121	GLN
1	B	137	ASN
1	B	144	HIS
1	B	147	GLN
1	B	204	ASN
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 carbohydrates in this entry.

5.6   Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is 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	364	A	1101	2	30,31,31	2.35	11 (36%)	43,47,47	0.97	2 (4%)
3	364	B	1102	-	30,31,31	2.32	11 (36%)	43,47,47	1.05	2 (4%)

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	364	A	1101	2	-	0/31/31/31	0/3/3/3
3	364	B	1102	-	-	0/31/31/31	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	364	CAW-CAV	-3.77	1.39	1.49
3	B	1102	364	CAW-CAV	-3.71	1.39	1.49
3	A	1101	364	CAY-CAX	-3.68	1.39	1.49
3	B	1102	364	CAY-CAX	-3.67	1.39	1.49
3	B	1102	364	PBB-OAA	-3.39	1.48	1.54
3	A	1101	364	PBB-OAA	-3.37	1.48	1.54
3	A	1101	364	CAR-NAZ	2.53	1.40	1.34
3	B	1102	364	CAR-NAZ	2.57	1.40	1.34
3	B	1102	364	PBC-CBA	2.78	1.87	1.85
3	B	1102	364	PBB-CBA	2.81	1.87	1.85
3	A	1101	364	PBB-CBA	3.00	1.87	1.85
3	A	1101	364	PBC-CBA	3.02	1.87	1.85
3	A	1101	364	PBB-OAE	3.52	1.61	1.54
3	B	1102	364	PBB-OAE	3.53	1.61	1.54
3	B	1102	364	PBC-OAF	3.59	1.61	1.54
3	B	1102	364	CAT-NAZ	3.60	1.40	1.34
3	A	1101	364	PBC-OAF	3.64	1.61	1.54
3	B	1102	364	PBC-OAG	3.66	1.61	1.54
3	A	1101	364	PBC-OAG	3.67	1.61	1.54
3	A	1101	364	CAT-NAZ	3.68	1.40	1.34
3	B	1102	364	PBB-OAD	6.70	1.61	1.50
3	A	1101	364	PBB-OAD	6.77	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	364	OAE-PBB-OAD	-3.48	105.26	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	364	OAE-PBB-OAD	-3.34	105.58	113.05
3	A	1101	364	OAA-PBB-CBA	3.06	112.81	106.04
3	B	1102	364	OAA-PBB-CBA	3.34	113.41	106.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	364	3	0
3	B	1102	364	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 ⓘ

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	303/340 (89%)	0.14	24 (7%)	13	14	17, 31, 77, 103	0
1	B	306/340 (90%)	0.17	25 (8%)	12	13	19, 35, 79, 100	0
All	All	609/680 (89%)	0.16	49 (8%)	13	13	17, 33, 79, 103	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	GLY	8.4
1	A	197	HIS	7.7
1	A	2	THR	7.3
1	B	43	PHE	6.9
1	A	42	ASN	6.3
1	B	42	ASN	5.8
1	A	39	PRO	5.7
1	B	3	LYS	5.6
1	B	40	GLY	5.1
1	B	39	PRO	5.0
1	A	191	PRO	4.7
1	A	193	SER	4.2
1	A	41	LYS	4.1
1	A	306	ASN	3.9
1	A	227	GLU	3.8
1	B	90	ARG	3.7
1	B	36	LEU	3.6
1	A	43	PHE	3.6
1	A	4	ASN	3.6
1	B	230	PHE	3.6
1	B	197	HIS	3.5
1	B	38	LYS	3.5
1	A	46	ASN	3.3
1	A	56	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	192	SER	3.1
1	A	226	SER	3.1
1	B	41	LYS	3.1
1	A	302	ASN	2.9
1	A	38	LYS	2.9
1	B	308	ASN	2.8
1	A	230	PHE	2.8
1	B	309	GLU	2.7
1	B	225	SER	2.7
1	B	191	PRO	2.7
1	A	90	ARG	2.7
1	A	3	LYS	2.6
1	A	53	ARG	2.5
1	B	4	ASN	2.5
1	B	226	SER	2.4
1	B	224	MET	2.3
1	B	37	LEU	2.2
1	B	192	SER	2.2
1	A	177	GLY	2.2
1	B	314	PRO	2.2
1	B	54	VAL	2.1
1	B	7	GLU	2.1
1	B	126	GLU	2.1
1	B	229	GLY	2.1
1	A	305	LYS	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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	364	B	1102	29/29	0.87	0.18	0.92	61,70,77,77	0
3	364	A	1101	29/29	0.94	0.13	-0.18	52,59,64,64	0
2	MG	A	1201	1/1	0.85	0.10	-	55,55,55,55	0

6.5　Other polymers ⓘ

There are no such residues in this entry.