Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:29 pm GMT

PDB ID	:	2E91
Title	:	S. cerevisiae geranylgeranyl pyrophosphate synthase in complex with magnesium and BPH-91
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	:	2.14 Å(reported)

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

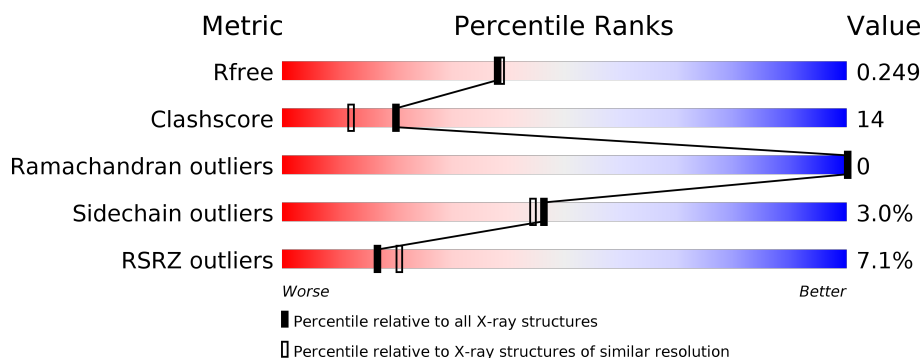|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.14 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	Percentile Ranks	Value
Rfree		0.249
Clashscore		14
Ramachandran outliers		0
Sidechain outliers		3.0%
RSRZ outliers		7.1%

Worse　Better

▮ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

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% 66% 20% · 13%
1	B	340	5% 64% 16% · 17%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5222 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.

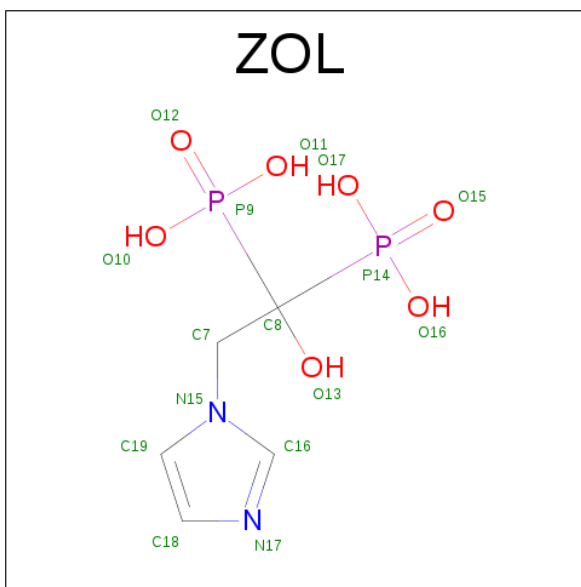| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2410	1548	409	443	10			
1	B	283	Total	C	N	O	S	0	0	0
			2306	1483	388	426	9			

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 ZOLEDRONIC ACID (three-letter code: ZOL) (formula: $C_5H_{10}N_2O_7P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 16	C 5	N 2	O 7	P 2	0	0
3	B	1	Total 16	C 5	N 2	O 7	P 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	231	Total 231	O 231	0	0
4	B	239	Total 239	O 239	0	0

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
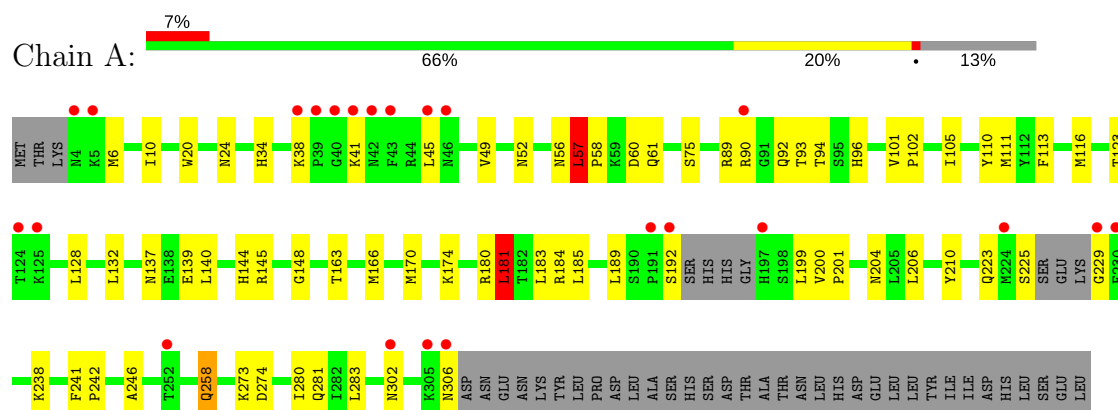
• Molecule 1: Geranylgeranyl pyrophosphate synthetase
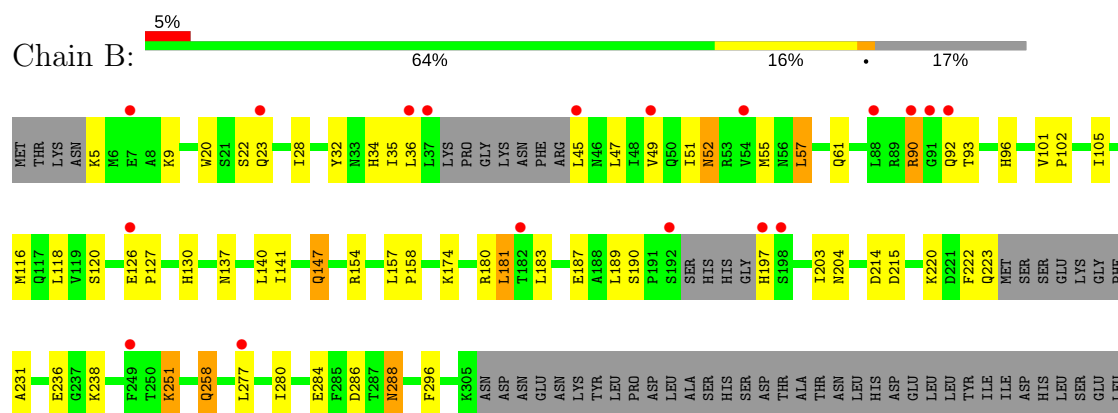
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.66Å 116.29Å 126.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.14 29.03 – 2.13	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.14) 93.9 (29.03-2.13)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.67 (at 2.14Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.249 0.197 , 0.249	Depositor DCC
R_{free} test set	1847 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5222	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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 (i)

5.1 Standard geometry (i)

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

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	0.81	0/2453	0.78	2/3319 (0.1%)
1	B	0.77	0/2345	0.81	2/3175 (0.1%)
All	All	0.79	0/4798	0.80	4/6494 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	LEU	CA-CB-CG	6.62	130.53	115.30
1	A	181	LEU	CA-CB-CG	6.18	129.53	115.30
1	B	215	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	57	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2410	0	2466	79	0
1	B	2306	0	2363	67	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	16	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	7	2	0
4	A	231	0	0	6	0
4	B	239	0	0	10	0
All	All	5222	0	4843	135	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 14.

All (135) 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	1.09
1:A:123:THR:HG21	1:A:128:LEU:HD23	1.33	1.06
1:A:163:THR:H	1:A:166:MET:CE	1.76	0.98
1:B:52:ASN:HD21	1:B:57:LEU:H	1.07	0.97
1:A:52:ASN:HD21	1:A:57:LEU:H	0.99	0.97
1:A:258:GLN:HE21	1:A:258:GLN:H	1.17	0.90
1:A:163:THR:N	1:A:166:MET:HE3	1.86	0.89
1:A:38:LYS:HE2	1:A:92:GLN:HB3	1.51	0.89
1:A:123:THR:HG21	1:A:128:LEU:CD2	2.04	0.87
1:B:5:LYS:CE	1:B:9:LYS:HE2	2.07	0.84
1:A:223:GLN:HE21	1:A:281:GLN:HE22	1.22	0.83
1:A:45:LEU:O	1:A:49:VAL:HG23	1.77	0.83
1:B:5:LYS:HE3	1:B:9:LYS:HE2	1.61	0.81
1:A:52:ASN:ND2	1:A:57:LEU:H	1.80	0.78
1:B:55:MET:CE	1:B:187:GLU:HA	2.15	0.76
1:A:140:LEU:O	1:A:144:HIS:HD2	1.70	0.74
1:A:105:ILE:HD11	1:B:105:ILE:HD11	1.70	0.73
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.36	0.73
1:B:52:ASN:ND2	1:B:57:LEU:H	1.86	0.73
1:A:183:LEU:HD21	1:A:199:LEU:HB2	1.70	0.72
1:A:56:ASN:HD22	1:A:192:SER:HB2	1.54	0.71
1:B:223:GLN:O	4:B:789:HOH:O	2.10	0.69
1:B:55:MET:HE2	1:B:187:GLU:HA	1.74	0.69
1:A:180:ARG:HD3	1:A:204:ASN:HD21	1.59	0.68
1:A:148:GLY:HA3	1:B:28:ILE:HD11	1.76	0.68
1:B:222:PHE:HB2	1:B:231:ALA:HB2	1.74	0.68
1:A:41:LYS:NZ	4:A:611:HOH:O	2.27	0.67
1:A:52:ASN:HD21	1:A:57:LEU:N	1.84	0.67
1:A:148:GLY:HA3	1:B:28:ILE:CD1	2.26	0.66
1:A:94:THR:HG21	1:A:96:HIS:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:HIS:HE1	4:B:645:HOH:O	1.78	0.65
1:A:94:THR:CG2	1:A:96:HIS:CD2	2.80	0.64
1:B:180:ARG:HH11	1:B:204:ASN:ND2	1.96	0.63
1:A:163:THR:N	1:A:166:MET:CE	2.51	0.63
1:A:223:GLN:NE2	1:A:281:GLN:HE22	1.97	0.62
1:B:222:PHE:HE2	1:B:277:LEU:HG	1.63	0.61
1:A:200:VAL:HB	1:A:201:PRO:HD3	1.83	0.60
1:A:38:LYS:HE2	1:A:92:GLN:CB	2.29	0.60
1:B:183:LEU:HD22	1:B:203:ILE:HB	1.81	0.60
1:B:5:LYS:HE2	1:B:9:LYS:HE2	1.81	0.60
3:B:902:ZOL:O12	4:B:651:HOH:O	2.16	0.60
1:A:163:THR:HG23	1:A:166:MET:HE2	1.84	0.59
1:A:38:LYS:HD2	1:A:89:ARG:O	2.02	0.59
1:A:34:HIS:HE1	1:A:93:THR:O	1.85	0.58
1:A:258:GLN:N	1:A:258:GLN:HE21	1.96	0.58
1:B:55:MET:HE1	1:B:187:GLU:HA	1.86	0.58
1:B:214:ASP:OD2	4:B:651:HOH:O	2.18	0.57
1:A:273:LYS:HD3	4:A:866:HOH:O	2.04	0.57
1:B:222:PHE:CE2	1:B:277:LEU:HG	2.40	0.56
1:A:180:ARG:HH11	1:A:204:ASN:ND2	2.04	0.56
1:B:55:MET:HE1	1:B:187:GLU:HG2	1.87	0.56
1:B:45:LEU:O	1:B:49:VAL:HG23	2.06	0.56
1:A:281:GLN:HA	1:A:281:GLN:NE2	2.21	0.56
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.54	0.55
1:A:163:THR:HG23	1:A:166:MET:CE	2.36	0.55
1:B:34:HIS:HE1	1:B:93:THR:O	1.90	0.54
1:B:96:HIS:HD2	4:B:811:HOH:O	1.89	0.54
1:B:180:ARG:HD3	1:B:204:ASN:HD21	1.72	0.54
1:A:183:LEU:HD21	1:A:199:LEU:CB	2.38	0.54
1:B:147:GLN:NE2	1:B:174:LYS:HG3	2.23	0.54
1:A:148:GLY:CA	1:B:28:ILE:HD11	2.38	0.54
1:A:145:ARG:HB3	1:B:20:TRP:CZ3	2.44	0.53
1:A:273:LYS:HG3	1:A:274:ASP:N	2.24	0.53
1:A:229:GLY:N	4:A:705:HOH:O	2.42	0.52
1:A:139:GLU:HB2	1:A:181:LEU:HD22	1.92	0.52
1:A:116:MET:HG2	1:B:137:ASN:ND2	2.24	0.51
1:B:23:GLN:H	1:B:23:GLN:CD	2.14	0.51
1:A:56:ASN:HD22	1:A:192:SER:CB	2.24	0.51
1:B:181:LEU:O	1:B:181:LEU:HD12	2.12	0.50
1:A:180:ARG:O	1:A:184:ARG:HG3	2.10	0.50
1:B:92:GLN:HG2	4:B:807:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:HD2	1:A:90:ARG:HB2	1.93	0.50
1:A:94:THR:HG22	1:A:96:HIS:CD2	2.46	0.50
1:B:22:SER:HB3	1:B:23:GLN:NE2	2.27	0.49
1:A:110:TYR:HE1	1:B:141:ILE:HG23	1.77	0.48
1:A:137:ASN:ND2	1:B:116:MET:HG2	2.28	0.48
1:B:157:LEU:HD12	1:B:158:PRO:HA	1.96	0.48
1:A:302:ASN:HB3	1:A:306:ASN:HD22	1.78	0.48
1:A:89:ARG:HD3	1:A:90:ARG:HD2	1.96	0.48
1:A:75:SER:OG	1:A:111:MET:HB2	2.13	0.47
1:B:92:GLN:NE2	4:B:808:HOH:O	2.47	0.47
1:A:223:GLN:HB2	1:A:280:ILE:HG21	1.95	0.47
1:A:246:ALA:HB2	1:A:283:LEU:HD22	1.96	0.46
1:A:89:ARG:HD3	1:A:90:ARG:CD	2.45	0.46
1:B:258:GLN:HG2	1:B:286:ASP:OD2	2.16	0.46
1:B:5:LYS:HD2	1:B:5:LYS:HA	1.64	0.46
3:B:902:ZOL:O16	4:B:651:HOH:O	2.01	0.46
1:A:20:TRP:CH2	1:A:24:ASN:HB3	2.51	0.46
1:B:47:LEU:O	1:B:51:ILE:HG13	2.16	0.45
1:A:148:GLY:C	1:B:28:ILE:HD11	2.37	0.45
1:A:206:LEU:HA	1:A:206:LEU:HD12	1.79	0.45
1:A:185:LEU:O	1:A:189:LEU:HG	2.16	0.45
1:B:220:LYS:HD2	1:B:220:LYS:HA	1.80	0.45
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.82	0.45
1:B:147:GLN:HE21	1:B:174:LYS:HG3	1.81	0.45
1:B:222:PHE:O	1:B:223:GLN:C	2.56	0.45
1:A:144:HIS:HE1	4:A:815:HOH:O	2.00	0.45
1:B:147:GLN:HA	1:B:147:GLN:HE21	1.83	0.44
1:B:284:GLU:OE1	1:B:284:GLU:HA	2.18	0.44
1:B:251:LYS:HD3	4:B:837:HOH:O	2.17	0.44
1:A:246:ALA:HB2	1:A:283:LEU:CD2	2.47	0.44
1:B:222:PHE:HD2	1:B:280:ILE:HD12	1.82	0.44
1:B:34:HIS:CE1	1:B:93:THR:O	2.70	0.43
1:A:132:LEU:HD11	1:A:189:LEU:HD21	1.99	0.43
1:A:34:HIS:CE1	1:A:93:THR:O	2.70	0.43
1:A:94:THR:HG21	1:A:96:HIS:NE2	2.32	0.43
1:A:210:TYR:CD2	1:A:210:TYR:C	2.91	0.43
1:A:241:PHE:HB3	1:A:242:PRO:HD3	2.00	0.43
4:A:849:HOH:O	1:B:130:HIS:HE1	2.01	0.43
1:A:170:MET:SD	1:A:174:LYS:HD3	2.59	0.42
1:B:288:ASN:HD22	1:B:288:ASN:HA	1.59	0.42
1:A:140:LEU:O	1:A:144:HIS:CD2	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLY:HA3	1:B:28:ILE:HD12	1.99	0.42
1:B:55:MET:HE3	1:B:190:SER:CB	2.49	0.42
1:A:94:THR:HG23	4:A:813:HOH:O	2.19	0.42
1:B:251:LYS:CE	4:B:837:HOH:O	2.67	0.42
1:B:32:TYR:O	1:B:35:ILE:HG22	2.18	0.42
1:B:90:ARG:NH1	1:B:90:ARG:HG3	2.34	0.42
1:A:280:ILE:HG22	1:A:281:GLN:HE21	1.84	0.42
1:A:58:PRO:HG2	1:A:61:GLN:HB2	2.01	0.42
1:A:101:VAL:N	1:A:102:PRO:CD	2.83	0.42
1:B:101:VAL:HB	1:B:102:PRO:HD3	2.02	0.41
1:A:302:ASN:HB3	1:A:306:ASN:ND2	2.36	0.41
1:A:281:GLN:CA	1:A:281:GLN:NE2	2.82	0.41
1:A:41:LYS:HB2	1:A:41:LYS:HE3	1.89	0.41
1:A:105:ILE:HD11	1:B:105:ILE:CD1	2.44	0.41
1:B:204:ASN:HA	1:B:204:ASN:HD22	1.66	0.41
1:A:113:PHE:CE2	1:B:140:LEU:HD13	2.56	0.41
1:B:61:GLN:NE2	1:B:189:LEU:HD22	2.35	0.41
1:B:154:ARG:HD2	1:B:236:GLU:O	2.20	0.41
1:A:10:ILE:HA	1:A:10:ILE:HD13	1.98	0.40
1:B:36:LEU:HD23	1:B:36:LEU:HA	1.89	0.40
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.97	0.40
1:B:126:GLU:N	1:B:127:PRO:CD	2.85	0.40
1:A:6:MET:HE2	1:B:296:PHE:CE2	2.56	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	290/340 (85%)	284 (98%)	6 (2%)	0	100	100
1	B	275/340 (81%)	273 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	565/680 (83%)	557 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	276/317 (87%)	270 (98%)	6 (2%)	57	59
1	B	265/317 (84%)	255 (96%)	10 (4%)	38	35
All	All	541/634 (85%)	525 (97%)	16 (3%)	46	44

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	60	ASP
1	A	181	LEU
1	A	225	SER
1	A	238	LYS
1	A	258	GLN
1	B	52	ASN
1	B	90	ARG
1	B	120	SER
1	B	147	GLN
1	B	181	LEU
1	B	197	HIS
1	B	238	LYS
1	B	251	LYS
1	B	258	GLN
1	B	288	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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	137	ASN
1	A	144	HIS
1	A	197	HIS
1	A	204	ASN
1	A	211	GLN
1	A	258	GLN
1	A	260	ASN
1	A	281	GLN
1	A	298	ASN
1	A	306	ASN
1	B	24	ASN
1	B	52	ASN
1	B	96	HIS
1	B	117	GLN
1	B	121	GLN
1	B	137	ASN
1	B	147	GLN
1	B	197	HIS
1	B	204	ASN
1	B	211	GLN
1	B	255	GLN
1	B	259	HIS
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 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	ZOL	A	901	2	14,16,16	2.30	7 (50%)	19,26,26	1.15	1 (5%)
3	ZOL	B	902	2	14,16,16	2.28	7 (50%)	19,26,26	1.13	1 (5%)

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	ZOL	A	901	2	-	0/23/23/23	0/1/1/1
3	ZOL	B	902	2	-	0/23/23/23	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	ZOL	C19-N15	-2.25	1.33	1.37
3	A	901	ZOL	C19-N15	-2.24	1.33	1.37
3	A	901	ZOL	P14-C8	2.11	1.86	1.85
3	B	902	ZOL	P14-C8	2.32	1.86	1.85
3	B	902	ZOL	P9-C8	2.52	1.86	1.85
3	A	901	ZOL	P9-C8	3.13	1.87	1.85
3	A	901	ZOL	P14-O17	3.36	1.61	1.54
3	A	901	ZOL	P9-O10	3.46	1.61	1.54
3	A	901	ZOL	P9-O11	3.49	1.61	1.54
3	B	902	ZOL	P14-O17	3.52	1.61	1.54
3	B	902	ZOL	P14-O16	3.55	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	ZOL	P9-O10	3.55	1.61	1.54
3	B	902	ZOL	P9-O11	3.60	1.61	1.54
3	A	901	ZOL	P14-O16	3.90	1.62	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	902	ZOL	P9-C8-P14	-4.01	105.28	112.70
3	A	901	ZOL	P9-C8-P14	-3.85	105.59	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	ZOL	2	0

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(Å²)	Q<0.9
1	A	296/340 (87%)	0.34	23 (7%)	14	17	24, 37, 68, 89	0
1	B	283/340 (83%)	0.29	18 (6%)	20	24	27, 40, 63, 85	0
All	All	579/680 (85%)	0.32	41 (7%)	17	21	24, 39, 66, 89	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	GLY	5.4
1	A	230	PHE	5.2
1	A	197	HIS	4.9
1	A	43	PHE	4.7
1	A	41	LYS	4.4
1	A	40	GLY	4.4
1	A	306	ASN	4.2
1	B	90	ARG	4.1
1	A	90	ARG	4.0
1	A	42	ASN	3.6
1	B	197	HIS	3.5
1	A	224	MET	3.3
1	A	38	LYS	3.2
1	A	192	SER	3.1
1	B	7	GLU	3.0
1	A	191	PRO	2.9
1	B	49	VAL	2.9
1	B	45	LEU	2.9
1	A	305	LYS	2.8
1	B	126	GLU	2.8
1	A	45	LEU	2.7
1	A	5	LYS	2.6
1	A	125	LYS	2.6
1	A	39	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	124	THR	2.6
1	B	37	LEU	2.6
1	A	46	ASN	2.5
1	B	91	GLY	2.5
1	B	198	SER	2.5
1	B	88	LEU	2.4
1	B	249	PHE	2.3
1	B	92	GLN	2.3
1	B	182	THR	2.2
1	B	54	VAL	2.2
1	B	23	GLN	2.2
1	A	302	ASN	2.1
1	A	252	THR	2.1
1	B	277	LEU	2.1
1	A	4	ASN	2.1
1	B	36	LEU	2.0
1	B	192	SER	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	ZOL	A	901	16/16	0.94	0.11	-0.91	30,36,40,41	0
3	ZOL	B	902	16/16	0.97	0.10	-1.08	36,40,45,46	0
2	MG	B	1304	1/1	0.93	0.08	-1.33	34,34,34,34	0
2	MG	B	1303	1/1	0.95	0.08	-1.54	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	A	1302	1/1	0.95	0.05	-1.76	35,35,35,35	0
2	MG	A	1301	1/1	0.97	0.04	-2.19	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.