



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:10 AM GMT

PDB ID : 2E93  
Title : *S. cerevisiae* geranylgeranyl pyrophosphate synthase in complex with BPH-629  
Authors : Guo, R.T.; Cao, R.; Ko, T.P.; Chen, C.K.-M.; Jeng, W.Y.; Chang, T.H.;  
Liang, P.H.; Oldfield, E.; Wang, A.H.-J.  
Deposited on : 2007-01-24  
Resolution : 2.12 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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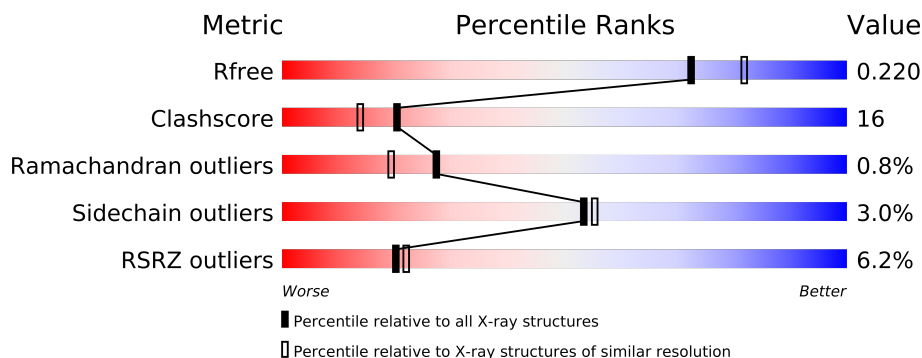
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.12 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	3409 (2.14-2.10)
Clashscore	79885	4090 (2.14-2.10)
Ramachandran outliers	78287	4048 (2.14-2.10)
Sidechain outliers	78261	4049 (2.14-2.10)
RSRZ outliers	66119	3410 (2.14-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5652 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

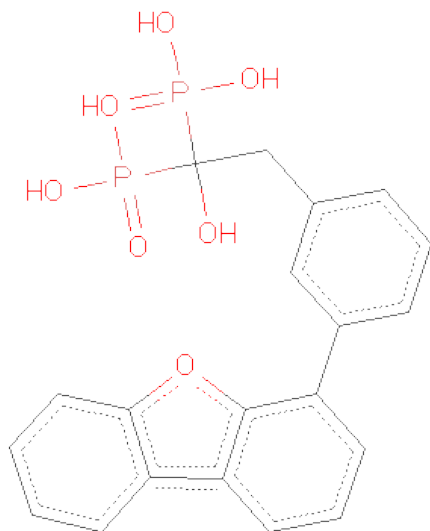
- Molecule 1 is a protein called Geranylgeranyl pyrophosphate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2442	1569	414	450	9			
1	B	314	Total	C	N	O	S	0	0	0
			2571	1652	432	477	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 [2-(3-DIBENZOFURAN-4-YL-PHENYL)-1-HYDROXY-1-PHOSPHONO-ETHYL]-PHOSPHONICACID (three-letter code: B29) (formula: C<sub>20</sub>H<sub>18</sub>O<sub>8</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			30	20	8	2		
2	A	1	Total	C	O	P	0	0
			30	20	8	2		
2	B	1	Total	C	O	P	0	0
			30	20	8	2		
2	B	1	Total	C	O	P	0	0
			30	20	8	2		

- Molecule 3 is water.

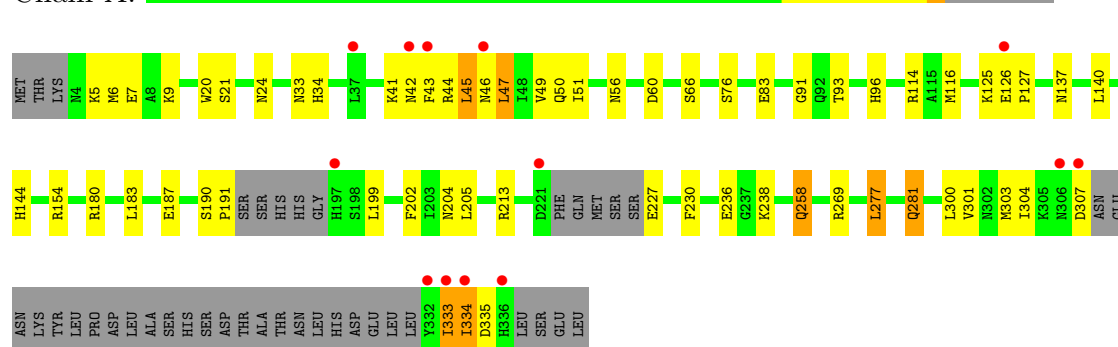
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	280	Total	O	0	0
			280	280		
3	B	239	Total	O	0	0
			239	239		

### 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 errors 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.

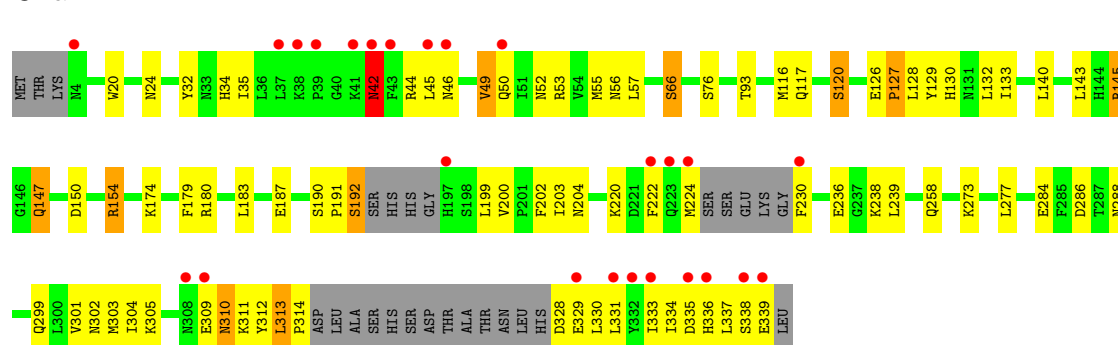
- Molecule 1: Geranylgeranyl pyrophosphate synthetase

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, $\alpha$ , $\beta$ , $\gamma$	45.79Å 115.82Å 130.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.96 – 2.12 28.96 – 2.12	Depositor EDS
% Data completeness (in resolution range)	93.6 (28.96-2.12) 94.1 (28.96-2.12)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.11 (at 2.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.167 , 0.217 0.167 , 0.220	Depositor DCC
$R_{free}$ test set	1873 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 37579 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5652	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B29

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	0.90	1/2485 (0.0%)	0.88	4/3362 (0.1%)
1	B	0.87	0/2617	0.83	3/3542 (0.1%)
All	All	0.88	1/5102 (0.0%)	0.86	7/6904 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLU	CB-CG	5.06	1.61	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	60	ASP	CB-CG-OD1	8.07	125.57	118.30
1	A	269	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	145	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	B	150	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	154	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	277	LEU	CA-CB-CG	-5.14	103.48	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2442	0	2494	73	0
1	B	2571	0	2615	96	0
2	A	60	0	28	6	0
2	B	60	0	28	9	0
3	A	280	0	0	12	0
3	B	239	0	0	8	0
All	All	5652	0	5165	163	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (163) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:304:ILE:HG21	1:B:334:ILE:HD13	1.28	1.14
1:B:126:GLU:HG3	3:B:1089:HOH:O	1.69	0.92
1:B:258:GLN:HG2	1:B:286:ASP:OD2	1.69	0.91
1:B:52:ASN:HD21	1:B:57:LEU:H	1.12	0.89
1:A:258:GLN:HE21	1:A:258:GLN:H	1.16	0.89
1:A:205:LEU:HD23	1:A:304:ILE:HD11	1.57	0.85
1:B:301:VAL:HG13	1:B:334:ILE:HG22	1.59	0.85
1:A:205:LEU:HD23	1:A:304:ILE:CD1	2.11	0.80
1:B:127:PRO:HG2	3:B:1090:HOH:O	1.85	0.77
1:A:281:GLN:HA	1:A:281:GLN:HE21	1.52	0.75
1:A:45:LEU:HD11	1:A:66:SER:HB3	1.69	0.75
1:A:43:PHE:O	1:A:46:ASN:HB3	1.86	0.74
1:B:313:LEU:HD11	1:B:330:LEU:HD23	1.68	0.73
1:B:49:VAL:HG12	1:B:50:GLN:HE21	1.51	0.73
1:B:304:ILE:HG22	1:B:331:LEU:HD13	1.72	0.72
1:B:55:MET:CE	1:B:187:GLU:HA	2.21	0.69
1:B:331:LEU:HA	1:B:334:ILE:HD12	1.74	0.69
1:B:45:LEU:HD13	1:B:66:SER:OG	1.93	0.69
1:A:304:ILE:CB	1:A:334:ILE:HD12	2.23	0.69
1:A:304:ILE:HB	1:A:334:ILE:HD12	1.75	0.69
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.40	0.68
1:A:44:ARG:HG3	2:A:902:B29:CAX	2.23	0.68
1:A:116:MET:CE	1:B:116:MET:SD	2.82	0.68
1:A:334:ILE:O	1:A:334:ILE:HG12	1.92	0.68
1:B:52:ASN:ND2	1:B:57:LEU:H	1.92	0.65
1:A:227:GLU:N	3:A:1121:HOH:O	2.29	0.65
1:A:116:MET:HE1	1:B:116:MET:SD	2.38	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:PHE:HA	3:A:1067:HOH:O	1.96	0.64
1:B:55:MET:HE2	1:B:187:GLU:HA	1.80	0.64
1:B:55:MET:HE3	1:B:190:SER:HB2	1.79	0.64
1:B:180:ARG:HH11	1:B:204:ASN:ND2	1.96	0.63
1:B:230:PHE:HZ	3:B:1023:HOH:O	1.81	0.63
1:A:7:GLU:HG3	1:B:303:MET:HG2	1.80	0.63
3:A:995:HOH:O	1:B:130:HIS:HE1	1.79	0.62
1:A:91:GLY:HA2	1:A:227:GLU:HB3	1.81	0.62
1:B:313:LEU:CD1	1:B:330:LEU:HD23	2.29	0.62
1:A:6:MET:SD	1:B:299:GLN:NE2	2.73	0.62
1:A:43:PHE:C	1:A:46:ASN:HB3	2.20	0.61
1:A:304:ILE:HB	1:A:334:ILE:CD1	2.31	0.60
1:B:335:ASP:O	1:B:338:SER:HB2	2.01	0.60
1:B:220:LYS:O	1:B:224:MET:HG2	2.01	0.60
1:B:50:GLN:OE1	1:B:329:GLU:HG2	2.02	0.59
1:B:330:LEU:HA	1:B:333:ILE:HD12	1.83	0.59
1:B:53:ARG:HD2	3:B:1108:HOH:O	2.03	0.58
1:B:147:GLN:HA	1:B:147:GLN:HE21	1.69	0.57
1:A:238:LYS:NZ	1:A:238:LYS:HB3	2.18	0.57
1:A:126:GLU:HB2	1:A:127:PRO:HD3	1.85	0.57
1:A:44:ARG:HD2	2:A:902:B29:CAZ	2.35	0.56
1:A:140:LEU:O	1:A:144:HIS:HD2	1.88	0.56
1:B:309:GLU:O	1:B:310:ASN:HB2	2.05	0.56
1:B:126:GLU:N	1:B:127:PRO:HD2	2.19	0.56
1:B:55:MET:HE3	1:B:190:SER:CB	2.35	0.56
1:B:273:LYS:NZ	1:B:277:LEU:HD11	2.20	0.56
1:B:55:MET:HE1	1:B:187:GLU:HA	1.87	0.56
1:A:333:ILE:O	1:A:335:ASP:N	2.38	0.56
1:A:213:ARG:NH1	3:A:1160:HOH:O	2.35	0.56
1:B:339:GLU:HA	1:B:339:GLU:OE2	2.05	0.56
1:A:6:MET:O	1:A:9:LYS:HG2	2.05	0.56
1:A:21:SER:H	1:A:24:ASN:HD22	1.54	0.56
1:A:258:GLN:N	1:A:258:GLN:HE21	1.96	0.55
1:A:281:GLN:HA	1:A:281:GLN:NE2	2.18	0.55
1:B:273:LYS:HZ1	1:B:277:LEU:HD11	1.72	0.55
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.53	0.54
1:B:120:SER:HA	1:B:129:TYR:HE1	1.73	0.54
1:B:179:PHE:HB3	1:B:203:ILE:HG13	1.89	0.53
1:A:180:ARG:HH11	1:A:204:ASN:ND2	2.06	0.53
1:A:227:GLU:N	3:A:1142:HOH:O	2.40	0.53
1:B:183:LEU:HD21	1:B:199:LEU:C	2.28	0.53
1:A:281:GLN:HE21	1:A:281:GLN:CA	2.21	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:46:ASN:O	1:A:50:GLN:HG2	2.09	0.53
1:A:116:MET:HE2	1:B:116:MET:SD	2.49	0.52
1:B:55:MET:CE	1:B:190:SER:HB2	2.39	0.52
1:B:55:MET:HE1	1:B:187:GLU:HG2	1.91	0.52
1:A:45:LEU:O	1:A:49:VAL:HG23	2.09	0.52
2:B:903:B29:OAT	2:B:903:B29:HAM	2.08	0.52
1:B:143:LEU:HD23	1:B:174:LYS:O	2.10	0.52
1:B:34:HIS:HE1	1:B:93:THR:O	1.93	0.52
1:B:304:ILE:HD13	1:B:334:ILE:HG12	1.91	0.51
1:A:202:PHE:CE1	1:A:304:ILE:HD12	2.45	0.51
1:A:180:ARG:HD3	1:A:204:ASN:HD21	1.76	0.51
1:A:83:GLU:O	1:A:154:ARG:NH2	2.43	0.51
1:B:202:PHE:CE1	1:B:334:ILE:HD11	2.45	0.51
1:A:114:ARG:NH1	3:A:931:HOH:O	2.43	0.51
1:A:43:PHE:HA	1:A:46:ASN:HB2	1.93	0.51
1:A:5:LYS:HD2	3:A:907:HOH:O	2.12	0.50
1:B:56:ASN:ND2	1:B:192:SER:OG	2.41	0.50
1:B:304:ILE:HG23	1:B:313:LEU:HD22	1.93	0.50
1:A:154:ARG:NH1	3:A:977:HOH:O	2.44	0.49
1:B:284:GLU:HG2	3:B:1058:HOH:O	2.11	0.49
1:B:191:PRO:HG2	1:B:192:SER:H	1.77	0.49
1:B:222:PHE:HD1	1:B:230:PHE:N	2.09	0.49
1:A:20:TRP:CH2	1:A:24:ASN:HB3	2.48	0.49
1:B:76:SER:HB2	2:B:904:B29:CAY	2.42	0.49
1:B:20:TRP:CH2	1:B:24:ASN:HB3	2.48	0.49
1:A:334:ILE:CG1	1:A:334:ILE:O	2.61	0.48
1:A:96:HIS:HD2	3:A:966:HOH:O	1.95	0.48
1:B:44:ARG:HH11	2:B:903:B29:HAJ	1.78	0.48
1:B:76:SER:HB2	2:B:904:B29:CAZ	2.43	0.48
1:B:202:PHE:CD1	1:B:313:LEU:HD13	2.49	0.48
1:A:304:ILE:HG13	1:A:334:ILE:HD12	1.96	0.48
1:B:329:GLU:O	1:B:333:ILE:HG13	2.13	0.48
1:B:147:GLN:HE22	1:B:174:LYS:NZ	2.11	0.48
1:A:33:ASN:ND2	3:A:1113:HOH:O	2.36	0.48
1:A:47:LEU:HG	1:A:51:ILE:HD12	1.96	0.48
1:B:76:SER:HB2	2:B:904:B29:CAX	2.44	0.48
1:B:273:LYS:NZ	1:B:277:LEU:CD1	2.77	0.47
1:B:202:PHE:CZ	1:B:334:ILE:HD11	2.48	0.47
1:A:137:ASN:HD21	1:B:117:GLN:N	2.12	0.47
1:A:34:HIS:HE1	1:A:93:THR:O	1.97	0.47
1:B:55:MET:O	1:B:191:PRO:HD2	2.15	0.47
1:A:125:LYS:HD2	3:A:1146:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:301:VAL:HG13	1:A:334:ILE:HD11	1.97	0.46
1:A:76:SER:HB2	2:A:901:B29:CAZ	2.45	0.46
1:A:42:ASN:C	1:A:44:ARG:H	2.18	0.46
1:B:313:LEU:HD12	1:B:314:PRO:CD	2.45	0.46
1:A:43:PHE:HA	1:A:46:ASN:CB	2.46	0.46
1:A:300:LEU:O	1:A:303:MET:HB2	2.15	0.46
1:A:277:LEU:HA	1:A:277:LEU:HD12	1.84	0.45
1:A:76:SER:HB2	2:A:901:B29:CAY	2.46	0.45
1:B:313:LEU:HD12	1:B:314:PRO:HD2	1.98	0.45
1:B:76:SER:HB2	2:B:904:B29:CBA	2.47	0.45
1:B:154:ARG:HD2	1:B:236:GLU:O	2.17	0.45
1:A:44:ARG:HD3	1:A:44:ARG:HA	1.45	0.44
1:A:304:ILE:CG2	1:A:334:ILE:HD12	2.47	0.44
2:A:901:B29:OAE	2:A:902:B29:OAE	2.35	0.44
1:B:32:TYR:O	1:B:35:ILE:HG22	2.18	0.44
1:B:313:LEU:HD12	1:B:313:LEU:HA	1.90	0.44
1:A:20:TRP:CZ3	1:B:145:ARG:HB3	2.53	0.44
1:B:301:VAL:HG13	1:B:334:ILE:CG2	2.39	0.43
1:B:309:GLU:O	1:B:310:ASN:CB	2.66	0.43
1:B:183:LEU:HD23	1:B:200:VAL:HA	2.00	0.43
1:A:187:GLU:OE2	3:A:1049:HOH:O	2.21	0.43
1:B:202:PHE:CZ	1:B:330:LEU:HG	2.52	0.43
1:A:304:ILE:HG21	1:A:334:ILE:HD12	1.99	0.43
1:B:310:ASN:HB3	1:B:313:LEU:O	2.18	0.43
1:A:44:ARG:HG3	2:A:902:B29:OAT	2.18	0.43
1:B:239:LEU:HA	1:B:239:LEU:HD13	1.81	0.43
1:B:302:ASN:HA	1:B:305:LYS:HB2	2.01	0.43
1:A:126:GLU:HB3	1:B:126:GLU:HB3	2.01	0.43
1:B:174:LYS:HE2	2:B:904:B29:OAG	2.18	0.43
1:B:46:ASN:O	1:B:50:GLN:HG2	2.19	0.42
1:B:44:ARG:HH11	2:B:903:B29:CAJ	2.32	0.42
2:B:903:B29:OAE	2:B:904:B29:OAA	2.37	0.42
1:B:52:ASN:HD22	1:B:55:MET:HB2	1.83	0.42
1:A:304:ILE:CG1	1:A:334:ILE:HD12	2.49	0.42
1:B:238:LYS:CE	3:B:1014:HOH:O	2.67	0.42
1:B:238:LYS:HE3	3:B:1014:HOH:O	2.19	0.42
1:A:47:LEU:O	1:A:51:ILE:HD12	2.20	0.42
1:B:128:LEU:O	1:B:132:LEU:HG	2.19	0.42
1:B:133:ILE:HA	1:B:133:ILE:HD13	1.80	0.42
1:A:190:SER:HA	1:A:191:PRO:HD3	1.83	0.42
1:B:126:GLU:N	1:B:127:PRO:CD	2.82	0.42
1:B:311:LYS:HE3	1:B:312:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:183:LEU:HD22	1:B:203:ILE:HB	2.01	0.42
1:A:183:LEU:HD21	1:A:199:LEU:HB2	2.02	0.42
1:B:130:HIS:O	1:B:130:HIS:HD2	2.03	0.41
1:B:333:ILE:O	1:B:337:LEU:HG	2.20	0.41
1:B:311:LYS:HE3	1:B:312:TYR:CE2	2.55	0.41
1:A:144:HIS:HE1	3:B:922:HOH:O	2.03	0.41
1:B:42:ASN:N	1:B:42:ASN:HD22	2.19	0.41
1:A:41:LYS:HA	1:A:41:LYS:HD3	1.89	0.40
1:B:180:ARG:HD3	1:B:204:ASN:HD21	1.86	0.40
1:A:137:ASN:CB	1:B:116:MET:HE1	2.52	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	291/340 (86%)	282 (97%)	7 (2%)	2 (1%)	30	23
1	B	306/340 (90%)	299 (98%)	4 (1%)	3 (1%)	22	14
All	All	597/680 (88%)	581 (97%)	11 (2%)	5 (1%)	27	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	ILE
1	B	42	ASN
1	B	310	ASN
1	B	127	PRO
1	A	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	279/317 (88%)	273 (98%)	6 (2%)	64	68
1	B	295/317 (93%)	284 (96%)	11 (4%)	45	45
All	All	574/634 (90%)	557 (97%)	17 (3%)	53	55

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	47	LEU
1	A	56	ASN
1	A	258	GLN
1	A	281	GLN
1	A	307	ASP
1	B	42	ASN
1	B	49	VAL
1	B	66	SER
1	B	120	SER
1	B	140	LEU
1	B	147	GLN
1	B	192	SER
1	B	288	ASN
1	B	313	LEU
1	B	328	ASP
1	B	336	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	34	HIS
1	A	61	GLN
1	A	67	GLN
1	A	85	ASN
1	A	96	HIS
1	A	109	ASN
1	A	137	ASN
1	A	144	HIS
1	A	164	GLN

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Mol	Chain	Res	Type
1	A	204	ASN
1	A	258	GLN
1	A	260	ASN
1	A	281	GLN
1	B	24	ASN
1	B	34	HIS
1	B	42	ASN
1	B	52	ASN
1	B	56	ASN
1	B	85	ASN
1	B	96	HIS
1	B	109	ASN
1	B	130	HIS
1	B	147	GLN
1	B	204	ASN
1	B	288	ASN
1	B	298	ASN
1	B	299	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	$\# Z  > 2$
2	B29	A	901	-	31,33,33	2.49	12 (38%)	48,52,52	1.17	5 (10%)
2	B29	A	902	-	31,33,33	2.47	10 (32%)	48,52,52	1.49	13 (27%)
2	B29	B	903	-	31,33,33	2.52	12 (38%)	48,52,52	1.20	5 (10%)
2	B29	B	904	-	31,33,33	2.48	10 (32%)	48,52,52	1.24	5 (10%)

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
2	B29	A	901	-	-	0/27/27/27	0/1/4/4
2	B29	A	902	-	-	0/27/27/27	0/1/4/4
2	B29	B	903	-	-	0/27/27/27	0/1/4/4
2	B29	B	904	-	-	0/27/27/27	0/1/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	903	B29	PBC-OAD	6.64	1.61	1.50
2	A	902	B29	PBD-OAF	6.54	1.61	1.50
2	B	904	B29	PBC-OAD	6.47	1.61	1.50
2	B	904	B29	PBD-OAF	6.47	1.61	1.50
2	B	903	B29	PBD-OAF	6.44	1.61	1.50
2	A	902	B29	PBC-OAD	6.42	1.61	1.50
2	A	901	B29	PBD-OAF	6.33	1.61	1.50
2	A	901	B29	PBC-OAD	6.25	1.60	1.50
2	B	903	B29	CAW-CAV	-5.50	1.39	1.49
2	A	901	B29	CAW-CAV	-5.44	1.39	1.49
2	B	904	B29	CAW-CAV	-5.22	1.39	1.49
2	A	902	B29	CAW-CAV	-5.22	1.39	1.49
2	B	904	B29	PBD-OAG	3.69	1.61	1.54
2	A	901	B29	PBD-OAG	3.57	1.61	1.54
2	B	903	B29	PBC-OAE	3.51	1.61	1.54
2	B	903	B29	PBD-OAG	3.42	1.61	1.54
2	A	901	B29	PBC-OAE	3.40	1.61	1.54
2	A	902	B29	PBC-OAE	3.34	1.61	1.54
2	A	901	B29	PBD-OAB	-3.33	1.48	1.54
2	B	904	B29	PBD-OAB	-3.32	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	B29	PBC-OAA	-3.25	1.48	1.54
2	B	904	B29	PBC-OAE	3.23	1.61	1.54
2	B	904	B29	PBC-OAA	-3.21	1.48	1.54
2	B	903	B29	PBC-OAA	-3.19	1.48	1.54
2	A	902	B29	PBD-OAB	-3.17	1.48	1.54
2	B	903	B29	PBD-OAB	-3.12	1.48	1.54
2	A	901	B29	PBC-OAA	-3.12	1.48	1.54
2	A	902	B29	PBC-CBB	3.11	1.87	1.85
2	A	902	B29	PBD-OAG	3.08	1.60	1.54
2	B	903	B29	CAS-CBB	-3.02	1.53	1.55
2	A	901	B29	PBD-CBB	2.66	1.87	1.85
2	A	901	B29	CAS-CBB	-2.64	1.53	1.55
2	B	904	B29	PBD-CBB	2.43	1.87	1.85
2	B	904	B29	CAS-CBB	-2.38	1.53	1.55
2	A	901	B29	PBC-CBB	2.13	1.86	1.85
2	A	902	B29	PBD-CBB	2.13	1.86	1.85
2	B	903	B29	PBC-CBB	2.12	1.86	1.85
2	B	903	B29	PBD-CBB	2.12	1.86	1.85
2	A	901	B29	CAZ-CAY	-2.11	1.39	1.45
2	A	902	B29	CAZ-CAY	-2.08	1.39	1.45
2	B	903	B29	CAW-CBA	-2.06	1.39	1.42
2	B	904	B29	CAW-CBA	-2.05	1.39	1.42
2	B	903	B29	CAZ-CAY	-2.03	1.39	1.45
2	A	901	B29	CAW-CBA	-2.03	1.39	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	904	B29	OAG-PBD-OAF	-3.91	104.41	113.14
2	A	902	B29	OAE-PBC-OAD	-3.67	104.94	113.14
2	A	902	B29	PBD-CBB-PBC	-3.51	106.56	112.78
2	B	903	B29	CBB-CAS-CAU	-3.51	110.67	115.72
2	A	901	B29	OAB-PBD-CBB	3.29	113.69	105.98
2	B	904	B29	OAB-PBD-CBB	3.22	113.55	105.98
2	A	901	B29	OAA-PBC-CBB	2.95	112.90	105.98
2	A	902	B29	OAA-PBC-CBB	2.78	112.51	105.98
2	A	901	B29	OAE-PBC-OAD	-2.78	106.93	113.14
2	B	904	B29	OAE-PBC-OAD	-2.72	107.07	113.14
2	A	902	B29	CAM-CAV-CAW	-2.68	116.34	120.85
2	A	902	B29	OAG-PBD-OAF	-2.57	107.39	113.14
2	B	903	B29	OAG-PBD-OAF	-2.53	107.48	113.14
2	A	902	B29	CAR-CAV-CAW	2.48	124.30	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	B29	OAB-PBD-CBB	2.40	111.63	105.98
2	B	903	B29	PBD-CBB-PBC	-2.31	108.69	112.78
2	A	901	B29	OAG-PBD-OAF	-2.30	108.00	113.14
2	A	902	B29	CAX-OAT-CBA	2.28	109.70	105.39
2	A	902	B29	CAS-CAU-CAL	-2.27	117.75	121.06
2	A	902	B29	OAB-PBD-OAG	2.27	114.39	107.93
2	A	902	B29	PBC-CBB-CAS	2.22	114.62	108.43
2	A	902	B29	OAE-PBC-OAA	2.20	114.20	107.93
2	B	904	B29	CAX-OAT-CBA	2.17	109.49	105.39
2	A	901	B29	OAE-PBC-CBB	-2.14	100.96	105.98
2	A	902	B29	CAQ-CAZ-CBA	2.02	120.70	118.45
2	B	904	B29	OAA-PBC-CBB	2.02	110.72	105.98
2	B	903	B29	CAX-OAT-CBA	2.02	109.21	105.39
2	B	903	B29	OAE-PBC-OAA	2.00	113.63	107.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	299/340 (87%)	0.06	13 (4%) 34 37	17, 27, 59, 102	0
1	B	314/340 (92%)	0.23	25 (7%) 12 13	17, 31, 78, 99	0
All	All	613/680 (90%)	0.15	38 (6%) 20 22	17, 29, 67, 102	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	PHE	7.2
1	B	332	TYR	6.4
1	B	43	PHE	6.0
1	A	42	ASN	5.3
1	A	46	ASN	5.3
1	B	197	HIS	4.8
1	B	230	PHE	4.6
1	A	332	TYR	4.3
1	B	45	LEU	4.2
1	A	334	ILE	3.9
1	B	309	GLU	3.8
1	B	335	ASP	3.5
1	B	4	ASN	3.3
1	A	333	ILE	3.1
1	B	50	GLN	3.1
1	B	329	GLU	3.1
1	A	197	HIS	3.0
1	B	339	GLU	3.0
1	B	39	PRO	2.9
1	B	42	ASN	2.9
1	B	46	ASN	2.8
1	B	308	ASN	2.8
1	A	306	ASN	2.6
1	B	222	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	307	ASP	2.6
1	A	37	LEU	2.6
1	B	336	HIS	2.5
1	B	37	LEU	2.4
1	A	221	ASP	2.4
1	A	126	GLU	2.4
1	B	224	MET	2.3
1	B	331	LEU	2.3
1	A	336	HIS	2.3
1	B	338	SER	2.1
1	B	41	LYS	2.1
1	B	223	GLN	2.0
1	B	38	LYS	2.0
1	B	333	ILE	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	B29	B	904	30/30	0.12	-0.28	26,30,36,37	0
2	B29	B	903	30/30	0.13	-0.71	34,50,55,56	0
2	B29	A	902	30/30	0.13	-0.81	31,37,44,46	0
2	B29	A	901	30/30	0.12	-0.88	24,27,30,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.