Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 09:00 PM EST

PDB ID	:	3RMG
Title	:	Crystal structure of geranylgeranyl pyrophosphate synthase from bacteroides thetaiotaomicron
Authors	:	Patskovsky, Y.; Toro, R.; Sauder, J.M.; Poulter, C.D.; Gerlt, J.A.; Burley, S.K.; Almo, S.C.; Enzyme Function Initiative (EFI); New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2011-04-20
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

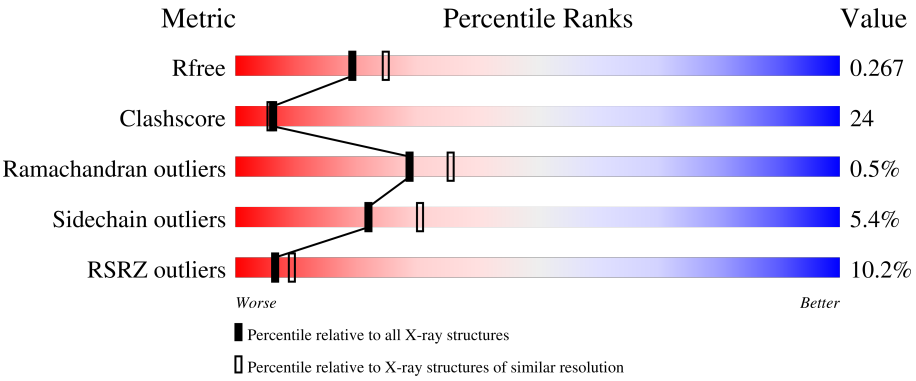
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	334	7%, 60%, 27%, ·, 10%
1	B	334	11%, 56%, 29%, ·, 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4627 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 Octaprenyl-diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	1	0
			2301	1472	369	453	7			
1	B	297	Total	C	N	O	S	0	2	0
			2257	1444	367	439	7			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q8A2P4
A	-1	SER	-	expression tag	UNP Q8A2P4
A	0	LEU	-	expression tag	UNP Q8A2P4
A	325	GLU	-	expression tag	UNP Q8A2P4
A	326	GLY	-	expression tag	UNP Q8A2P4
A	327	HIS	-	expression tag	UNP Q8A2P4
A	328	HIS	-	expression tag	UNP Q8A2P4
A	329	HIS	-	expression tag	UNP Q8A2P4
A	330	HIS	-	expression tag	UNP Q8A2P4
A	331	HIS	-	expression tag	UNP Q8A2P4
A	332	HIS	-	expression tag	UNP Q8A2P4
B	-2	MET	-	expression tag	UNP Q8A2P4
B	-1	SER	-	expression tag	UNP Q8A2P4
B	0	LEU	-	expression tag	UNP Q8A2P4
B	325	GLU	-	expression tag	UNP Q8A2P4
B	326	GLY	-	expression tag	UNP Q8A2P4
B	327	HIS	-	expression tag	UNP Q8A2P4
B	328	HIS	-	expression tag	UNP Q8A2P4
B	329	HIS	-	expression tag	UNP Q8A2P4
B	330	HIS	-	expression tag	UNP Q8A2P4
B	331	HIS	-	expression tag	UNP Q8A2P4
B	332	HIS	-	expression tag	UNP Q8A2P4

- Molecule 2 is water.

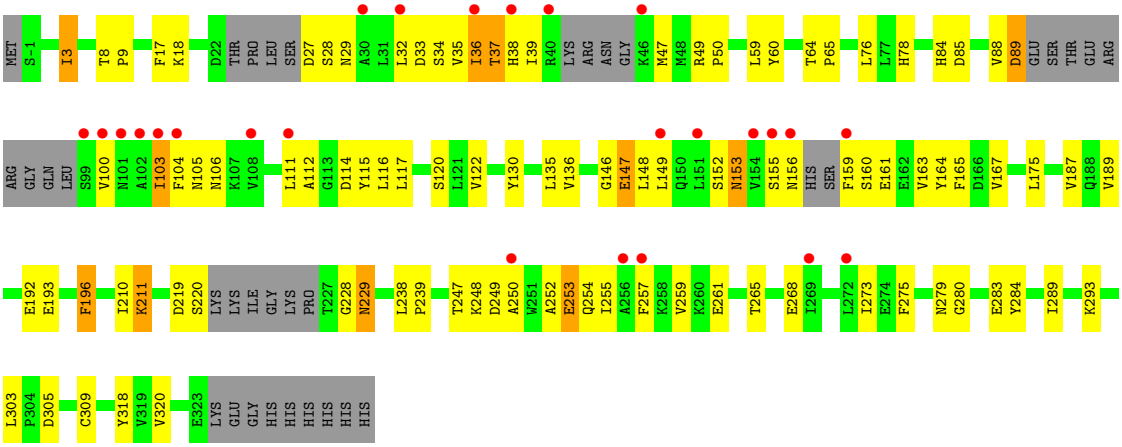
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	43	Total O 43 43	0	0
2	B	26	Total O 26 26	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

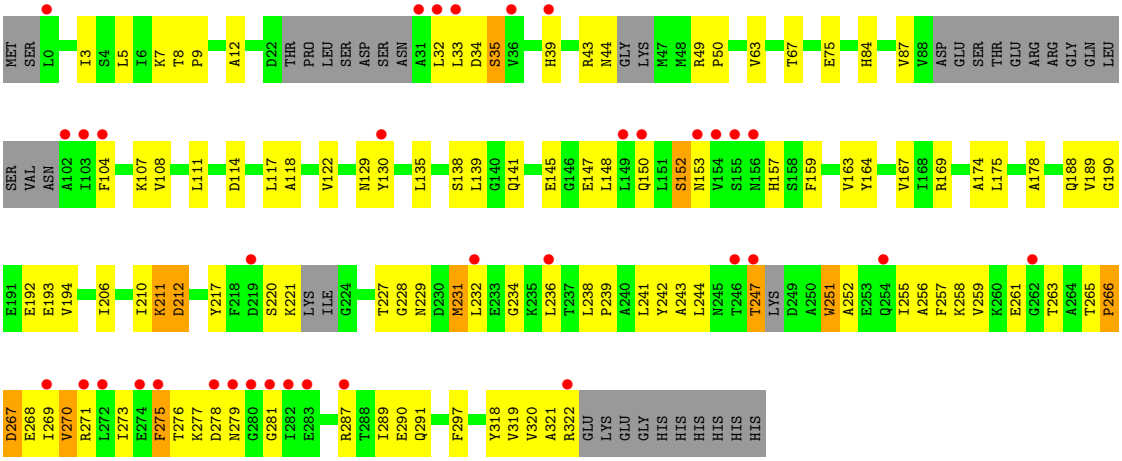
• Molecule 1: Octaprenyl-diphosphate synthase

Chain A:



• Molecule 1: Octaprenyl-diphosphate synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.62Å 111.41Å 83.38Å 90.00° 92.56° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 44.57 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.30) 99.2 (44.57-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.258 0.217 , 0.267	Depositor DCC
R_{free} test set	1287 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å^2)	46.5	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4627	wwPDB-VP
Average B, all atoms (Å^2)	67.0	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.*

[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

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	0.48	0/2335	0.59	0/3168
1	B	0.47	0/2295	0.53	0/3119
All	All	0.48	0/4630	0.56	0/6287

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2301	0	2283	112	0
1	B	2257	0	2216	123	0
2	A	43	0	0	0	0
2	B	26	0	0	3	0
All	All	4627	0	4499	221	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 24.

All (221) 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:36:ILE:HD12	1:A:36:ILE:C	1.55	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD22	1:B:145:GLU:HG3	1.25	1.15
1:A:33:ASP:O	1:A:37:THR:HB	1.46	1.15
1:A:88:VAL:HG13	1:A:89:ASP:OD1	1.49	1.12
1:B:49:ARG:HD3	1:B:175:LEU:HD12	1.25	1.07
1:A:103:ILE:O	1:A:103:ILE:HD12	1.56	1.04
1:A:275:PHE:CE1	1:A:279:ASN:ND2	2.30	0.99
1:B:269:ILE:O	1:B:273:ILE:HG13	1.62	0.99
1:A:36:ILE:HD12	1:A:36:ILE:O	1.61	0.98
1:A:249:ASP:O	1:A:253:GLU:HG3	1.64	0.96
1:A:255:ILE:HD12	1:A:268:GLU:OE2	1.65	0.96
1:A:36:ILE:C	1:A:36:ILE:CD1	2.29	0.93
1:A:32:LEU:O	1:A:36:ILE:HG23	1.67	0.93
1:B:251:TRP:CD1	1:B:255:ILE:HD11	2.04	0.91
1:A:293:LYS:HD2	1:A:320:VAL:HG21	1.52	0.90
1:B:49:ARG:HD3	1:B:175:LEU:CD1	1.99	0.90
1:A:117:LEU:HD23	1:B:117:LEU:HD23	1.54	0.89
1:B:243:ALA:HB1	1:B:275:PHE:CZ	2.08	0.88
1:A:36:ILE:HD12	1:A:37:THR:N	1.89	0.87
1:A:85:ASP:O	1:A:88:VAL:HG12	1.75	0.86
1:A:29:ASN:HB3	1:A:32:LEU:HB3	1.57	0.86
1:A:103:ILE:C	1:A:103:ILE:HD12	1.96	0.85
1:B:267:ASP:O	1:B:270:VAL:HB	1.76	0.85
1:A:29:ASN:HB3	1:A:32:LEU:CB	2.09	0.83
1:B:227:THR:HG22	1:B:273:ILE:CD1	2.09	0.83
1:B:104:PHE:O	1:B:108:VAL:HG23	1.78	0.82
1:A:146:GLY:O	1:A:149:LEU:HB3	1.82	0.79
1:A:34:SER:O	1:A:38:HIS:HB2	1.85	0.77
1:A:29:ASN:CB	1:A:32:LEU:HB3	2.14	0.77
1:A:103:ILE:HG13	1:A:104:PHE:N	1.98	0.76
1:B:251:TRP:CD1	1:B:252:ALA:N	2.55	0.75
1:B:227:THR:CG2	1:B:273:ILE:HD13	2.17	0.75
1:B:232:LEU:O	1:B:232:LEU:HD12	1.87	0.74
1:B:231:MET:O	1:B:259:VAL:HG13	1.86	0.74
1:A:255:ILE:CD1	1:A:268:GLU:OE2	2.37	0.72
1:B:243:ALA:CB	1:B:275:PHE:CZ	2.73	0.71
1:B:270:VAL:HG12	1:B:271:ARG:N	2.06	0.70
1:A:76:LEU:CB	1:A:120[A]:SER:OG	2.39	0.69
1:B:251:TRP:HD1	1:B:255:ILE:HD11	1.57	0.69
1:B:227:THR:HG22	1:B:273:ILE:HD13	1.73	0.69
1:B:148:LEU:CD1	1:B:148:LEU:N	2.56	0.68
1:B:251:TRP:C	1:B:251:TRP:CD1	2.65	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ILE:HG22	1:B:277:LYS:HE3	1.75	0.67
1:A:117:LEU:HD23	1:B:117:LEU:CD2	2.24	0.67
1:B:273:ILE:O	1:B:277:LYS:HG3	1.94	0.67
1:B:211:LYS:HB3	1:B:322:ARG:HH12	1.59	0.67
1:A:280:GLY:HA2	1:A:283:GLU:OE1	1.96	0.66
1:A:106:ASN:HD22	1:A:106:ASN:N	1.91	0.66
1:B:163:VAL:O	1:B:167:VAL:HG23	1.94	0.66
1:A:275:PHE:CD1	1:A:279:ASN:ND2	2.63	0.65
1:A:36:ILE:CD1	1:A:37:THR:N	2.53	0.65
1:B:321:ALA:O	1:B:322:ARG:C	2.36	0.64
1:B:148:LEU:HD12	1:B:148:LEU:N	2.12	0.64
1:B:236:LEU:O	1:B:241:LEU:HG	1.98	0.64
1:B:164:TYR:CE2	1:B:238:LEU:HB2	2.33	0.64
1:B:239:PRO:HB3	1:B:281:GLY:O	1.99	0.63
1:A:29:ASN:CB	1:A:32:LEU:CB	2.74	0.63
1:A:229:ASN:HD22	1:A:229:ASN:C	1.99	0.62
1:A:76:LEU:HB3	1:A:120[A]:SER:OG	2.00	0.62
1:A:228:GLY:HA2	1:A:273:ILE:HD11	1.81	0.62
1:B:227:THR:CG2	1:B:273:ILE:CD1	2.75	0.62
1:B:43:ARG:O	1:B:44:ASN:C	2.38	0.61
1:A:147:GLU:HG3	1:A:147:GLU:O	1.99	0.61
1:A:36:ILE:CG1	1:A:37:THR:N	2.62	0.61
1:A:103:ILE:C	1:A:103:ILE:CD1	2.58	0.61
1:A:117:LEU:CD2	1:B:117:LEU:HD23	2.28	0.61
1:B:257:PHE:O	1:B:261:GLU:CB	2.49	0.61
1:B:75:GLU:OE1	1:B:75:GLU:HA	2.01	0.60
1:A:18:LYS:CE	1:A:47:MET:SD	2.89	0.60
1:A:34:SER:O	1:A:38:HIS:CB	2.50	0.60
1:A:155:SER:O	1:A:156:ASN:C	2.40	0.60
1:A:228:GLY:CA	1:A:273:ILE:HD11	2.32	0.59
1:A:103:ILE:CG1	1:A:104:PHE:N	2.64	0.59
1:A:100:VAL:O	1:A:103:ILE:HG23	2.03	0.59
1:B:217:TYR:CE1	1:B:276:THR:HG21	2.38	0.59
1:B:243:ALA:O	1:B:247:THR:HB	2.02	0.59
1:A:122:VAL:HG13	2:B:333:HOH:O	2.02	0.58
1:B:275:PHE:CD1	1:B:279:ASN:ND2	2.71	0.58
1:A:250:ALA:O	1:A:254:GLN:HB2	2.02	0.58
1:A:160:SER:OG	1:A:163:VAL:HG23	2.03	0.58
1:A:76:LEU:HB2	1:A:120[A]:SER:OG	2.02	0.58
1:B:3:ILE:H	1:B:3:ILE:HD12	1.67	0.58
1:A:104:PHE:O	1:A:105:ASN:C	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HD12	1:A:37:THR:CA	2.33	0.58
1:B:231:MET:O	1:B:259:VAL:CG1	2.51	0.58
1:B:290:GLU:HG3	2:B:350:HOH:O	2.04	0.57
1:A:135:LEU:C	1:A:135:LEU:HD23	2.25	0.57
1:B:243:ALA:CB	1:B:275:PHE:CE2	2.88	0.56
1:B:251:TRP:CD1	1:B:255:ILE:CD1	2.84	0.56
1:A:29:ASN:HB3	1:A:32:LEU:H	1.71	0.56
1:B:3:ILE:N	1:B:3:ILE:HD12	2.21	0.56
1:B:227:THR:CG2	1:B:228:GLY:N	2.68	0.56
1:A:36:ILE:HG13	1:A:37:THR:N	2.21	0.55
1:A:59:LEU:HD22	1:A:303:LEU:HD13	1.88	0.55
1:B:275:PHE:CD2	1:B:276:THR:N	2.74	0.55
1:B:159:PHE:CE2	1:B:244:LEU:HD13	2.41	0.55
1:A:18:LYS:HE2	1:A:47:MET:SD	2.47	0.55
1:A:18:LYS:HE3	1:A:47:MET:SD	2.47	0.55
1:A:163:VAL:O	1:A:167:VAL:HG23	2.06	0.55
1:A:252:ALA:O	1:A:254:GLN:N	2.40	0.54
1:B:265:THR:O	1:B:267:ASP:N	2.40	0.54
1:B:251:TRP:CG	1:B:252:ALA:N	2.75	0.53
1:A:164:TYR:CE2	1:A:238:LEU:HB2	2.43	0.53
1:B:32:LEU:O	1:B:34:ASP:N	2.42	0.53
1:B:227:THR:HG22	1:B:228:GLY:N	2.23	0.53
1:A:114:ASP:OD2	1:B:84:HIS:ND1	2.40	0.53
1:A:88:VAL:CG1	1:A:89:ASP:OD1	2.40	0.53
1:A:252:ALA:C	1:A:254:GLN:N	2.62	0.52
1:B:266:PRO:O	1:B:270:VAL:HG23	2.09	0.52
1:A:84:HIS:ND1	1:B:114:ASP:OD2	2.29	0.52
1:A:148:LEU:HD13	1:B:111:LEU:HB3	1.92	0.52
1:A:192:GLU:HG2	1:A:193:GLU:N	2.25	0.52
1:A:211:LYS:HD2	1:A:320:VAL:O	2.09	0.52
1:A:3:ILE:HD11	1:A:318:TYR:CE1	2.45	0.51
1:B:135:LEU:HD23	1:B:135:LEU:C	2.31	0.51
1:A:28:SER:N	1:B:145:GLU:OE1	2.43	0.51
1:B:243:ALA:HB3	1:B:275:PHE:CE2	2.46	0.51
1:A:252:ALA:C	1:A:254:GLN:H	2.13	0.51
1:B:217:TYR:HE1	1:B:276:THR:HG21	1.75	0.51
1:A:39:ILE:HD11	1:A:116:LEU:HD11	1.92	0.50
1:A:32:LEU:CD2	1:B:145:GLU:HG3	2.18	0.50
1:B:319:VAL:O	1:B:319:VAL:CG1	2.60	0.50
1:A:161:GLU:OE2	1:A:284:TYR:OH	2.30	0.50
1:B:243:ALA:HB1	1:B:275:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ASP:OD1	1:B:278:ASP:O	2.30	0.50
1:A:130:TYR:CE2	1:B:130:TYR:CE2	2.99	0.49
1:B:3:ILE:HG23	1:B:7:LYS:HE3	1.94	0.49
1:B:150:GLN:O	1:B:153:ASN:HB3	2.11	0.49
1:B:267:ASP:O	1:B:270:VAL:CB	2.56	0.48
1:B:32:LEU:O	1:B:35:SER:N	2.36	0.48
1:A:149:LEU:O	1:A:153:ASN:ND2	2.45	0.48
1:B:212:ASP:OD1	1:B:322:ARG:NH2	2.46	0.48
1:B:234:GLY:HA2	1:B:259:VAL:HG12	1.95	0.48
1:B:211:LYS:CB	1:B:322:ARG:HH12	2.27	0.48
1:B:251:TRP:NE1	1:B:255:ILE:HD11	2.28	0.48
1:B:270:VAL:CG1	1:B:271:ARG:N	2.73	0.48
1:A:36:ILE:HD12	1:A:37:THR:HA	1.95	0.48
1:B:49:ARG:CD	1:B:175:LEU:CD1	2.85	0.48
1:B:265:THR:H	1:B:268:GLU:HG3	1.79	0.47
1:A:85:ASP:OD1	1:A:147:GLU:OE1	2.32	0.47
1:A:219:ASP:O	1:A:220:SER:C	2.52	0.47
1:A:8:THR:N	1:A:9:PRO:CD	2.76	0.47
1:B:135:LEU:HD23	1:B:135:LEU:O	2.14	0.47
1:A:196:PHE:CD1	1:A:196:PHE:C	2.88	0.47
1:B:229:ASN:ND2	1:B:232:LEU:HD23	2.29	0.47
1:A:106:ASN:ND2	1:A:106:ASN:N	2.58	0.47
1:A:89:ASP:N	1:A:89:ASP:OD1	2.47	0.47
1:B:189:VAL:HG23	1:B:193:GLU:HB2	1.96	0.47
1:B:49:ARG:HB2	1:B:50:PRO:HD3	1.96	0.47
1:A:76:LEU:HB3	1:A:120[A]:SER:HG	1.78	0.47
1:B:129:ASN:OD1	1:B:129:ASN:C	2.53	0.47
1:B:138:SER:O	1:B:141:GLN:HB2	2.14	0.46
1:B:206:ILE:O	1:B:210:ILE:HG13	2.15	0.46
1:A:36:ILE:CD1	1:A:36:ILE:O	2.48	0.46
1:B:12:ALA:HB3	2:B:343:HOH:O	2.15	0.46
1:B:269:ILE:O	1:B:273:ILE:CG1	2.48	0.46
1:B:319:VAL:O	1:B:319:VAL:HG12	2.15	0.46
1:A:283:GLU:CD	1:A:283:GLU:H	2.19	0.46
1:B:231:MET:HA	1:B:259:VAL:HG11	1.97	0.46
1:A:29:ASN:HD21	1:B:148:LEU:C	2.19	0.46
1:A:229:ASN:C	1:A:229:ASN:ND2	2.68	0.45
1:B:139:LEU:HD21	1:B:175:LEU:HD23	1.97	0.45
1:A:111:LEU:HD13	1:B:147:GLU:HB3	1.98	0.45
1:B:268:GLU:C	1:B:270:VAL:H	2.20	0.45
1:B:3:ILE:H	1:B:3:ILE:CD1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:HG13	1:B:67:THR:HB	1.99	0.45
1:A:3:ILE:CD1	1:A:3:ILE:N	2.79	0.45
1:B:190:GLY:O	1:B:194:VAL:HG23	2.17	0.44
1:B:263:THR:OG1	1:B:263:THR:O	2.30	0.44
1:A:152:SER:O	1:A:153:ASN:C	2.56	0.44
1:B:135:LEU:HD21	1:B:178:ALA:HB1	2.00	0.44
1:B:229:ASN:O	1:B:232:LEU:HB3	2.18	0.44
1:A:64:THR:HB	1:A:65:PRO:HD2	2.00	0.43
1:B:234:GLY:HA2	1:B:259:VAL:O	2.18	0.43
1:B:118:ALA:O	1:B:122:VAL:HG23	2.17	0.43
1:A:78:HIS:HB2	1:A:175:LEU:HD21	2.00	0.43
1:B:192:GLU:CD	1:B:192:GLU:H	2.22	0.43
1:B:287:ARG:O	1:B:291:GLN:HG3	2.17	0.43
1:B:211:LYS:HG2	1:B:289:ILE:HD13	1.99	0.43
1:A:159:PHE:CD1	1:A:159:PHE:N	2.85	0.43
1:A:210:ILE:HG22	1:A:289:ILE:HD11	1.99	0.43
1:B:220:SER:O	1:B:221:LYS:C	2.57	0.43
1:A:165:PHE:HE2	1:A:210:ILE:HD11	1.84	0.43
1:B:244:LEU:HD23	1:B:275:PHE:CZ	2.53	0.43
1:B:242:TYR:CD2	1:B:242:TYR:C	2.93	0.42
1:B:84:HIS:CE1	1:B:114:ASP:OD1	2.72	0.42
1:B:8:THR:HB	1:B:9:PRO:HD3	2.01	0.42
1:B:32:LEU:C	1:B:34:ASP:N	2.73	0.42
1:A:135:LEU:HD23	1:A:136:VAL:N	2.34	0.42
1:A:60:TYR:HB2	1:A:187:VAL:HG21	2.02	0.42
1:A:130:TYR:CZ	1:B:130:TYR:CE2	3.07	0.42
1:A:64:THR:HB	1:A:65:PRO:CD	2.50	0.42
1:B:318:TYR:CD2	1:B:318:TYR:C	2.92	0.42
1:A:88:VAL:HG23	1:B:107:LYS:CB	2.50	0.42
1:B:251:TRP:O	1:B:255:ILE:HG13	2.20	0.42
1:A:247:THR:O	1:A:248:LYS:CB	2.67	0.42
1:A:255:ILE:O	1:A:259:VAL:HG23	2.20	0.42
1:B:5:LEU:HA	1:B:5:LEU:HD23	1.81	0.42
1:A:238:LEU:N	1:A:239:PRO:CD	2.83	0.41
1:B:148:LEU:O	1:B:152:SER:HB2	2.19	0.41
1:B:189:VAL:HG21	1:B:193:GLU:HB3	2.02	0.41
1:B:268:GLU:C	1:B:270:VAL:N	2.73	0.41
1:A:29:ASN:CB	1:A:32:LEU:HB2	2.49	0.41
1:B:211:LYS:HD2	1:B:320:VAL:O	2.20	0.41
1:A:189:VAL:HB	1:A:193:GLU:OE1	2.21	0.41
1:A:49:ARG:HB2	1:A:50:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LEU:HD11	1:B:256:ALA:HB2	2.01	0.41
1:A:32:LEU:HD11	1:A:115:TYR:CE2	2.56	0.41
1:B:257:PHE:O	1:B:261:GLU:N	2.48	0.41
1:B:258:LYS:CB	1:B:263:THR:O	2.68	0.41
1:A:17:PHE:C	1:A:17:PHE:CD2	2.94	0.41
1:A:252:ALA:O	1:A:253:GLU:C	2.58	0.41
1:B:169:ARG:O	1:B:174:ALA:HB2	2.20	0.41
1:A:305:ASP:OD2	1:A:309:CYS:HB3	2.20	0.41
1:A:228:GLY:HA3	1:A:273:ILE:HD11	2.03	0.41
1:A:257:PHE:O	1:A:261:GLU:HB2	2.21	0.41
1:B:153:ASN:O	1:B:153:ASN:OD1	2.39	0.41
1:B:84:HIS:O	1:B:87:VAL:HG12	2.21	0.40
1:A:35:VAL:HG11	1:A:112:ALA:HB2	2.03	0.40
1:A:39:ILE:CD1	1:A:116:LEU:HD11	2.51	0.40
1:B:148:LEU:HD13	1:B:148:LEU:N	2.36	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	288/334 (86%)	277 (96%)	10 (4%)	1 (0%)	41	50
1	B	287/334 (86%)	267 (93%)	18 (6%)	2 (1%)	22	26
All	All	575/668 (86%)	544 (95%)	28 (5%)	3 (0%)	29	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	LEU
1	A	253	GLU
1	B	266	PRO

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	246/282 (87%)	234 (95%)	12 (5%)	25 35
1	B	235/282 (83%)	221 (94%)	14 (6%)	19 26
All	All	481/564 (85%)	455 (95%)	26 (5%)	22 30

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	27	ASP
1	A	36	ILE
1	A	37	THR
1	A	89	ASP
1	A	103	ILE
1	A	147	GLU
1	A	153	ASN
1	A	196	PHE
1	A	211	LYS
1	A	229	ASN
1	A	265	THR
1	B	35	SER
1	B	39	HIS
1	B	152	SER
1	B	157	HIS
1	B	188	GLN
1	B	211	LYS
1	B	212	ASP
1	B	231	MET
1	B	247	THR
1	B	251	TRP
1	B	267	ASP
1	B	270	VAL
1	B	275	PHE
1	B	297	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	106	ASN
1	A	229	ASN
1	A	245	ASN
1	A	291	GLN
1	B	106	ASN
1	B	126	GLN
1	B	141	GLN
1	B	150	GLN
1	B	229	ASN
1	B	279	ASN
1	B	291	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} 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	299/334 (89%)	0.42	25 (8%)	11	15	31, 59, 110, 132	0
1	B	297/334 (88%)	0.59	36 (12%)	4	6	31, 63, 122, 133	0
All	All	596/668 (89%)	0.51	61 (10%)	6	9	31, 60, 118, 133	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	VAL	7.8
1	B	31	ALA	7.7
1	A	32	LEU	7.1
1	B	280	GLY	6.6
1	A	100	VAL	6.6
1	A	101	ASN	6.4
1	A	40	ARG	6.2
1	B	154	VAL	6.2
1	A	151	LEU	5.9
1	A	256	ALA	5.5
1	A	99	SER	5.3
1	B	103	ILE	5.0
1	B	281	GLY	4.8
1	A	257	PHE	4.8
1	B	39	HIS	4.8
1	A	36	ILE	4.4
1	A	111	LEU	4.4
1	B	275	PHE	4.4
1	A	103	ILE	4.4
1	A	102	ALA	4.2
1	B	282	ILE	4.1
1	A	149	LEU	3.9
1	A	104	PHE	3.8
1	B	269	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	33	LEU	3.7
1	B	278	ASP	3.7
1	B	155	SER	3.7
1	B	246	THR	3.5
1	B	219	ASP	3.5
1	B	271	ARG	3.4
1	A	46	LYS	3.4
1	A	30	ALA	3.3
1	A	108	VAL	3.3
1	B	283	GLU	3.2
1	B	0	LEU	3.2
1	B	156	ASN	3.2
1	B	322	ARG	3.1
1	B	149	LEU	3.1
1	B	32	LEU	3.0
1	A	155	SER	3.0
1	B	279	ASN	2.9
1	B	232	LEU	2.9
1	A	156	ASN	2.8
1	B	254	GLN	2.7
1	B	247	THR	2.6
1	B	150	GLN	2.6
1	A	38	HIS	2.5
1	B	104	PHE	2.4
1	B	287	ARG	2.3
1	A	269	ILE	2.3
1	B	36	VAL	2.3
1	A	250	ALA	2.3
1	A	159	PHE	2.2
1	B	236	LEU	2.2
1	B	272	LEU	2.2
1	B	274	GLU	2.2
1	A	272	LEU	2.1
1	B	102	ALA	2.1
1	B	130	TYR	2.1
1	B	262	GLY	2.0
1	B	153	ASN	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.