Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:09 am BST

PDB ID	:	2VG4
Title	:	Rv2361 native
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Deposited on	:	2007-11-08
Resolution	:	2.60 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 ①) were used in the production of this report:

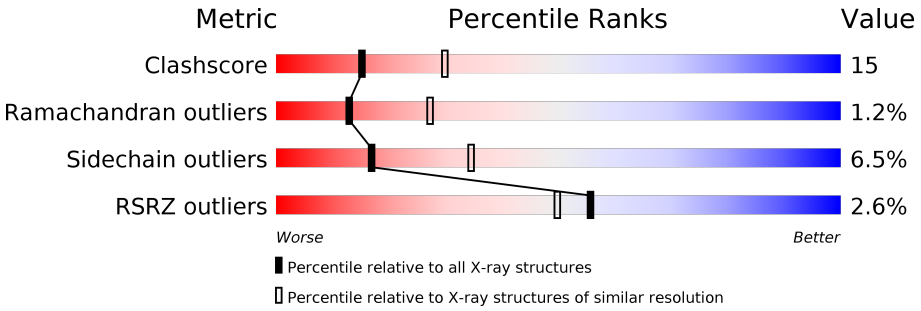
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	284	64% 35%
1	B	284	62% 35%
1	C	284	4% 65% 32%
1	D	284	5% 60% 37%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18112 atoms, of which 8956 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 UNDECAPRENYL PYROPHOSPHATE SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	H	N	O	S	0	0	0
			4529	1443	2241	422	414	9			
1	B	284	Total	C	H	N	O	S	0	0	0
			4529	1443	2241	422	414	9			
1	C	284	Total	C	H	N	O	S	0	0	0
			4529	1443	2241	422	414	9			
1	D	283	Total	C	H	N	O	S	0	0	0
			4510	1434	2233	421	413	9			

- Molecule 2 is water.

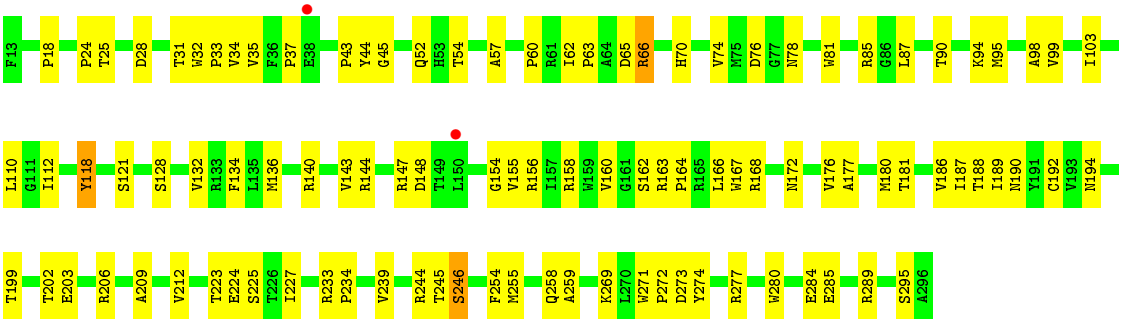
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		
2	B	6	Total	O	0	0
			6	6		
2	C	1	Total	O	0	0
			1	1		
2	D	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

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.

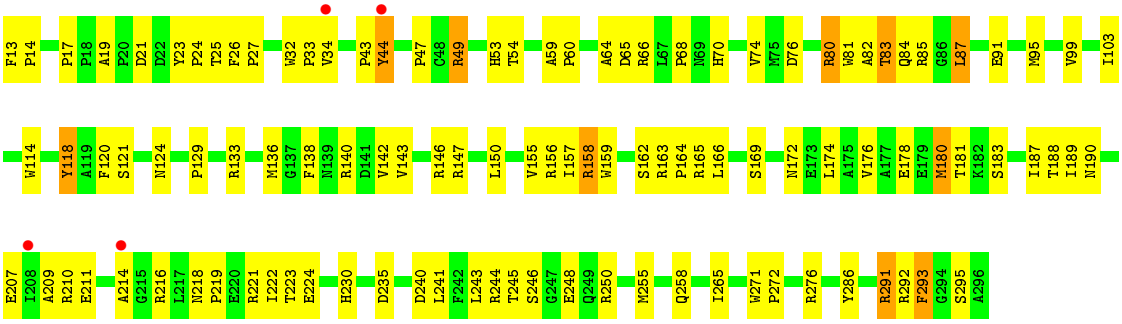
- Molecule 1: UNDECAPRENYL PYROPHOSPHATE SYNTHETASE

Chain A:



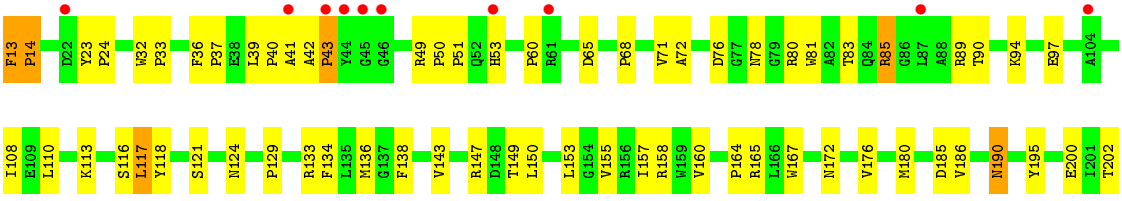
- Molecule 1: UNDECAPRENYL PYROPHOSPHATE SYNTHETASE

Chain B:



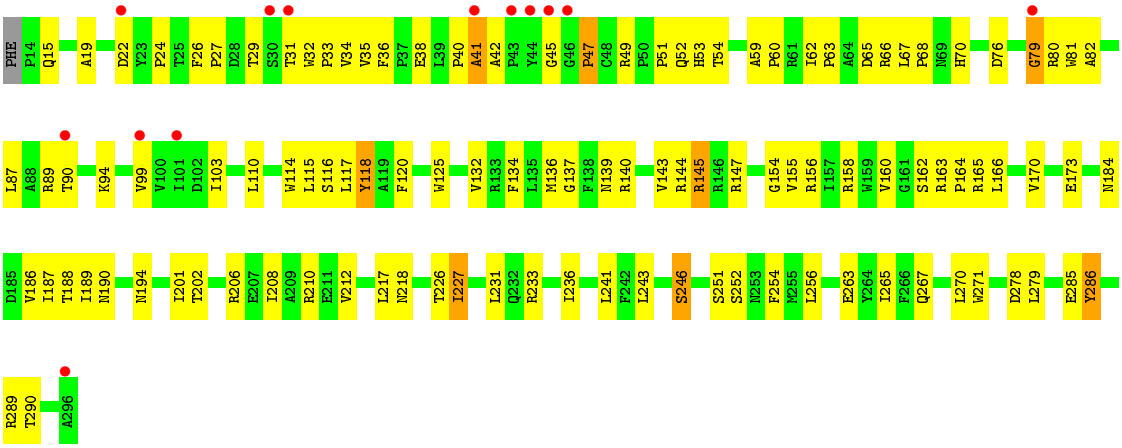
- Molecule 1: UNDECAPRENYL PYROPHOSPHATE SYNTHETASE

Chain C:



• Molecule 1: UNDECAPRENYL PYROPHOSPHATE SYNTHETASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	87.30Å 87.30Å 183.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.00 – 2.60 69.92 – 2.61	Depositor EDS
% Data completeness (in resolution range)	84.0 (52.00-2.60) 92.3 (69.92-2.61)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.62Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.216 , 0.255 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 15.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.065 for -h,-k,l 0.270 for h,-h-k,-l 0.066 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18112	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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	0.24	0/2350	0.46	0/3196
1	B	0.23	0/2350	0.45	0/3196
1	C	0.23	0/2350	0.46	0/3196
1	D	0.23	0/2338	0.45	0/3179
All	All	0.23	0/9388	0.45	0/12767

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	2288	2241	2245	79	0
1	B	2288	2241	2245	73	0
1	C	2288	2241	2245	67	0
1	D	2277	2233	2237	61	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
All	All	9156	8956	8972	272	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 (272) 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:B:43:PRO:O	1:B:44:TYR:HB2	1.84	0.77
1:A:245:THR:HG23	1:A:269:LYS:O	1.88	0.72
1:C:13:PHE:N	1:C:14:PRO:HA	2.05	0.71
1:A:66:ARG:HH11	1:A:66:ARG:HG2	1.55	0.71
1:A:44:TYR:HB2	1:A:45:GLY:HA3	1.73	0.69
1:D:144:ARG:HA	1:D:147:ARG:HD3	1.73	0.68
1:C:13:PHE:N	1:C:14:PRO:CA	2.57	0.68
1:B:255:MET:HE3	1:B:258:GLN:HB2	1.77	0.67
1:A:60:PRO:HD2	1:A:110:LEU:HD13	1.78	0.66
1:C:172:ASN:O	1:C:176:VAL:HG23	1.96	0.65
1:A:34:VAL:HG21	1:A:98:ALA:HB2	1.78	0.65
1:A:70:HIS:CE1	1:A:239:VAL:HG22	2.32	0.64
1:A:44:TYR:HB2	1:A:45:GLY:CA	2.28	0.64
1:A:110:LEU:HD23	1:A:112:ILE:HD11	1.80	0.64
1:C:85:ARG:CG	1:C:85:ARG:HH11	2.11	0.63
1:C:42:ALA:N	1:C:43:PRO:HD3	2.15	0.61
1:C:245:THR:HB	1:C:269:LYS:O	2.00	0.61
1:C:39:LEU:HD21	1:C:51:PRO:HG3	1.82	0.61
1:A:160:VAL:HG21	1:A:190:ASN:HB3	1.84	0.59
1:C:243:LEU:HD11	1:C:282:ALA:CB	2.32	0.59
1:B:155:VAL:HG11	1:B:189:ILE:HD12	1.85	0.58
1:A:81:TRP:CZ3	1:A:95:MET:HG3	2.39	0.58
1:D:67:LEU:HD12	1:D:68:PRO:HD2	1.86	0.58
1:A:31:THR:HG21	1:A:35:VAL:HG23	1.85	0.58
1:A:43:PRO:N	1:A:44:TYR:HA	2.19	0.58
1:D:243:LEU:HD23	1:D:265:ILE:HB	1.85	0.58
1:C:239:VAL:HG23	1:C:258:GLN:HB3	1.85	0.58
1:D:166:LEU:HD11	1:D:170:VAL:HG11	1.84	0.57
1:D:155:VAL:HG22	1:D:187:ILE:CG2	2.35	0.57
1:A:110:LEU:HD22	1:A:280:TRP:CD1	2.40	0.57
1:B:53:HIS:HB2	1:B:276:ARG:HD2	1.88	0.56
1:C:160:VAL:HA	1:C:232:GLN:OE1	2.05	0.56
1:D:53:HIS:CG	1:D:54:THR:H	2.22	0.56
1:B:23:TYR:CD2	1:B:24:PRO:HD2	2.41	0.56
1:D:62:ILE:HD12	1:D:110:LEU:HD11	1.88	0.56
1:A:63:PRO:HB2	1:A:65:ASP:OD1	2.05	0.56
1:D:36:PHE:CE1	1:D:51:PRO:HG3	2.41	0.56
1:B:87:LEU:HD12	1:B:91:GLU:HB2	1.88	0.56
1:D:233:ARG:O	1:D:236:ILE:HG13	2.06	0.56
1:B:19:ALA:HB2	1:B:49:ARG:NH2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HA	1:A:52:GLN:O	2.06	0.55
1:A:223:THR:HG22	1:A:224:GLU:N	2.20	0.55
1:B:85:ARG:HB2	1:B:87:LEU:HD21	1.88	0.55
1:B:163:ARG:N	1:B:164:PRO:CD	2.69	0.55
1:C:176:VAL:O	1:C:180:MET:HG3	2.07	0.55
1:C:24:PRO:HB3	1:C:37:PRO:HB2	1.89	0.55
1:A:103:ILE:HD11	1:A:274:TYR:CD2	2.42	0.54
1:B:74:VAL:HB	1:B:244:ARG:HD2	1.88	0.54
1:C:164:PRO:O	1:C:165:ARG:HB2	2.07	0.54
1:D:32:TRP:NE1	1:D:94:LYS:HB3	2.22	0.54
1:A:144:ARG:HD3	1:B:293:PHE:CD1	2.42	0.54
1:D:82:ALA:HB3	1:D:89:ARG:HA	1.89	0.54
1:B:99:VAL:O	1:B:103:ILE:HD13	2.08	0.54
1:A:32:TRP:HA	1:A:33:PRO:C	2.26	0.54
1:B:209:ALA:HB1	1:D:212:VAL:HG21	1.89	0.54
1:A:60:PRO:HD2	1:A:110:LEU:CD1	2.38	0.53
1:D:29:THR:HA	1:D:34:VAL:HG22	1.90	0.53
1:D:76:ASP:O	1:D:271:TRP:HB2	2.08	0.53
1:C:39:LEU:HD11	1:C:51:PRO:HD3	1.90	0.53
1:C:23:TYR:CG	1:C:24:PRO:HD2	2.43	0.53
1:A:160:VAL:O	1:A:192:CYS:HA	2.08	0.53
1:C:242:PHE:HB3	1:C:264:TYR:HD1	1.72	0.53
1:A:76:ASP:HB3	1:A:245:THR:O	2.09	0.53
1:B:157:ILE:HD12	1:B:189:ILE:O	2.09	0.53
1:A:160:VAL:HG22	1:A:233:ARG:HG3	1.90	0.53
1:D:33:PRO:HG2	1:D:145:ARG:NH1	2.24	0.53
1:B:23:TYR:CE2	1:B:49:ARG:HG2	2.44	0.52
1:C:206:ARG:O	1:C:210:ARG:HG3	2.08	0.52
1:A:118:TYR:CZ	1:A:121:SER:HB3	2.45	0.52
1:A:172:ASN:O	1:A:176:VAL:HG23	2.09	0.52
1:B:140:ARG:HD3	1:B:169:SER:HB3	1.91	0.51
1:A:176:VAL:O	1:A:180:MET:HG3	2.10	0.51
1:D:53:HIS:CG	1:D:54:THR:N	2.78	0.51
1:B:138:PHE:O	1:B:142:VAL:HG23	2.09	0.51
1:D:90:THR:HB	1:D:134:PHE:CE2	2.46	0.51
1:B:14:PRO:HG3	1:B:64:ALA:HB2	1.91	0.51
1:D:19:ALA:HB2	1:D:49:ARG:CZ	2.41	0.51
1:C:113:LYS:O	1:C:113:LYS:HG3	2.11	0.51
1:B:155:VAL:O	1:B:181:THR:HB	2.11	0.50
1:B:87:LEU:HD12	1:B:91:GLU:CB	2.41	0.50
1:A:156:ARG:HG3	1:A:181:THR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:SER:HB3	1:D:270:LEU:HD22	1.93	0.50
1:B:118:TYR:CZ	1:B:121:SER:HB3	2.46	0.50
1:C:269:LYS:HD3	1:C:274:TYR:HA	1.94	0.50
1:A:223:THR:HG22	1:A:225:SER:H	1.76	0.50
1:C:110:LEU:HD22	1:C:280:TRP:CD1	2.47	0.50
1:A:147:ARG:HG2	1:A:177:ALA:HB2	1.93	0.50
1:B:129:PRO:O	1:B:133:ARG:HB2	2.12	0.49
1:D:160:VAL:HG21	1:D:190:ASN:HB3	1.92	0.49
1:B:241:LEU:HD11	1:B:265:ILE:HD12	1.95	0.49
1:B:255:MET:HE3	1:B:258:GLN:CB	2.42	0.49
1:B:293:PHE:CD2	1:B:293:PHE:C	2.85	0.49
1:C:212:VAL:HG22	1:C:217:LEU:HG	1.94	0.49
1:A:269:LYS:HD3	1:A:273:ASP:O	2.13	0.49
1:A:271:TRP:N	1:A:272:PRO:CD	2.75	0.49
1:D:251:SER:O	1:D:252:SER:HB2	2.12	0.49
1:A:162:SER:OG	1:A:164:PRO:HD2	2.13	0.49
1:C:143:VAL:O	1:C:147:ARG:HD3	2.13	0.48
1:C:264:TYR:HB3	1:C:266:PHE:CE2	2.48	0.48
1:B:85:ARG:HB2	1:B:87:LEU:CD2	2.43	0.48
1:A:44:TYR:CB	1:A:45:GLY:HA3	2.39	0.48
1:B:53:HIS:HB2	1:B:276:ARG:CD	2.44	0.48
1:D:65:ASP:OD1	1:D:65:ASP:C	2.50	0.48
1:A:285:GLU:HG2	1:A:289:ARG:HH22	1.78	0.48
1:A:163:ARG:N	1:A:164:PRO:CD	2.77	0.47
1:A:34:VAL:HG21	1:A:98:ALA:CB	2.44	0.47
1:B:219:PRO:HA	1:B:222:ILE:HG13	1.95	0.47
1:C:49:ARG:HG2	1:C:50:PRO:HD2	1.96	0.47
1:D:155:VAL:N	1:D:184:ASN:HD22	2.12	0.47
1:A:110:LEU:HD22	1:A:280:TRP:HD1	1.78	0.47
1:A:28:ASP:O	1:A:34:VAL:HG13	2.14	0.47
1:D:120:PHE:HB3	1:D:194:ASN:H	1.79	0.47
1:B:23:TYR:CZ	1:B:49:ARG:HG2	2.49	0.47
1:D:164:PRO:O	1:D:165:ARG:HB2	2.14	0.47
1:B:81:TRP:CD1	1:B:272:PRO:HB2	2.49	0.47
1:A:144:ARG:HA	1:A:147:ARG:HD3	1.96	0.47
1:D:26:PHE:CG	1:D:27:PRO:HA	2.50	0.47
1:A:44:TYR:HD2	1:A:45:GLY:O	1.98	0.47
1:B:146:ARG:O	1:B:150:LEU:HG	2.14	0.47
1:C:41:ALA:O	1:C:42:ALA:HB3	2.14	0.47
1:D:63:PRO:HB2	1:D:66:ARG:HB2	1.97	0.47
1:C:242:PHE:CD2	1:C:264:TYR:CD1	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG11	1:A:189:ILE:HD12	1.97	0.47
1:B:25:THR:HB	1:B:54:THR:HA	1.97	0.47
1:C:76:ASP:HB3	1:C:246:SER:HB3	1.97	0.47
1:C:241:LEU:HG	1:C:243:LEU:HD23	1.96	0.46
1:B:157:ILE:O	1:B:178:GLU:HA	2.14	0.46
1:B:172:ASN:O	1:B:176:VAL:HG23	2.15	0.46
1:B:211:GLU:OE2	1:B:230:HIS:NE2	2.48	0.46
1:B:291:ARG:HG3	1:B:295:SER:CB	2.45	0.46
1:D:154:GLY:HA3	1:D:186:VAL:CG2	2.46	0.46
1:C:242:PHE:HB3	1:C:264:TYR:CD1	2.50	0.46
1:D:137:GLY:O	1:D:140:ARG:HB3	2.15	0.46
1:B:207:GLU:HA	1:B:210:ARG:HD2	1.97	0.46
1:A:212:VAL:CG1	1:C:213:ALA:HB2	2.46	0.46
1:B:164:PRO:O	1:B:165:ARG:HB2	2.14	0.46
1:C:149:THR:O	1:C:153:LEU:HG	2.16	0.46
1:C:241:LEU:HD11	1:C:265:ILE:HD12	1.98	0.46
1:C:78:ASN:OD1	1:C:271:TRP:HB3	2.16	0.46
1:B:43:PRO:O	1:B:44:TYR:CB	2.60	0.46
1:C:85:ARG:HG3	1:C:85:ARG:HH11	1.79	0.46
1:D:36:PHE:CZ	1:D:51:PRO:HG3	2.51	0.46
1:A:255:MET:O	1:A:259:ALA:HB3	2.16	0.46
1:C:60:PRO:CG	1:C:280:TRP:HB3	2.46	0.46
1:D:118:TYR:CE1	1:D:254:PHE:HB2	2.51	0.46
1:B:80:ARG:O	1:B:84:GLN:HG3	2.16	0.46
1:B:87:LEU:H	1:B:87:LEU:HD23	1.81	0.45
1:A:166:LEU:HD13	1:A:194:ASN:HB2	1.98	0.45
1:D:70:HIS:CD2	1:D:114:TRP:HB3	2.51	0.45
1:B:162:SER:HB2	1:B:164:PRO:HD2	1.98	0.45
1:C:24:PRO:HG2	1:C:39:LEU:HD22	1.99	0.45
1:D:241:LEU:HD22	1:D:286:TYR:CB	2.46	0.45
1:B:23:TYR:CG	1:B:24:PRO:CD	3.00	0.45
1:C:228:ALA:O	1:C:234:PRO:HB3	2.17	0.45
1:C:68:PRO:HB2	1:C:71:VAL:CG2	2.47	0.45
1:D:32:TRP:CZ2	1:D:94:LYS:HG2	2.51	0.45
1:C:249:GLN:HA	1:C:266:PHE:CE1	2.52	0.45
1:A:99:VAL:HG11	1:A:274:TYR:HB3	1.98	0.45
1:C:23:TYR:CE1	1:C:40:PRO:HG2	2.52	0.45
1:C:116:SER:O	1:C:117:LEU:HD12	2.17	0.45
1:A:110:LEU:HD23	1:A:112:ILE:CD1	2.47	0.44
1:B:156:ARG:HG2	1:B:188:THR:HG23	1.99	0.44
1:A:255:MET:HB3	1:A:258:GLN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:CG2	1:A:98:ALA:HB2	2.46	0.44
1:B:211:GLU:HG2	1:B:216:ARG:HE	1.81	0.44
1:C:286:TYR:C	1:C:286:TYR:CD2	2.90	0.44
1:A:147:ARG:HG2	1:A:177:ALA:CB	2.48	0.44
1:A:245:THR:CG2	1:A:246:SER:N	2.80	0.44
1:B:70:HIS:CD2	1:B:114:TRP:HB3	2.52	0.44
1:D:45:GLY:O	1:D:47:PRO:HD2	2.17	0.44
1:A:25:THR:HB	1:A:54:THR:HA	1.99	0.44
1:A:66:ARG:HH11	1:A:66:ARG:CG	2.28	0.44
1:B:76:ASP:OD2	1:B:248:GLU:HG3	2.18	0.44
1:A:103:ILE:HD11	1:A:274:TYR:CE2	2.53	0.44
1:B:147:ARG:HD2	1:B:180:MET:SD	2.58	0.44
1:B:114:TRP:CH2	1:B:235:ASP:O	2.71	0.44
1:B:250:ARG:HD3	1:D:263:GLU:OE2	2.17	0.44
1:A:95:MET:HB2	1:A:272:PRO:HB3	2.00	0.43
1:C:97:GLU:HB2	1:C:138:PHE:HZ	1.83	0.43
1:D:286:TYR:C	1:D:286:TYR:CD2	2.91	0.43
1:B:271:TRP:N	1:B:272:PRO:CD	2.80	0.43
1:D:15:GLN:HG3	1:D:110:LEU:HD12	1.99	0.43
1:A:154:GLY:HA3	1:A:186:VAL:CG2	2.49	0.43
1:B:59:ALA:HA	1:B:60:PRO:HD3	1.90	0.43
1:D:217:LEU:HG	1:D:218:ASN:N	2.33	0.43
1:D:82:ALA:HB1	1:D:87:LEU:HB2	2.00	0.43
1:B:68:PRO:HG3	1:B:286:TYR:CD2	2.53	0.43
1:A:209:ALA:HB1	1:C:212:VAL:HG21	2.00	0.43
1:C:271:TRP:HB3	1:C:272:PRO:HD3	1.99	0.43
1:A:85:ARG:HB2	1:A:87:LEU:HD12	1.99	0.43
1:D:206:ARG:O	1:D:210:ARG:HG3	2.18	0.43
1:A:187:ILE:HG12	1:A:188:THR:N	2.33	0.43
1:B:23:TYR:CG	1:B:24:PRO:HD2	2.53	0.43
1:D:116:SER:O	1:D:117:LEU:HD23	2.18	0.43
1:D:278:ASP:O	1:D:279:LEU:C	2.57	0.43
1:C:85:ARG:CG	1:C:85:ARG:NH1	2.76	0.43
1:D:136:MET:HA	1:D:136:MET:CE	2.48	0.43
1:D:59:ALA:HA	1:D:60:PRO:HD3	1.88	0.43
1:C:241:LEU:HG	1:C:243:LEU:CD2	2.49	0.43
1:C:255:MET:HB3	1:C:258:GLN:HB2	2.01	0.43
1:D:115:LEU:O	1:D:189:ILE:HA	2.19	0.43
1:D:201:ILE:HD11	1:D:256:LEU:HD23	2.01	0.43
1:A:24:PRO:HB3	1:A:37:PRO:HB3	2.01	0.43
1:C:81:TRP:CD1	1:C:273:ASP:OD1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ILE:HG23	1:D:217:LEU:CD2	2.48	0.43
1:A:57:ALA:HB2	1:A:277:ARG:HD3	2.01	0.42
1:A:74:VAL:HB	1:A:244:ARG:HD2	2.01	0.42
1:C:136:MET:HB3	1:C:167:TRP:CD2	2.54	0.42
1:A:147:ARG:CG	1:A:177:ALA:HB2	2.49	0.42
1:A:254:PHE:O	1:A:255:MET:C	2.58	0.42
1:C:108:ILE:HG12	1:C:186:VAL:HG12	2.01	0.42
1:C:72:ALA:HB1	1:C:254:PHE:HE2	1.84	0.42
1:B:120:PHE:CE1	1:B:124:ASN:CB	3.02	0.42
1:B:83:THR:C	1:B:85:ARG:H	2.22	0.42
1:D:227:ILE:O	1:D:231:LEU:HG	2.19	0.42
1:C:32:TRP:HA	1:C:33:PRO:C	2.39	0.42
1:C:68:PRO:HB2	1:C:71:VAL:HG22	2.00	0.42
1:A:223:THR:CG2	1:A:224:GLU:N	2.82	0.42
1:A:76:ASP:O	1:A:245:THR:HG22	2.20	0.42
1:B:158:ARG:NE	1:B:190:ASN:OD1	2.52	0.42
1:C:121:SER:O	1:C:124:ASN:HB2	2.19	0.42
1:A:94:LYS:HE3	1:A:134:PHE:CZ	2.55	0.42
1:C:200:GLU:HG2	1:C:231:LEU:HD22	2.01	0.42
1:B:159:TRP:HB2	1:B:174:LEU:HD13	2.02	0.42
1:C:36:PHE:CZ	1:C:149:THR:HG23	2.55	0.42
1:D:163:ARG:N	1:D:164:PRO:HD2	2.35	0.42
1:B:136:MET:SD	1:B:166:LEU:HD12	2.60	0.42
1:B:224:GLU:N	1:D:202:THR:HG21	2.35	0.42
1:C:39:LEU:HD11	1:C:51:PRO:HG3	2.01	0.42
1:D:125:TRP:CE3	1:D:132:VAL:HG11	2.54	0.42
1:A:43:PRO:CD	1:A:44:TYR:HA	2.50	0.41
1:B:157:ILE:HG22	1:B:181:THR:OG1	2.20	0.41
1:B:99:VAL:HG12	1:B:271:TRP:CZ2	2.56	0.41
1:C:116:SER:O	1:C:117:LEU:CD1	2.68	0.41
1:C:129:PRO:O	1:C:133:ARG:HB2	2.20	0.41
1:C:53:HIS:HB2	1:C:276:ARG:HD2	2.02	0.41
1:D:156:ARG:O	1:D:188:THR:HA	2.21	0.41
1:A:233:ARG:HA	1:A:234:PRO:HD3	1.86	0.41
1:C:195:TYR:OH	1:C:255:MET:HA	2.20	0.41
1:A:143:VAL:HG12	1:A:144:ARG:N	2.35	0.41
1:A:66:ARG:NH1	1:A:66:ARG:HG2	2.31	0.41
1:B:214:ALA:CB	1:B:216:ARG:NH1	2.83	0.41
1:B:82:ALA:O	1:B:87:LEU:HG	2.20	0.41
1:C:150:LEU:HB3	1:C:155:VAL:HB	2.01	0.41
1:B:120:PHE:CE1	1:B:124:ASN:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:TRP:HA	1:B:33:PRO:C	2.40	0.41
1:C:160:VAL:HG21	1:C:190:ASN:HB3	2.03	0.41
1:A:140:ARG:NH1	1:B:291:ARG:HB3	2.35	0.41
1:B:218:ASN:HB3	1:B:221:ARG:HB2	2.02	0.41
1:B:26:PHE:CG	1:B:27:PRO:HA	2.55	0.41
1:D:79:GLY:O	1:D:80:ARG:C	2.59	0.41
1:A:227:ILE:HD11	1:C:202:THR:HA	2.03	0.41
1:C:264:TYR:HB3	1:C:266:PHE:CZ	2.56	0.41
1:A:60:PRO:CD	1:A:110:LEU:HD13	2.49	0.41
1:A:90:THR:HB	1:A:134:PHE:CD2	2.56	0.41
1:B:34:VAL:O	1:B:34:VAL:HG23	2.21	0.41
1:C:90:THR:O	1:C:94:LYS:HG3	2.20	0.41
1:D:139:ASN:O	1:D:143:VAL:HG23	2.21	0.41
1:D:241:LEU:HD22	1:D:286:TYR:HB3	2.03	0.41
1:D:285:GLU:O	1:D:289:ARG:HG2	2.21	0.40
1:A:128:SER:O	1:A:132:VAL:HG23	2.22	0.40
1:A:199:THR:O	1:A:203:GLU:HG3	2.21	0.40
1:A:63:PRO:HB2	1:A:66:ARG:HG3	2.04	0.40
1:B:81:TRP:CZ3	1:B:95:MET:HG3	2.56	0.40
1:D:80:ARG:O	1:D:81:TRP:C	2.59	0.40
1:A:62:ILE:HD11	1:A:284:GLU:HG2	2.04	0.40
1:B:222:ILE:HG22	1:B:223:THR:N	2.36	0.40
1:A:136:MET:HB3	1:A:167:TRP:CD2	2.57	0.40
1:B:120:PHE:CE1	1:B:124:ASN:HB3	2.56	0.40
1:D:40:PRO:O	1:D:41:ALA:C	2.59	0.40
1:D:41:ALA:O	1:D:42:ALA:HB3	2.22	0.40
1:D:99:VAL:O	1:D:103:ILE:HD13	2.22	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	282/284 (99%)	257 (91%)	24 (8%)	1 (0%)	34 57
1	B	282/284 (99%)	256 (91%)	21 (7%)	5 (2%)	8 16
1	C	282/284 (99%)	248 (88%)	32 (11%)	2 (1%)	22 43
1	D	281/284 (99%)	245 (87%)	30 (11%)	6 (2%)	7 13
All	All	1127/1136 (99%)	1006 (89%)	107 (10%)	14 (1%)	13 27

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	TYR
1	D	41	ALA
1	D	246	SER
1	B	187	ILE
1	D	24	PRO
1	B	17	PRO
1	C	185	ASP
1	D	52	GLN
1	D	79	GLY
1	C	43	PRO
1	A	18	PRO
1	B	47	PRO
1	B	143	VAL
1	D	47	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	239/239 (100%)	229 (96%)	10 (4%)	30 55
1	B	239/239 (100%)	220 (92%)	19 (8%)	12 24
1	C	239/239 (100%)	220 (92%)	19 (8%)	12 24
1	D	238/239 (100%)	224 (94%)	14 (6%)	19 39
All	All	955/956 (100%)	893 (94%)	62 (6%)	17 34

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	78	ASN
1	A	118	TYR
1	A	148	ASP
1	A	158	ARG
1	A	168	ARG
1	A	202	THR
1	A	206	ARG
1	A	246	SER
1	A	295	SER
1	B	13	PHE
1	B	21	ASP
1	B	49	ARG
1	B	65	ASP
1	B	66	ARG
1	B	80	ARG
1	B	83	THR
1	B	87	LEU
1	B	118	TYR
1	B	158	ARG
1	B	180	MET
1	B	183	SER
1	B	240	ASP
1	B	243	LEU
1	B	245	THR
1	B	246	SER
1	B	291	ARG
1	B	292	ARG
1	B	293	PHE
1	C	13	PHE
1	C	14	PRO
1	C	65	ASP
1	C	80	ARG
1	C	83	THR
1	C	85	ARG
1	C	89	ARG
1	C	117	LEU
1	C	118	TYR
1	C	134	PHE
1	C	157	ILE
1	C	158	ARG
1	C	190	ASN

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Mol	Chain	Res	Type
1	C	243	LEU
1	C	249	GLN
1	C	268	ASP
1	C	273	ASP
1	C	285	GLU
1	C	290	THR
1	D	22	ASP
1	D	31	THR
1	D	35	VAL
1	D	38	GLU
1	D	118	TYR
1	D	145	ARG
1	D	158	ARG
1	D	162	SER
1	D	173	GLU
1	D	226	THR
1	D	227	ILE
1	D	267	GLN
1	D	286	TYR
1	D	290	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	124	ASN
1	A	249	GLN
1	C	184	ASN
1	D	93	HIS
1	D	184	ASN
1	D	249	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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	284/284 (100%)	0.12	2 (0%)	87 86	18, 27, 37, 62	0
1	B	284/284 (100%)	0.20	4 (1%)	75 71	22, 30, 43, 76	0
1	C	284/284 (100%)	0.32	10 (3%)	44 36	20, 33, 55, 84	0
1	D	283/284 (99%)	0.34	13 (4%)	32 26	23, 37, 55, 80	0
All	All	1135/1136 (99%)	0.24	29 (2%)	56 50	18, 31, 51, 84	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	44	TYR	9.3
1	D	43	PRO	7.3
1	C	43	PRO	5.6
1	C	44	TYR	4.4
1	B	44	TYR	4.0
1	C	104	ALA	3.8
1	C	87	LEU	3.6
1	D	101	ILE	3.3
1	C	41	ALA	3.3
1	D	30	SER	3.1
1	C	45	GLY	3.1
1	D	99	VAL	3.0
1	B	214	ALA	2.9
1	B	34	VAL	2.8
1	C	53	HIS	2.7
1	D	79	GLY	2.7
1	D	46	GLY	2.6
1	D	31	THR	2.5
1	C	22	ASP	2.5
1	B	208	ILE	2.4
1	A	150	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	41	ALA	2.3
1	D	90	THR	2.3
1	D	296	ALA	2.3
1	C	61	ARG	2.3
1	D	45	GLY	2.2
1	A	38	GLU	2.1
1	C	46	GLY	2.1
1	D	22	ASP	2.1

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 carbohydrates 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.