



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:17 am GMT

PDB ID : 3WYJ
Title : Structure of E. coli undecaprenyl diphosphate synthase in complex with BPH-789
Authors : Gao, J.; Ko, T.P.; Huang, C.H.; Oldfield, E.; Guo, R.T.
Deposited on : 2014-08-29
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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
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

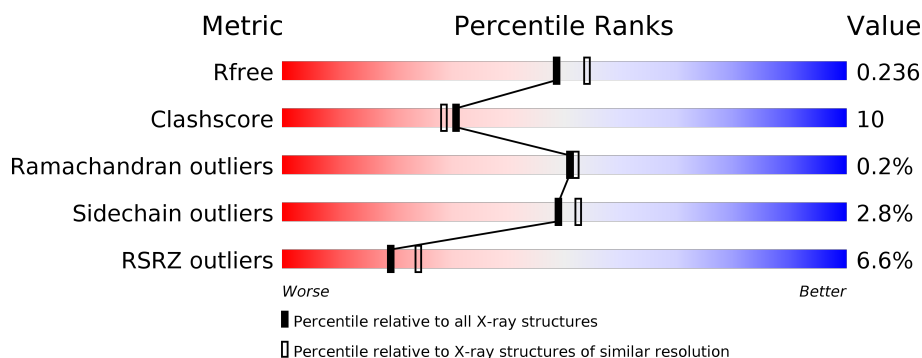
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 ≥ 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 $\leq 5\%$. 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.

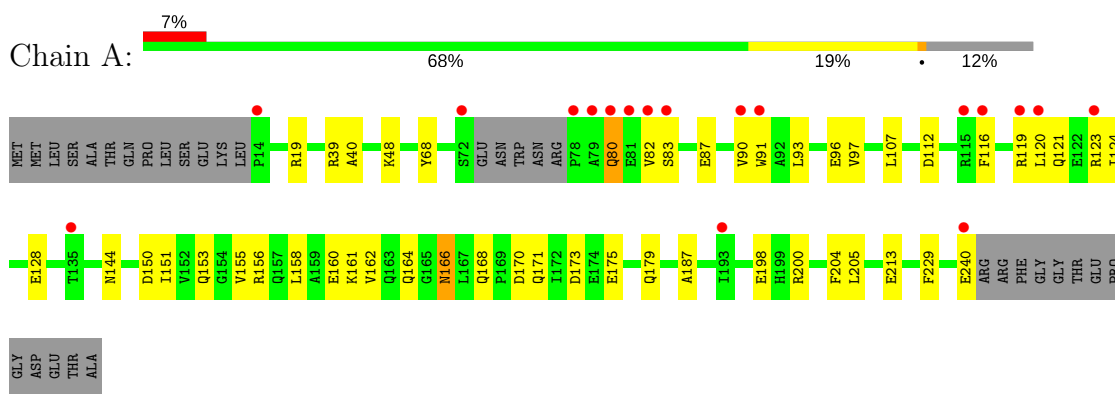
Mol	Chain	Length	Quality of chain
1	A	253	
1	B	253	

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	193	Total 193	O 193	0	0
3	B	232	Total 232	O 232	0	0

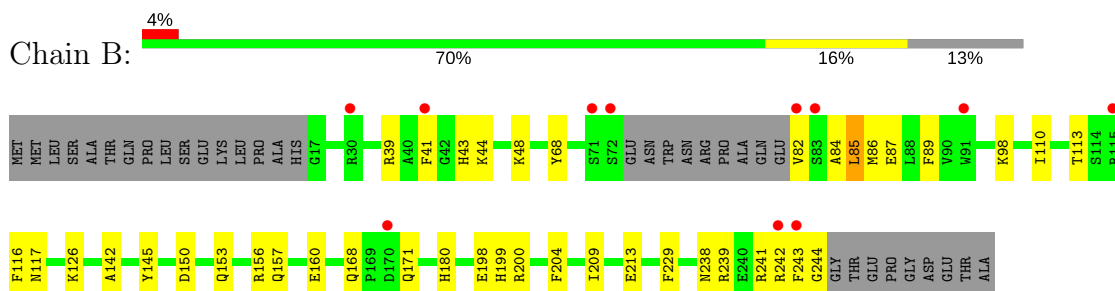
3 Residue-property plots [i](#)

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: Ditrans, polycis-undecaprenyl-diphosphate synthase ((2E,6E)-farnesyl-diphosphate specific)



- Molecule 1: Ditrans, polycis-undecaprenyl-diphosphate synthase ((2E,6E)-farnesyl-diphosphate specific)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.71Å 69.00Å 108.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 23.53 – 2.09	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.10) 97.7 (23.53-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.90 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.241 0.196 , 0.236	Depositor DCC
R_{free} test set	1361 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3988	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H78

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	0.32	0/1794	0.55	0/2421
1	B	0.32	0/1777	0.55	0/2395
All	All	0.32	0/3571	0.55	0/4816

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	1759	0	1726	42	0
1	B	1744	0	1717	33	0
2	A	60	0	30	0	0
3	A	193	0	0	3	0
3	B	232	0	0	4	0
All	All	3988	0	3473	73	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 10.

All (73) 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:86:MET:HE1	1:B:117:ASN:H	1.12	1.08
1:B:86:MET:HE1	1:B:117:ASN:N	1.91	0.86
1:A:116:PHE:HB3	1:A:120:LEU:HD11	1.63	0.79
1:A:123:ARG:HA	1:A:123:ARG:HH11	1.51	0.76
1:A:83:SER:O	1:A:87:GLU:HG2	1.89	0.72
1:A:93:LEU:HD11	1:A:107:LEU:HD21	1.72	0.71
1:A:93:LEU:O	1:A:97:VAL:HG23	1.92	0.69
1:B:156:ARG:O	1:B:160:GLU:HG3	1.93	0.67
1:A:161:LYS:HA	1:A:164:GLN:HG2	1.77	0.66
1:B:150:ASP:O	1:B:153:GLN:HG3	1.99	0.63
1:A:213:GLU:OE2	1:B:199:HIS:HB2	1.99	0.63
1:A:124:ILE:O	1:A:128:GLU:HG3	1.99	0.62
1:A:156:ARG:O	1:A:160:GLU:HG2	1.99	0.61
1:A:200:ARG:HH21	1:B:213:GLU:HB2	1.67	0.59
1:A:164:GLN:HG3	1:A:166:ASN:ND2	2.17	0.58
1:B:239:ARG:O	1:B:242:ARG:O	2.21	0.58
1:A:173:ASP:HB2	3:A:1131:HOH:O	2.03	0.58
1:B:82:VAL:HG12	1:B:85:LEU:HD23	1.86	0.57
1:A:80:GLN:NE2	1:A:80:GLN:H	2.03	0.56
1:B:213:GLU:OE2	1:B:239:ARG:HD3	2.06	0.56
1:B:44:LYS:HE3	1:B:48:LYS:HZ3	1.70	0.56
1:B:168:GLN:O	1:B:171:GLN:HB3	2.06	0.56
1:B:113:THR:HG22	1:B:116:PHE:CE2	2.41	0.56
1:A:120:LEU:HD12	1:A:120:LEU:C	2.26	0.55
1:A:168:GLN:HB2	1:A:171:GLN:HG3	1.90	0.54
1:A:175:GLU:O	1:A:179:GLN:HG3	2.08	0.54
1:A:93:LEU:HD11	1:A:107:LEU:CD2	2.38	0.54
1:A:164:GLN:HE21	1:A:166:ASN:HD21	1.55	0.54
1:B:44:LYS:HE3	1:B:48:LYS:NZ	2.22	0.54
1:B:98:LYS:HD2	3:B:368:HOH:O	2.08	0.53
1:B:126:LYS:HD3	3:B:477:HOH:O	2.07	0.53
1:A:116:PHE:HB3	1:A:120:LEU:CD1	2.38	0.52
1:A:119:ARG:HG2	1:A:119:ARG:HH11	1.75	0.51
1:A:48:LYS:HD3	1:A:48:LYS:C	2.31	0.51
1:A:198:GLU:OE1	1:A:200:ARG:HD2	2.11	0.51
1:A:164:GLN:HG3	1:A:166:ASN:HD21	1.75	0.51
1:A:90:VAL:HG21	1:A:120:LEU:HB2	1.93	0.50
1:A:123:ARG:HH11	1:A:123:ARG:CA	2.24	0.50
1:A:82:VAL:HG23	1:A:83:SER:N	2.27	0.50
1:A:19:ARG:NH2	1:A:187:ALA:HB2	2.28	0.48
1:A:68:TYR:HB2	1:A:204:PHE:CE1	2.48	0.48
1:B:242:ARG:C	1:B:244:GLY:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:O	1:A:121:GLN:NE2	2.47	0.47
1:A:204:PHE:CG	1:A:205:LEU:N	2.82	0.47
1:B:242:ARG:O	1:B:244:GLY:N	2.45	0.47
1:A:96:GLU:HG2	3:A:1015:HOH:O	2.13	0.47
1:B:84:ALA:HB3	3:B:531:HOH:O	2.14	0.47
1:B:39:ARG:HH21	1:B:43:HIS:HE1	1.63	0.46
1:B:86:MET:CE	1:B:117:ASN:H	2.03	0.45
1:B:110:ILE:HG13	1:B:142:ALA:HA	1.97	0.45
1:B:142:ALA:HB1	1:B:145:TYR:HB3	1.99	0.45
1:B:41:PHE:HB2	3:B:491:HOH:O	2.17	0.45
1:B:157:GLN:OE1	1:B:180:HIS:HD2	2.01	0.44
1:A:161:LYS:HA	1:A:164:GLN:CG	2.45	0.44
1:B:85:LEU:HG	1:B:86:MET:N	2.33	0.44
1:B:238:ASN:OD1	1:B:241:ARG:NH2	2.49	0.43
1:A:121:GLN:HG3	3:A:1174:HOH:O	2.18	0.43
1:A:164:GLN:NE2	1:A:166:ASN:HD21	2.14	0.43
1:A:39:ARG:CG	1:A:40:ALA:N	2.82	0.43
1:A:164:GLN:HE21	1:A:166:ASN:ND2	2.16	0.43
1:A:158:LEU:O	1:A:162:VAL:HG23	2.18	0.42
1:B:209:ILE:HD12	1:B:209:ILE:C	2.39	0.42
1:B:85:LEU:C	1:B:85:LEU:HD12	2.39	0.42
1:B:86:MET:CE	1:B:116:PHE:HA	2.49	0.41
1:A:112:ASP:HB3	1:A:144:ASN:ND2	2.35	0.41
1:A:150:ASP:O	1:A:153:GLN:HG3	2.20	0.41
1:A:164:GLN:CG	1:A:166:ASN:HD21	2.33	0.41
1:A:119:ARG:HG2	1:A:119:ARG:NH1	2.35	0.41
1:A:151:ILE:O	1:A:155:VAL:HG23	2.21	0.41
1:B:68:TYR:HB2	1:B:204:PHE:CE1	2.56	0.41
1:B:198:GLU:CD	1:B:200:ARG:HH21	2.25	0.40
1:B:39:ARG:HE	1:B:43:HIS:CE1	2.39	0.40
1:B:198:GLU:CD	1:B:200:ARG:NH2	2.75	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	218/253 (86%)	209 (96%)	9 (4%)	0	100	100
1	B	215/253 (85%)	209 (97%)	5 (2%)	1 (0%)	32	28
All	All	433/506 (86%)	418 (96%)	14 (3%)	1 (0%)	51	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	PHE

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	180/206 (87%)	174 (97%)	6 (3%)	43	45
1	B	178/206 (86%)	174 (98%)	4 (2%)	57	62
All	All	358/412 (87%)	348 (97%)	10 (3%)	49	52

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	91	TRP
1	A	166	ASN
1	A	170	ASP
1	A	229	PHE
1	A	240	GLU
1	B	85	LEU
1	B	87	GLU
1	B	89	PHE
1	B	229	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	121	GLN
1	A	164	GLN
1	A	166	ASN
1	A	238	ASN
1	B	43	HIS
1	B	157	GLN
1	B	180	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	H78	A	900	-	64,64,64	8.63	58 (90%)	102,102,102	3.77	36 (35%)

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	H78	A	900	-	-	0/76/76/76	0/5/5/5

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	H78	CBN-CCB	-58.58	1.10	1.55
2	A	900	H78	CBM-CCA	-12.87	1.45	1.55
2	A	900	H78	PCE-CCB	-9.04	1.78	1.85
2	A	900	H78	PCF-CCB	-8.39	1.79	1.85
2	A	900	H78	CBZ-SCH	-7.88	1.65	1.76
2	A	900	H78	PCD-CCA	-6.86	1.80	1.85
2	A	900	H78	CBM-CBQ	-5.56	1.41	1.51
2	A	900	H78	CBT-NBP	-5.56	1.34	1.43
2	A	900	H78	CBN-CBR	-5.35	1.42	1.51
2	A	900	H78	CBV-CBX	-5.03	1.36	1.49
2	A	900	H78	CBW-CBU	-4.27	1.38	1.49
2	A	900	H78	CBS-NBO	-3.54	1.37	1.43
2	A	900	H78	OAO-SCG	-2.88	1.40	1.43
2	A	900	H78	PCC-CCA	-2.29	1.83	1.85
2	A	900	H78	CBK-CBX	2.09	1.43	1.39
2	A	900	H78	CBK-CBT	2.12	1.43	1.39
2	A	900	H78	CAV-CBE	2.22	1.43	1.38
2	A	900	H78	CAS-CBB	2.25	1.43	1.38
2	A	900	H78	CBJ-CBW	2.47	1.44	1.39
2	A	900	H78	CBI-CBV	2.50	1.44	1.39
2	A	900	H78	PCE-OAK	2.57	1.59	1.54
2	A	900	H78	CBB-CBU	2.58	1.44	1.39
2	A	900	H78	CAY-CBR	2.62	1.44	1.38
2	A	900	H78	CBH-CBQ	2.62	1.43	1.39
2	A	900	H78	PCE-OAI	2.65	1.59	1.54
2	A	900	H78	CAU-CBD	2.66	1.44	1.38
2	A	900	H78	CAS-CAX	2.68	1.44	1.38
2	A	900	H78	CBE-CBX	2.71	1.45	1.39
2	A	900	H78	CAT-CAY	2.71	1.44	1.38
2	A	900	H78	CAW-CBG	2.73	1.44	1.38
2	A	900	H78	CBJ-CBS	2.81	1.44	1.39
2	A	900	H78	CAT-CBC	2.81	1.44	1.38
2	A	900	H78	PCC-OAE	2.86	1.60	1.54
2	A	900	H78	CAU-CAZ	2.87	1.44	1.38
2	A	900	H78	CBI-CBR	2.90	1.44	1.39
2	A	900	H78	CAX-CBQ	2.97	1.45	1.38
2	A	900	H78	CBD-CBW	3.02	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	H78	CBA-CBT	3.03	1.44	1.39
2	A	900	H78	CBF-CBY	3.05	1.43	1.38
2	A	900	H78	CAV-CBA	3.05	1.44	1.38
2	A	900	H78	PCD-OAF	3.06	1.60	1.54
2	A	900	H78	CBC-CBV	3.11	1.45	1.39
2	A	900	H78	CAZ-CBS	3.15	1.44	1.39
2	A	900	H78	CBL-CBZ	3.20	1.45	1.39
2	A	900	H78	CBG-CBZ	3.26	1.44	1.38
2	A	900	H78	CBL-CBY	3.29	1.45	1.39
2	A	900	H78	PCF-OAN	3.38	1.61	1.54
2	A	900	H78	PCD-OAH	3.45	1.61	1.54
2	A	900	H78	PCF-OAL	3.52	1.61	1.54
2	A	900	H78	CBH-CBU	3.70	1.46	1.39
2	A	900	H78	PCC-OAD	3.73	1.61	1.54
2	A	900	H78	PCF-OAM	5.42	1.59	1.50
2	A	900	H78	PCD-OAG	5.52	1.59	1.50
2	A	900	H78	PCE-OAJ	6.25	1.60	1.50
2	A	900	H78	PCC-OAC	7.00	1.61	1.50
2	A	900	H78	OAR-SCH	9.12	1.53	1.43
2	A	900	H78	SCG-NBO	9.28	1.79	1.63
2	A	900	H78	OAQ-SCH	10.39	1.54	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	H78	PCF-CCB-PCE	-15.24	84.51	112.70
2	A	900	H78	PCD-CCA-PCC	-10.99	92.37	112.70
2	A	900	H78	OAP-SCG-OAO	-10.54	106.07	119.55
2	A	900	H78	OAR-SCH-OAQ	-7.19	110.35	119.55
2	A	900	H78	CBD-CBW-CBU	-6.62	109.69	121.38
2	A	900	H78	OAE-PCC-CCA	-5.02	94.95	106.04
2	A	900	H78	OAN-PCF-OAM	-4.93	102.01	113.05
2	A	900	H78	CBK-CBX-CBV	-4.38	113.45	120.88
2	A	900	H78	OAL-PCF-OAM	-4.11	103.86	113.05
2	A	900	H78	OAE-PCC-OAC	-3.84	104.45	113.05
2	A	900	H78	CBF-CBY-SCG	-2.84	116.64	119.77
2	A	900	H78	OAI-PCE-OAJ	-2.75	106.89	113.05
2	A	900	H78	OAF-PCD-OAG	-2.60	107.23	113.05
2	A	900	H78	CBB-CBU-CBW	-2.19	117.51	121.38
2	A	900	H78	OAB-CCB-CBN	-2.15	105.67	110.69
2	A	900	H78	OAM-PCF-CCB	-2.07	104.41	109.92
2	A	900	H78	CBS-NBO-SCG	-2.05	116.84	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	H78	OAQ-SCH-CBZ	2.07	110.52	107.95
2	A	900	H78	CBG-CBZ-SCH	2.08	122.07	119.77
2	A	900	H78	CAW-CBF-CBY	2.19	121.27	118.96
2	A	900	H78	CAZ-CBS-NBO	2.24	125.03	120.11
2	A	900	H78	CAW-CBG-CBZ	2.44	121.53	118.96
2	A	900	H78	CBE-CBX-CBV	2.96	126.61	121.38
2	A	900	H78	OAH-PCD-CCA	3.05	112.78	106.04
2	A	900	H78	CBL-CBY-SCG	3.33	123.16	119.19
2	A	900	H78	CBT-NBP-SCH	3.38	133.93	123.30
2	A	900	H78	OAJ-PCE-CCB	3.40	118.95	109.92
2	A	900	H78	PCE-CCB-CBN	3.41	118.42	109.23
2	A	900	H78	PCD-CCA-CBM	5.29	123.49	109.23
2	A	900	H78	OAP-SCG-CBY	5.76	115.08	107.95
2	A	900	H78	CBJ-CBW-CBU	5.82	130.75	120.88
2	A	900	H78	PCF-CCB-CBN	5.83	124.94	109.23
2	A	900	H78	CBY-SCG-NBO	6.17	114.75	106.83
2	A	900	H78	OAD-PCC-CCA	9.46	126.93	106.04
2	A	900	H78	OAN-PCF-CCB	10.66	129.58	106.04
2	A	900	H78	CCB-CBN-CBR	15.13	141.69	116.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å ²)	Q<0.9
1	A	222/253 (87%)	0.42	18 (8%) 13 16	18, 35, 70, 101	0
1	B	219/253 (86%)	0.06	11 (5%) 30 36	17, 30, 59, 75	0
All	All	441/506 (87%)	0.24	29 (6%) 19 24	17, 32, 64, 101	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	TRP	8.2
1	B	82	VAL	6.4
1	A	82	VAL	6.0
1	A	80	GLN	5.7
1	B	72	SER	5.3
1	A	81	GLU	5.2
1	A	78	PRO	4.1
1	B	83	SER	4.0
1	A	14	PRO	3.8
1	A	120	LEU	3.5
1	B	115	ARG	3.5
1	A	115	ARG	3.4
1	A	240	GLU	3.3
1	B	170	ASP	3.1
1	A	90	VAL	2.8
1	A	79	ALA	2.8
1	B	91	TRP	2.8
1	A	135	THR	2.7
1	B	30	ARG	2.7
1	A	72	SER	2.6
1	A	83	SER	2.6
1	A	123	ARG	2.6
1	A	119	ARG	2.5
1	A	116	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	193	ILE	2.4
1	B	71	SER	2.3
1	B	242	ARG	2.1
1	B	41	PHE	2.1
1	B	243	PHE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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
2	H78	A	900	60/60	0.86	0.17	0.56	32,61,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.