Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:57 AM GMT

PDB ID	:	3GNN
Title	:	Crystal structure of nicotinate-nucleotide pyrophosphorylase from Burkholderi pseudomallei
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2009-03-17
Resolution	:	2.25 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

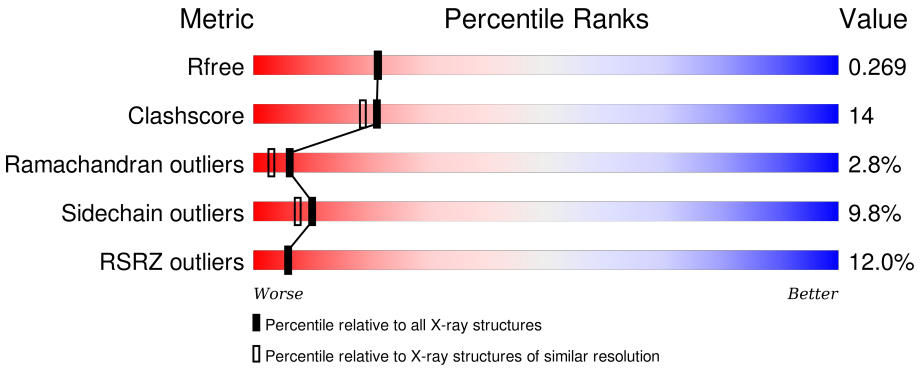
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.25 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	298	9% 61% 24% • 11%
1	B	298	11% 57% 21% • 18%
2	D	4	100%
2	E	4	100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3879 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 Nicotinate-nucleotide pyrophosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			1960	1213	363	378	6			
1	B	244	Total	C	N	O	S	0	0	0
			1773	1096	321	350	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q3JV59
A	-2	PRO	-	EXPRESSION TAG	UNP Q3JV59
A	-1	GLY	-	EXPRESSION TAG	UNP Q3JV59
A	0	SER	-	EXPRESSION TAG	UNP Q3JV59
B	-3	GLY	-	EXPRESSION TAG	UNP Q3JV59
B	-2	PRO	-	EXPRESSION TAG	UNP Q3JV59
B	-1	GLY	-	EXPRESSION TAG	UNP Q3JV59
B	0	SER	-	EXPRESSION TAG	UNP Q3JV59

- Molecule 2 is a protein called Unknown Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			20	12	4	4			
2	E	4	Total	C	N	O	0	0	0
			20	12	4	4			

- Molecule 3 is water.

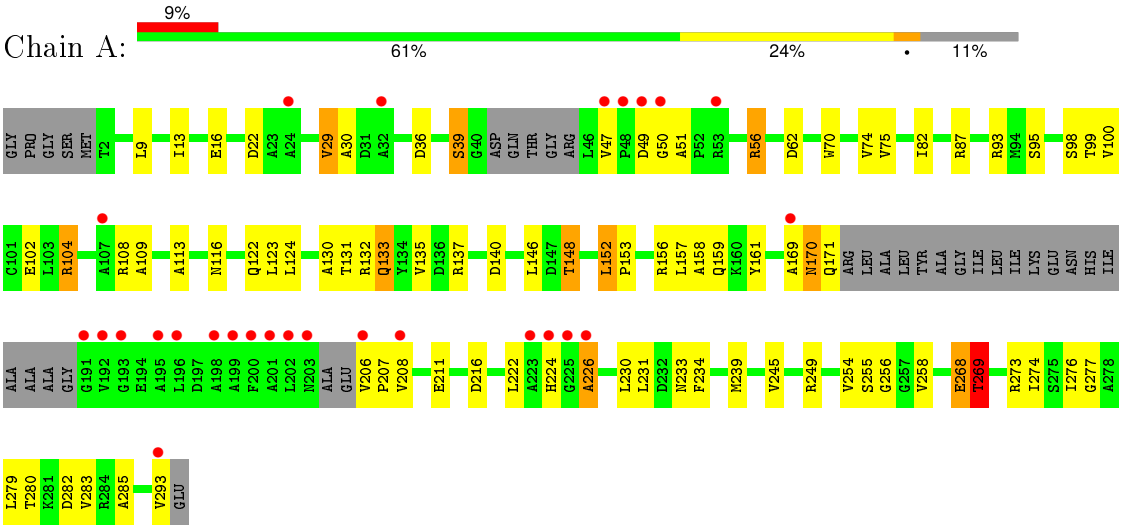
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	44	Total	O	0	0
			44	44		

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 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.

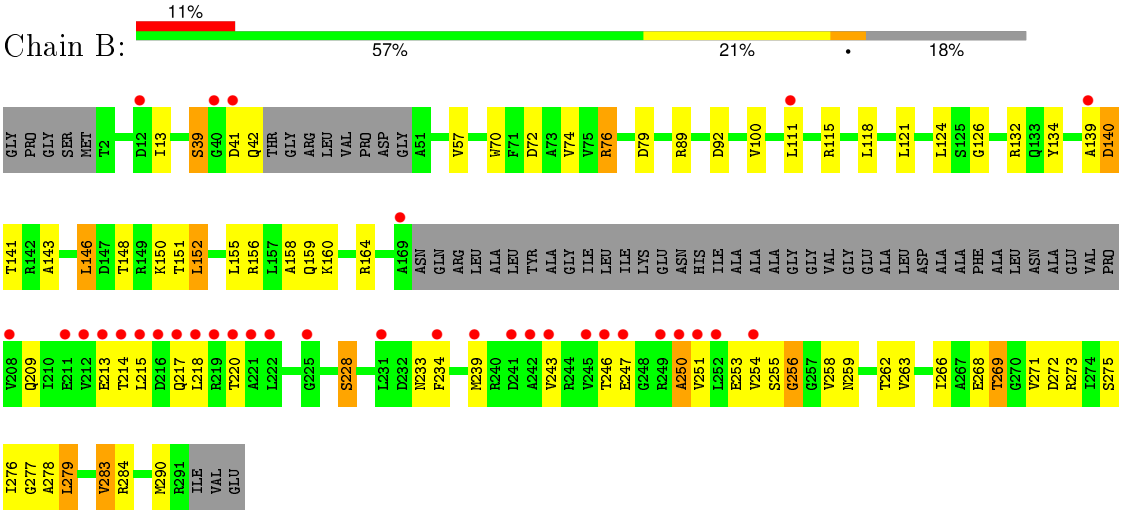
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase

Chain A:



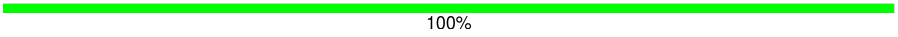
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase

Chain B:



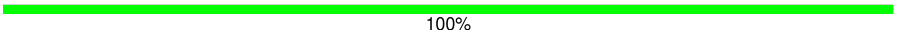
- Molecule 2: Unknown Peptide

Chain D:



There are no outlier residues recorded for this chain.

- Molecule 2: Unknown Peptide

Chain E: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	160.98Å 57.41Å 66.24Å 90.00° 106.74° 90.00°	Depositor
Resolution (Å)	39.14 – 2.25 39.14 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.14-2.25) 98.7 (39.14-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.214 , 0.273 0.213 , 0.269	Depositor DCC
R_{free} test set	1366 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 27260 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3879	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.02	4/1980 (0.2%)	1.01	5/2692 (0.2%)
1	B	0.89	0/1790	0.93	4/2436 (0.2%)
All	All	0.96	4/3770 (0.1%)	0.97	9/5128 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	ALA	CA-CB	6.51	1.66	1.52
1	A	268	GLU	CG-CD	-6.23	1.42	1.51
1	A	29	VAL	CB-CG2	5.33	1.64	1.52
1	A	30	ALA	CA-CB	-5.30	1.41	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	89	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	92	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	157	LEU	CB-CG-CD1	6.02	121.23	111.00
1	B	72	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	62	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	89	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	22	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	87	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	104	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	1960	0	1934	60	0
1	B	1773	0	1715	52	0
2	D	20	0	6	0	0
2	E	20	0	6	0	0
3	A	62	0	0	4	0
3	B	44	0	0	2	0
All	All	3879	0	3661	106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (106) 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:152:LEU:HD23	1:A:159:GLN:HE22	1.00	1.15
1:A:169:ALA:O	1:A:171:GLN:HG3	1.50	1.11
1:A:152:LEU:CD2	1:A:159:GLN:HE22	1.63	1.11
1:A:152:LEU:HD23	1:A:159:GLN:NE2	1.67	1.10
1:A:239:MET:HB3	1:A:269:THR:HG21	1.55	0.87
1:B:151:THR:HG21	1:B:156:ARG:HG3	1.56	0.86
1:A:276:ILE:HB	1:A:279:LEU:HG	1.57	0.85
1:A:282:ASP:OD1	3:A:341:HOH:O	1.95	0.83
1:B:259:ASN:O	1:B:263:VAL:HG23	1.79	0.83
1:A:169:ALA:O	1:A:171:GLN:CG	2.30	0.77
1:B:258:VAL:HG23	1:B:263:VAL:HG22	1.66	0.77
1:B:254:VAL:HG12	1:B:256:GLY:H	1.49	0.77
1:A:9:LEU:O	1:A:13:ILE:HD12	1.89	0.72
1:A:258:VAL:HG11	1:A:276:ILE:HD12	1.73	0.70
1:A:133:GLN:NE2	3:A:346:HOH:O	2.24	0.70
1:B:152:LEU:HD11	1:B:279:LEU:HD13	1.74	0.69
1:A:56:ARG:CZ	1:A:99:THR:HG21	2.23	0.69
1:B:262:THR:O	1:B:266:ILE:HG13	1.93	0.69
1:B:151:THR:HG22	1:B:159:GLN:NE2	2.09	0.68
1:B:57:VAL:HG22	1:B:290:MET:HE2	1.77	0.67
1:B:151:THR:HG22	1:B:159:GLN:HE22	1.59	0.66
1:A:231:LEU:HD22	1:A:234:PHE:CE1	2.32	0.65
1:B:283:VAL:O	1:B:283:VAL:CG2	2.45	0.65
1:A:152:LEU:HD23	1:A:159:GLN:CD	2.19	0.63
1:A:146:LEU:HD22	1:A:171:GLN:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:CD1	1:B:279:LEU:HD13	2.30	0.62
1:B:118:LEU:HD13	1:B:290:MET:CE	2.31	0.61
1:A:239:MET:HB3	1:A:269:THR:CG2	2.29	0.60
1:A:156:ARG:NH2	1:B:39:SER:OG	2.26	0.60
1:A:13:ILE:HD13	1:A:161:TYR:CD1	2.36	0.59
1:B:139:ALA:O	1:B:140:ASP:CG	2.42	0.58
1:A:36:ASP:HB2	1:A:116:ASN:HD21	1.69	0.58
1:A:123:LEU:HD13	1:B:279:LEU:HD11	1.86	0.57
1:B:239:MET:HB3	1:B:269:THR:HG21	1.87	0.57
1:B:76:ARG:NH2	3:B:304:HOH:O	2.38	0.56
1:A:102:GLU:OE2	1:A:104:ARG:NH1	2.38	0.56
1:B:57:VAL:HG22	1:B:290:MET:CE	2.34	0.56
1:A:148:THR:OG1	1:A:277:GLY:HA2	2.08	0.53
1:B:134:TYR:CE2	1:B:263:VAL:HG21	2.44	0.52
1:A:131:THR:O	1:A:135:VAL:HG23	2.08	0.52
1:B:278:ALA:HA	1:B:283:VAL:HG21	1.91	0.52
1:A:122:GLN:HB3	1:A:285:ALA:HB1	1.91	0.52
1:A:276:ILE:N	1:A:276:ILE:HD13	2.25	0.51
1:A:206:VAL:HB	1:A:207:PRO:HD3	1.93	0.51
1:A:156:ARG:HH22	1:B:39:SER:CB	2.24	0.50
1:B:269:THR:HG22	1:B:271:VAL:HG13	1.94	0.50
1:A:93:ARG:NH1	1:A:132:ARG:HD2	2.27	0.50
1:B:151:THR:HG21	1:B:156:ARG:CG	2.38	0.49
1:B:259:ASN:O	1:B:263:VAL:CG2	2.55	0.49
1:B:164:ARG:NE	3:B:338:HOH:O	2.39	0.49
1:B:246:THR:HG21	1:B:250:ALA:HA	1.95	0.48
1:A:124:LEU:HD21	1:A:158:ALA:HB1	1.94	0.48
1:B:13:ILE:HD11	1:B:164:ARG:HG3	1.95	0.48
1:A:156:ARG:HG2	1:A:156:ARG:HH21	1.78	0.48
1:A:13:ILE:HD13	1:A:161:TYR:HD1	1.76	0.48
1:B:70:TRP:O	1:B:74:VAL:HG23	2.13	0.48
1:A:39:SER:HB2	1:B:156:ARG:HD2	1.96	0.47
1:A:75:VAL:HG22	1:A:113:ALA:HB1	1.97	0.47
1:B:276:ILE:HD12	1:B:276:ILE:O	2.14	0.47
1:B:269:THR:CG2	1:B:271:VAL:HG13	2.44	0.47
1:A:133:GLN:OE1	3:A:334:HOH:O	2.20	0.47
1:A:156:ARG:HG2	1:A:156:ARG:NH2	2.30	0.46
1:A:231:LEU:HD22	1:A:234:PHE:CZ	2.49	0.46
1:B:283:VAL:HG22	1:B:283:VAL:O	2.16	0.46
1:A:285:ALA:HB2	1:B:279:LEU:HG	1.98	0.46
1:A:123:LEU:HD12	1:A:283:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD11	1:A:109:ALA:HB1	1.98	0.46
1:B:283:VAL:O	1:B:283:VAL:HG23	2.15	0.46
1:A:146:LEU:CD2	1:A:171:GLN:HA	2.46	0.45
1:B:239:MET:O	1:B:243:VAL:HG23	2.15	0.45
1:A:29:VAL:HG22	1:A:74:VAL:HG22	1.98	0.45
1:B:255:SER:O	1:B:256:GLY:O	2.35	0.45
1:A:245:VAL:O	1:A:249:ARG:NH2	2.49	0.45
1:B:140:ASP:C	1:B:140:ASP:OD1	2.55	0.45
1:B:253:GLU:HA	1:B:273:ARG:O	2.17	0.45
1:B:124:LEU:HD21	1:B:158:ALA:HB1	1.99	0.45
1:A:231:LEU:HB2	1:A:254:VAL:HG12	1.99	0.44
1:B:126:GLY:HA3	1:B:284:ARG:O	2.17	0.44
1:A:274:ILE:HG22	1:A:276:ILE:CD1	2.47	0.44
1:B:143:ALA:HA	1:B:272:ASP:O	2.17	0.44
1:A:146:LEU:HD11	1:A:273:ARG:HD3	1.98	0.44
1:B:134:TYR:CD2	1:B:263:VAL:HG21	2.52	0.43
1:A:211:GLU:HA	1:A:230:LEU:HB3	2.00	0.43
1:A:258:VAL:CG1	1:A:276:ILE:HD12	2.46	0.43
1:A:152:LEU:HD23	1:A:159:GLN:OE1	2.18	0.43
1:B:277:GLY:O	1:B:283:VAL:HG21	2.18	0.43
1:B:290:MET:HB2	1:B:290:MET:HE2	1.90	0.43
1:A:47:VAL:O	1:A:108:ARG:NH2	2.51	0.43
1:A:170:ASN:C	1:A:171:GLN:HG3	2.38	0.43
1:A:70:TRP:O	1:A:74:VAL:HG23	2.19	0.42
1:A:233:ASN:OD1	1:A:256:GLY:HA3	2.19	0.42
1:A:222:LEU:HA	1:A:226:ALA:HB2	2.01	0.42
1:A:140:ASP:N	3:A:320:HOH:O	2.28	0.42
1:A:153:PRO:HG2	1:B:155:LEU:HD11	2.00	0.42
1:B:148:THR:HG23	1:B:150:LYS:O	2.19	0.42
1:A:152:LEU:CD2	1:A:280:THR:O	2.68	0.42
1:B:118:LEU:HD13	1:B:290:MET:HE2	2.02	0.42
1:B:146:LEU:O	1:B:275:SER:HA	2.19	0.42
1:B:118:LEU:HD12	1:B:121:LEU:HD12	2.02	0.41
1:A:146:LEU:HD23	1:A:169:ALA:HB3	2.02	0.41
1:B:209:GLN:HG3	1:B:228:SER:OG	2.20	0.41
1:B:139:ALA:C	1:B:141:THR:H	2.23	0.41
1:A:293:VAL:O	1:A:293:VAL:HG13	2.21	0.41
1:A:170:ASN:O	1:A:171:GLN:HB2	2.22	0.40
1:A:133:GLN:HG2	1:A:137:ARG:HH21	1.85	0.40
1:B:79:ASP:C	1:B:79:ASP:OD1	2.59	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	258/298 (87%)	245 (95%)	6 (2%)	7 (3%)	6	3
1	B	238/298 (80%)	219 (92%)	12 (5%)	7 (3%)	6	3
All	All	496/596 (83%)	464 (94%)	18 (4%)	14 (3%)	6	3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	ASP
1	B	250	ALA
1	B	256	GLY
1	A	50	GLY
1	B	234	PHE
1	A	170	ASN
1	A	224	HIS
1	B	247	GLU
1	A	226	ALA
1	A	49	ASP
1	A	269	THR
1	B	233	ASN
1	B	251	VAL
1	A	51	ALA

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	195/227 (86%)	181 (93%)	14 (7%)	18 16
1	B	173/227 (76%)	151 (87%)	22 (13%)	5 3
All	All	368/454 (81%)	332 (90%)	36 (10%)	10 7

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	39	SER
1	A	56	ARG
1	A	95	SER
1	A	98	SER
1	A	100	VAL
1	A	133	GLN
1	A	148	THR
1	A	152	LEU
1	A	208	VAL
1	A	216	ASP
1	A	255	SER
1	A	268	GLU
1	A	269	THR
1	B	39	SER
1	B	42	GLN
1	B	76	ARG
1	B	100	VAL
1	B	111	LEU
1	B	115	ARG
1	B	132	ARG
1	B	140	ASP
1	B	146	LEU
1	B	152	LEU
1	B	160	LYS
1	B	213	GLU
1	B	214	THR
1	B	215	LEU
1	B	217	GLN
1	B	218	LEU
1	B	220	THR
1	B	228	SER
1	B	268	GLU
1	B	269	THR
1	B	279	LEU

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Mol	Chain	Res	Type
1	B	283	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	266/298 (89%)	0.60	27 (10%)	9	9	20, 43, 84, 97	0
1	B	244/298 (81%)	0.69	34 (13%)	4	4	22, 46, 88, 91	0
2	D	0/4	-	-			-	-
2	E	0/4	-	-			-	-
All	All	510/604 (84%)	0.64	61 (11%)	6	6	20, 44, 87, 97	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	PRO	7.2
1	A	47	VAL	6.6
1	A	50	GLY	5.3
1	A	201	ALA	5.2
1	B	234	PHE	4.5
1	A	192	VAL	4.5
1	B	213	GLU	4.5
1	B	250	ALA	4.4
1	B	254	VAL	4.3
1	B	211	GLU	4.3
1	B	214	THR	4.3
1	A	200	PHE	4.2
1	A	195	ALA	4.1
1	B	252	LEU	4.1
1	B	241	ASP	4.0
1	A	198	ALA	3.9
1	A	202	LEU	3.8
1	A	226	ALA	3.8
1	A	225	GLY	3.8
1	B	40	GLY	3.4
1	B	220	THR	3.3
1	B	41	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	239	MET	3.2
1	B	217	GLN	3.0
1	B	111	LEU	3.0
1	B	242	ALA	3.0
1	B	247	GLU	2.9
1	B	216	ASP	2.9
1	A	49	ASP	2.9
1	B	221	ALA	2.9
1	A	169	ALA	2.8
1	B	215	LEU	2.8
1	A	206	VAL	2.7
1	A	199	ALA	2.7
1	B	231	LEU	2.7
1	B	249	ARG	2.6
1	B	222	LEU	2.6
1	B	208	VAL	2.6
1	A	224	HIS	2.5
1	A	107	ALA	2.5
1	A	53	ARG	2.5
1	B	218	LEU	2.4
1	A	293	VAL	2.4
1	B	245	VAL	2.4
1	B	251	VAL	2.3
1	B	212	VAL	2.3
1	A	223	ALA	2.3
1	A	208	VAL	2.2
1	A	191	GLY	2.2
1	B	139	ALA	2.2
1	B	219	ARG	2.2
1	B	243	VAL	2.2
1	B	225	GLY	2.2
1	A	24	ALA	2.1
1	A	32	ALA	2.1
1	B	169	ALA	2.0
1	A	203	ASN	2.0
1	B	12	ASP	2.0
1	A	193	GLY	2.0
1	B	246	THR	2.0
1	A	196	LEU	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.