Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 02:31 PM EDT

PDB ID	:	2R5W
Title	:	Crystal structure of a bifunctional NMN adenylyltransferase/ADP ribose pyrophosphatase from Francisella tularensis
Authors	:	Huang, N.; Sorci, L.; Zhang, X.; Brautigan, C.; Li, X.; Raffaelli, N.; Grishin, N.; Osterman, A.; Zhang, H.
Deposited on	:	2007-09-04
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

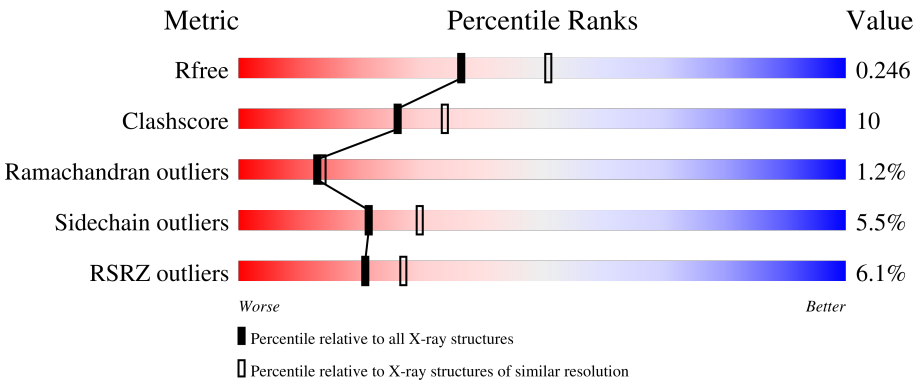
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	352	8% 79% 16%
1	B	352	4% 76% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	351	-	-	X	-
3	CL	B	351	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6097 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 Nicotinamide-nucleotide adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	345	2836	1826	478	520	12	0	0	0
1	A	344	2827	1820	476	519	12	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP Q5NHR1
B	-3	ALA	-	EXPRESSION TAG	UNP Q5NHR1
B	-2	MET	-	EXPRESSION TAG	UNP Q5NHR1
B	-1	ASP	-	EXPRESSION TAG	UNP Q5NHR1
B	0	PRO	-	EXPRESSION TAG	UNP Q5NHR1
A	-4	GLY	-	EXPRESSION TAG	UNP Q5NHR1
A	-3	ALA	-	EXPRESSION TAG	UNP Q5NHR1
A	-2	MET	-	EXPRESSION TAG	UNP Q5NHR1
A	-1	ASP	-	EXPRESSION TAG	UNP Q5NHR1
A	0	PRO	-	EXPRESSION TAG	UNP Q5NHR1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	B	3	3	3	0	0
2	A	3	3	3	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	B	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0

- Molecule 4 is water.

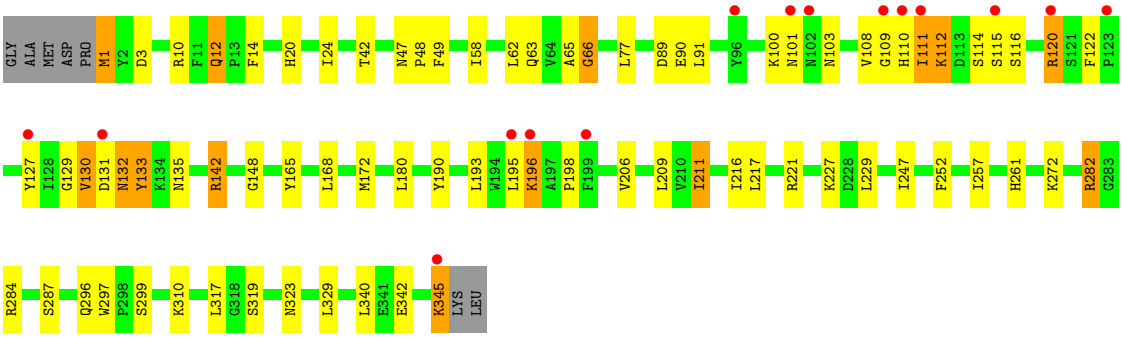
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	214	214	214	0	0
			Total	O		
4	A	211	211	211	0	0

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.

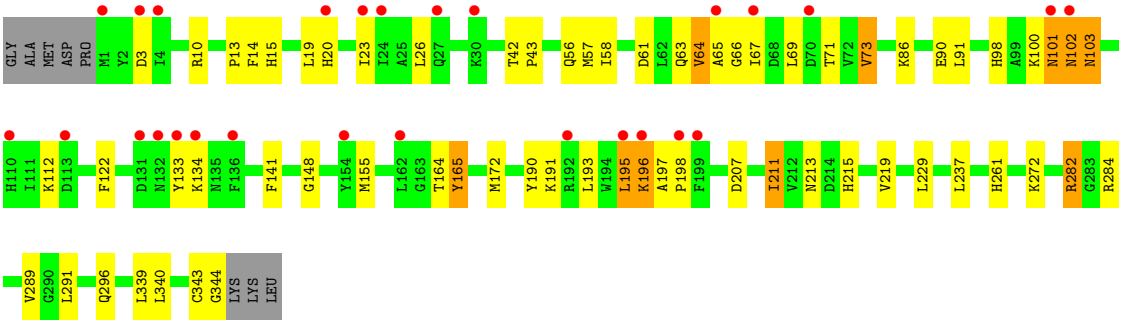
• Molecule 1: Nicotinamide-nucleotide adenylyltransferase

Chain B:



• Molecule 1: Nicotinamide-nucleotide adenylyltransferase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	124.91Å 163.15Å 180.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 2.30 39.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.53-2.30) 98.0 (39.37-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.194 , 0.253 0.185 , 0.246	Depositor DCC
R_{free} test set	2025 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6097	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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 (i)

5.1 Standard geometry (i)

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

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	0.72	0/2897	0.73	0/3924
1	B	0.69	0/2906	0.70	2/3935 (0.1%)
All	All	0.70	0/5803	0.71	2/7859 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	GLY	N-CA-C	-5.54	99.25	113.10
1	B	142	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ASN	Peptide
1	B	65	ALA	Peptide

5.2 Too-close contacts (i)

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	2827	0	2778	59	0
1	B	2836	0	2791	55	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	3	0
3	B	2	0	0	2	0
4	A	211	0	0	7	0
4	B	214	0	0	9	0
All	All	6097	0	5569	117	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 (117) 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:42:THR:HG21	1:A:229:LEU:HD21	1.34	1.04
3:A:351:CL:CL	4:A:355:HOH:O	2.12	1.03
1:A:65:ALA:H	1:A:66:GLY:HA2	1.29	0.98
3:A:351:CL:CL	4:A:447:HOH:O	2.18	0.96
3:B:351:CL:CL	4:B:386:HOH:O	2.22	0.95
1:B:42:THR:HG21	1:B:229:LEU:HD13	1.55	0.88
3:B:351:CL:CL	4:B:461:HOH:O	2.39	0.78
1:A:197:ALA:HB3	4:A:442:HOH:O	1.83	0.77
1:A:42:THR:HG21	1:A:229:LEU:CD2	2.14	0.76
1:B:116:SER:O	1:B:120:ARG:HD2	1.85	0.75
1:B:148:GLY:HA2	1:B:172:MET:HE3	1.68	0.75
1:A:211:ILE:HD11	1:A:340:LEU:HD21	1.69	0.74
3:A:351:CL:CL	4:A:357:HOH:O	2.44	0.72
1:A:103:ASN:ND2	1:A:103:ASN:H	1.88	0.72
1:A:193:LEU:O	1:A:196:LYS:HB2	1.89	0.72
1:A:61:ASP:OD2	1:A:164:THR:HG23	1.89	0.72
1:B:110:HIS:HA	1:B:131:ASP:OD1	1.91	0.71
1:B:131:ASP:HB3	1:B:132:ASN:HB2	1.73	0.71
1:A:155:MET:HE1	1:A:165:TYR:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:O	1:A:64:VAL:HG12	1.91	0.69
1:B:131:ASP:CB	1:B:132:ASN:HB2	2.23	0.69
1:A:343:CYS:H	1:A:344:GLY:HA3	1.58	0.68
1:B:131:ASP:HA	1:B:132:ASN:CB	2.22	0.68
1:A:101:ASN:H	1:A:103:ASN:HD21	1.42	0.67
1:B:133:TYR:CD1	1:B:133:TYR:N	2.48	0.67
1:B:190:TYR:CZ	1:B:282:ARG:HD2	2.30	0.67
1:A:272:LYS:HG3	1:A:339:LEU:HD21	1.77	0.66
1:A:57:MET:HB3	1:A:164:THR:HG22	1.78	0.66
1:B:340:LEU:O	1:B:345:LYS:HG3	1.97	0.65
1:B:198:PRO:HG3	1:A:193:LEU:HB3	1.79	0.64
1:A:63:GLN:HE21	1:A:69:LEU:HD11	1.63	0.64
1:B:148:GLY:HA2	1:B:172:MET:CE	2.27	0.63
1:A:211:ILE:CD1	1:A:340:LEU:HD21	2.28	0.63
1:A:343:CYS:N	1:A:344:GLY:HA3	2.14	0.63
1:B:1:MET:N	4:B:530:HOH:O	2.30	0.62
1:B:319:SER:O	1:B:323:ASN:HB2	1.99	0.61
1:B:109:GLY:O	1:B:130:VAL:HG22	2.01	0.61
1:B:142:ARG:NH2	4:B:387:HOH:O	2.33	0.61
1:A:272:LYS:HG3	1:A:339:LEU:CD2	2.31	0.60
1:B:24:ILE:HG21	1:B:130:VAL:HG12	1.84	0.60
1:B:131:ASP:HA	1:B:132:ASN:CG	2.23	0.60
1:B:216:ILE:HD11	1:B:317:LEU:HD21	1.84	0.60
1:B:89:ASP:OD2	4:B:442:HOH:O	2.17	0.59
1:B:10:ARG:NH1	4:B:425:HOH:O	2.35	0.59
1:B:131:ASP:CA	1:B:132:ASN:HB2	2.32	0.59
1:B:110:HIS:N	1:B:127:TYR:OH	2.36	0.58
1:A:26:LEU:HD22	1:A:71:THR:CG2	2.34	0.58
1:A:65:ALA:N	1:A:66:GLY:HA2	2.04	0.58
1:A:261:HIS:HD2	4:A:368:HOH:O	1.87	0.57
1:B:42:THR:HG23	4:B:428:HOH:O	2.04	0.56
1:B:100:LYS:H	1:B:103:ASN:ND2	2.04	0.56
1:B:190:TYR:CE2	1:B:282:ARG:HD2	2.41	0.55
1:A:148:GLY:HA2	1:A:172:MET:HE2	1.88	0.55
1:B:272:LYS:HE2	4:B:497:HOH:O	2.07	0.55
1:B:131:ASP:CA	1:B:132:ASN:CB	2.85	0.55
1:B:12:GLN:HE22	1:B:49:PHE:H	1.53	0.54
1:A:3:ASP:OD1	1:A:103:ASN:HA	2.08	0.54
1:A:42:THR:HG23	1:A:43:PRO:HD2	1.91	0.52
1:A:190:TYR:CE2	1:A:282:ARG:HG2	2.44	0.52
1:A:91:LEU:HD23	1:A:122:PHE:CZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:O	1:A:90:GLU:HG2	2.10	0.52
1:A:155:MET:CE	1:A:165:TYR:N	2.72	0.52
1:B:297:TRP:HD1	1:B:299:SER:O	1.94	0.51
1:A:103:ASN:H	1:A:103:ASN:HD22	1.54	0.51
1:A:291:LEU:HD23	1:A:343:CYS:HB3	1.93	0.50
1:B:110:HIS:HB3	1:B:131:ASP:OD2	2.11	0.50
1:A:42:THR:CG2	1:A:43:PRO:HD2	2.41	0.50
1:A:191:LYS:O	1:A:195:LEU:HD13	2.12	0.50
1:A:42:THR:CG2	1:A:229:LEU:HD21	2.24	0.49
1:B:77:LEU:HD23	1:B:90:GLU:HG2	1.93	0.49
1:B:48:PRO:HB3	1:B:180:LEU:HD13	1.95	0.48
1:B:62:LEU:O	1:B:66:GLY:HA2	2.14	0.48
1:A:19:LEU:O	1:A:23:ILE:HG13	2.13	0.48
1:B:196:LYS:HD2	1:B:196:LYS:HA	1.69	0.48
1:A:57:MET:HB3	1:A:164:THR:CG2	2.44	0.47
1:A:103:ASN:ND2	1:A:103:ASN:N	2.58	0.47
1:B:206:VAL:HB	1:B:247:ILE:HG12	1.96	0.47
1:A:61:ASP:CG	1:A:164:THR:HG23	2.33	0.47
1:A:64:VAL:O	1:A:64:VAL:CG1	2.61	0.47
1:B:42:THR:HG21	1:B:229:LEU:CD1	2.37	0.47
1:B:112:LYS:HE2	1:B:131:ASP:HB3	1.97	0.47
1:B:110:HIS:O	1:B:115:SER:HB3	2.15	0.46
1:A:26:LEU:HD21	1:A:71:THR:HG22	1.98	0.46
1:A:112:LYS:HA	1:A:112:LYS:HD2	1.83	0.46
1:A:26:LEU:CD2	1:A:71:THR:CG2	2.94	0.46
1:B:221:ARG:HD2	1:B:329:LEU:HD22	1.98	0.45
1:A:63:GLN:HE21	1:A:69:LEU:CD1	2.29	0.45
1:B:3:ASP:OD2	1:B:103:ASN:HA	2.16	0.45
1:B:63:GLN:NE2	4:B:446:HOH:O	2.49	0.45
1:A:13:PRO:HG3	1:A:141:PHE:CE2	2.51	0.45
1:B:193:LEU:HB3	1:A:198:PRO:HG3	1.99	0.45
1:A:20:HIS:HA	1:A:23:ILE:HD12	1.98	0.45
1:A:56:GLN:NE2	4:A:535:HOH:O	2.50	0.44
1:A:272:LYS:HE2	1:A:343:CYS:SG	2.58	0.44
1:A:207:ASP:HB2	1:A:289:VAL:HG22	1.99	0.44
1:B:10:ARG:HH12	1:B:47:ASN:CG	2.22	0.43
1:B:216:ILE:HD11	1:B:317:LEU:CD2	2.48	0.43
1:B:14:PHE:CD1	1:B:58:ILE:HG12	2.54	0.43
1:A:190:TYR:CD2	1:A:282:ARG:HG2	2.54	0.43
1:A:65:ALA:H	1:A:66:GLY:CA	2.13	0.43
1:A:10:ARG:NH2	4:A:418:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ILE:HD11	1:B:340:LEU:HD21	2.01	0.42
1:A:14:PHE:CD1	1:A:58:ILE:HG12	2.54	0.42
1:A:26:LEU:CD2	1:A:71:THR:HG22	2.49	0.42
1:A:155:MET:HE1	1:A:164:THR:C	2.40	0.42
1:B:252:PHE:HE1	1:B:261:HIS:CD2	2.38	0.42
1:A:73:VAL:HG21	1:A:98:HIS:CE1	2.55	0.42
1:A:213:ASN:OD1	1:A:296:GLN:HA	2.20	0.41
1:B:108:VAL:HG22	1:B:108:VAL:O	2.20	0.41
1:B:91:LEU:HD23	1:B:122:PHE:CZ	2.56	0.41
1:A:211:ILE:HA	1:A:215:HIS:O	2.20	0.41
1:B:168:LEU:O	1:B:172:MET:HG3	2.20	0.41
1:B:217:LEU:HD22	1:B:257:ILE:HD12	2.02	0.41
1:A:197:ALA:HA	1:A:198:PRO:HD3	1.79	0.41
1:B:110:HIS:H	1:B:127:TYR:HH	1.68	0.40
1:B:111:ILE:HG12	1:B:129:GLY:HA3	2.04	0.40
1:B:20:HIS:NE2	1:B:24:ILE:HD11	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	342/352 (97%)	323 (94%)	14 (4%)	5 (2%)	10 10
1	B	343/352 (97%)	329 (96%)	11 (3%)	3 (1%)	17 20
All	All	685/704 (97%)	652 (95%)	25 (4%)	8 (1%)	13 14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	ASN
1	A	133	TYR

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Mol	Chain	Res	Type
1	B	101	ASN
1	B	112	LYS
1	A	67	ILE
1	A	102	ASN
1	A	196	LYS
1	A	64	VAL

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	311/317 (98%)	298 (96%)	13 (4%)	30	42
1	B	312/317 (98%)	291 (93%)	21 (7%)	16	21
All	All	623/634 (98%)	589 (94%)	34 (6%)	21	30

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	12	GLN
1	B	111	ILE
1	B	114	SER
1	B	120	ARG
1	B	130	VAL
1	B	133	TYR
1	B	135	ASN
1	B	165	TYR
1	B	195	LEU
1	B	196	LYS
1	B	209	LEU
1	B	211	ILE
1	B	227	LYS
1	B	282	ARG
1	B	284	ARG
1	B	287	SER

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Mol	Chain	Res	Type
1	B	296	GLN
1	B	310	LYS
1	B	342	GLU
1	B	345	LYS
1	A	15	HIS
1	A	73	VAL
1	A	100	LYS
1	A	102	ASN
1	A	103	ASN
1	A	134	LYS
1	A	165	TYR
1	A	195	LEU
1	A	211	ILE
1	A	219	VAL
1	A	237	LEU
1	A	282	ARG
1	A	284	ARG

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

Mol	Chain	Res	Type
1	B	12	GLN
1	B	103	ASN
1	B	261	HIS
1	A	63	GLN
1	A	88	GLN
1	A	103	ASN
1	A	261	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	344/352 (97%)	0.29	27 (7%)	13	17	21, 40, 82, 108	0
1	B	345/352 (98%)	0.06	15 (4%)	35	42	24, 38, 71, 97	0
All	All	689/704 (97%)	0.17	42 (6%)	21	27	21, 39, 78, 108	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	TYR	12.2
1	B	111	ILE	6.9
1	A	113	ASP	5.2
1	B	110	HIS	5.1
1	B	195	LEU	5.0
1	A	110	HIS	5.0
1	A	101	ASN	4.6
1	A	199	PHE	4.2
1	A	20	HIS	4.1
1	A	192	ARG	4.1
1	A	27	GLN	4.0
1	A	136	PHE	3.9
1	A	198	PRO	3.8
1	A	30	LYS	3.5
1	B	115	SER	3.5
1	B	196	LYS	3.5
1	B	102	ASN	3.4
1	A	131	ASP	3.2
1	A	23	ILE	3.1
1	A	65	ALA	3.1
1	A	134	LYS	2.8
1	B	345	LYS	2.7
1	A	24	ILE	2.7
1	B	123	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	109	GLY	2.6
1	B	101	ASN	2.6
1	A	132	ASN	2.6
1	A	3	ASP	2.5
1	A	102	ASN	2.5
1	A	162	LEU	2.4
1	B	199	PHE	2.4
1	A	195	LEU	2.4
1	A	196	LYS	2.4
1	A	1	MET	2.4
1	A	70	ASP	2.2
1	B	127	TYR	2.2
1	A	4	ILE	2.2
1	B	131	ASP	2.1
1	A	154	TYR	2.1
1	B	120	ARG	2.1
1	A	67	ILE	2.1
1	B	96	TYR	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)

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. 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	B-factors(Å^2)	Q<0.9
2	MG	B	350	1/1	0.87	0.12	39,39,39,39	0
2	MG	A	349	1/1	0.88	0.09	30,30,30,30	0
2	MG	B	349	1/1	0.90	0.11	39,39,39,39	0
3	CL	A	351	1/1	0.90	0.16	31,31,31,31	0
2	MG	A	350	1/1	0.96	0.11	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	B	351	1/1	0.98	0.14	37,37,37,37	0
2	MG	A	348	1/1	0.98	0.08	31,31,31,31	0
3	CL	B	352	1/1	0.99	0.08	37,37,37,37	0
2	MG	B	348	1/1	0.99	0.06	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.