Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:45 PM GMT

PDB ID	:	1YKD
Title	:	Crystal Structure of the Tandem GAF Domains from a Cyanobacterial Adenylyl Cyclase: Novel Modes of Ligand-Binding and Dimerization
Authors	:	Martinez, S.E.; Bruder, S.; Schultz, A.; Zheng, N.; Schultz, J.E.; Beavo, J.A.; Linder, J.U.
Deposited on	:	2005-01-17
Resolution	:	1.90 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:

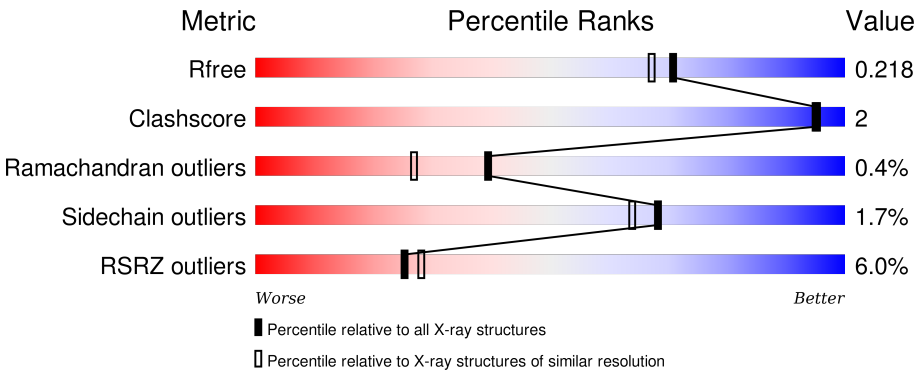
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	398	7% 92% • •
1	B	398	4% 89% 6% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6601 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.

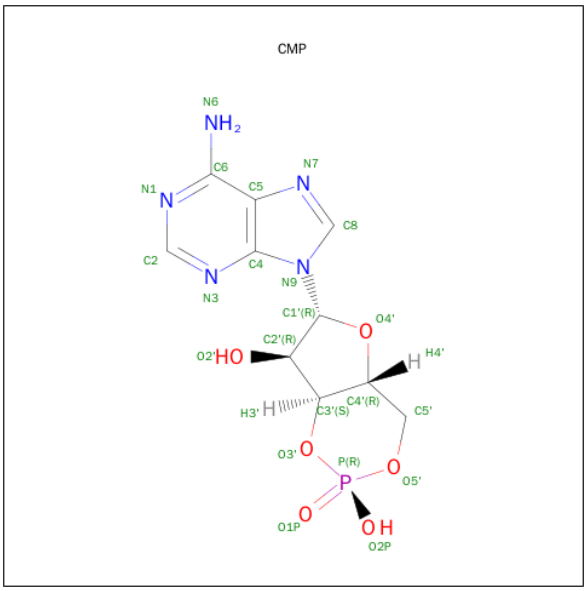
- Molecule 1 is a protein called adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	3029	1919	512	585	13	0	1	0
1	B	380	3009	1910	507	580	12	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	GLY	-	CLONING ARTIFACT	UNP P94182
A	447	SER	-	CLONING ARTIFACT	UNP P94182
A	448	ARG	-	CLONING ARTIFACT	UNP P94182
A	449	SER	-	CLONING ARTIFACT	UNP P94182
A	450	HIS	-	CLONING ARTIFACT	UNP P94182
A	451	HIS	-	CLONING ARTIFACT	UNP P94182
A	452	HIS	-	CLONING ARTIFACT	UNP P94182
A	453	HIS	-	CLONING ARTIFACT	UNP P94182
A	454	HIS	-	CLONING ARTIFACT	UNP P94182
A	455	HIS	-	CLONING ARTIFACT	UNP P94182
B	446	GLY	-	CLONING ARTIFACT	UNP P94182
B	447	SER	-	CLONING ARTIFACT	UNP P94182
B	448	ARG	-	CLONING ARTIFACT	UNP P94182
B	449	SER	-	CLONING ARTIFACT	UNP P94182
B	450	HIS	-	CLONING ARTIFACT	UNP P94182
B	451	HIS	-	CLONING ARTIFACT	UNP P94182
B	452	HIS	-	CLONING ARTIFACT	UNP P94182
B	453	HIS	-	CLONING ARTIFACT	UNP P94182
B	454	HIS	-	CLONING ARTIFACT	UNP P94182
B	455	HIS	-	CLONING ARTIFACT	UNP P94182

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 3 is water.

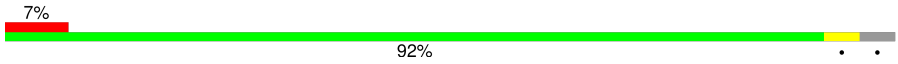
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	228	Total	O	0	0
			228	228		
3	B	247	Total	O	0	0
			247	247		

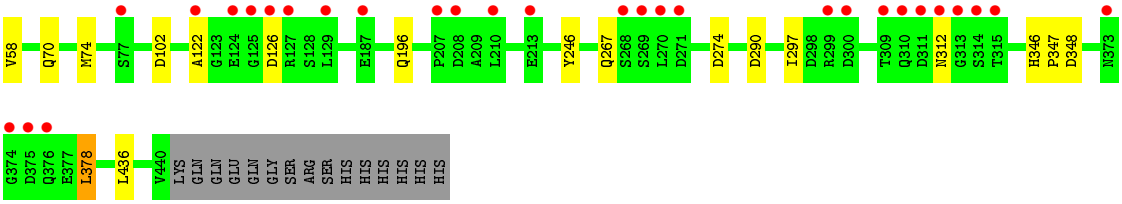
3 Residue-property plots (i)

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: adenylate cyclase

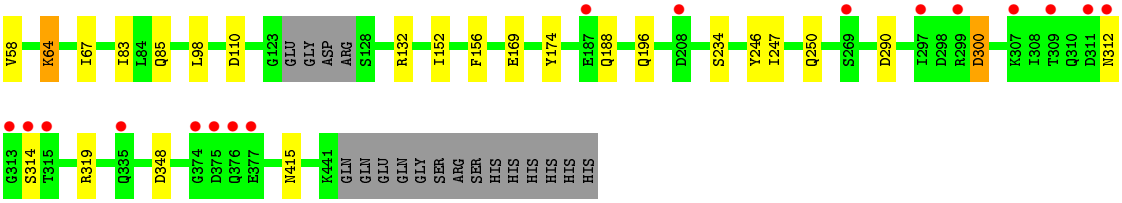
Chain A:





- Molecule 1: adenylate cyclase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.96Å 66.27Å 70.21Å 103.57° 96.56° 115.15°	Depositor
Resolution (Å)	48.20 – 1.90 48.17 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (48.20-1.90) 83.4 (48.17-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.182 , 0.215 0.190 , 0.218	Depositor DCC
R_{free} test set	3743 reflections (5.66%)	DCC
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.5	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 73121 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6601	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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 (i)

5.1 Standard geometry (i)

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

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	0.35	0/3089	0.68	5/4181 (0.1%)
1	B	0.36	0/3068	0.68	3/4151 (0.1%)
All	All	0.35	0/6157	0.68	8/8332 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	348	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	102	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	348	ASP	CB-CG-OD2	5.36	123.13	118.30
1	B	290	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	290	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	110	ASP	CB-CG-OD2	5.09	122.89	118.30
1	A	274	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	126	ASP	CB-CG-OD2	5.02	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3029	0	3016	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3009	0	3002	11	0
2	A	44	0	22	3	0
2	B	44	0	22	3	0
3	A	228	0	0	1	1
3	B	247	0	0	1	0
All	All	6601	0	6062	19	1

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 2.

All (19) 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)
2:B:503:CMP:H2	2:B:503:CMP:C2	0.97	1.48
2:A:501:CMP:H2	2:A:501:CMP:C2	0.97	1.48
2:A:502:CMP:C2	2:A:502:CMP:H2	0.97	1.48
2:B:504:CMP:C2	2:B:504:CMP:H2	0.97	1.47
1:A:297:ILE:HD11	1:A:378:LEU:HD23	1.53	0.91
1:A:58:VAL:N	1:B:246:TYR:HH	1.71	0.87
1:A:246:TYR:HH	1:B:58:VAL:N	1.77	0.83
1:B:169:GLU:HG3	1:B:174:TYR:O	1.95	0.67
1:A:122:ALA:HB2	3:A:612:HOH:O	1.95	0.66
1:B:64:LYS:HD2	1:B:67:ILE:HD12	1.87	0.56
1:B:247:ILE:O	1:B:250:GLN:HG2	2.10	0.51
1:B:152:ILE:HG21	1:B:156:PHE:CD1	2.47	0.50
1:A:196:GLN:OE1	2:A:501:CMP:H8	2.13	0.48
1:A:267:GLN:HE21	1:B:83:ILE:HD11	1.79	0.47
1:B:169:GLU:CG	1:B:174:TYR:O	2.62	0.47
1:A:436:LEU:HD23	1:B:234:SER:OG	2.16	0.46
1:B:196:GLN:OE1	2:B:503:CMP:H8	2.16	0.45
1:B:132:ARG:NH2	3:B:551:HOH:O	2.48	0.44
1:A:346:HIS:CG	1:A:347:PRO:HD2	2.55	0.42

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:561:HOH:O	3:A:686:HOH:O[1_655]	2.17	0.03

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	382/398 (96%)	376 (98%)	5 (1%)	1 (0%)	46	35
1	B	377/398 (95%)	368 (98%)	7 (2%)	2 (0%)	34	21
All	All	759/796 (95%)	744 (98%)	12 (2%)	3 (0%)	39	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	ASN
1	B	300	ASP
1	B	312	ASN

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	331/344 (96%)	328 (99%)	3 (1%)	84	83
1	B	329/344 (96%)	321 (98%)	8 (2%)	57	49
All	All	660/688 (96%)	649 (98%)	11 (2%)	68	64

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	74	MET
1	A	378	LEU

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Mol	Chain	Res	Type
1	B	64	LYS
1	B	85	GLN
1	B	98	LEU
1	B	188	GLN
1	B	300	ASP
1	B	314	SER
1	B	319	ARG
1	B	415	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	312	ASN
1	A	432	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are 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	CMP	A	501	-	19,25,25	1.54	2 (10%)	18,39,39	3.39	5 (27%)
2	CMP	A	502	-	19,25,25	1.80	4 (21%)	18,39,39	3.41	7 (38%)
2	CMP	B	503	-	19,25,25	1.53	4 (21%)	18,39,39	3.54	7 (38%)
2	CMP	B	504	-	19,25,25	1.81	3 (15%)	18,39,39	3.46	8 (44%)

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	CMP	A	501	-	-	0/0/31/31	0/4/4/4
2	CMP	A	502	-	-	0/0/31/31	0/4/4/4
2	CMP	B	503	-	-	0/0/31/31	0/4/4/4
2	CMP	B	504	-	-	0/0/31/31	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	CMP	O5'-C5'	-2.47	1.42	1.46
2	B	503	CMP	C5-N7	-2.06	1.32	1.39
2	B	503	CMP	P-O3'	2.47	1.62	1.58
2	A	502	CMP	P-O3'	2.57	1.62	1.58
2	B	504	CMP	P-O3'	3.30	1.63	1.58
2	A	501	CMP	C2-N1	3.48	1.40	1.33
2	B	503	CMP	C2-N1	3.51	1.40	1.33
2	B	503	CMP	O4'-C1'	3.56	1.45	1.41
2	B	504	CMP	C2-N1	3.64	1.40	1.33
2	A	502	CMP	C2-N1	3.64	1.40	1.33
2	A	501	CMP	O4'-C1'	4.47	1.46	1.41
2	B	504	CMP	O4'-C1'	4.83	1.47	1.41
2	A	502	CMP	O4'-C1'	4.91	1.47	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	CMP	N3-C2-N1	-12.12	119.62	128.89
2	B	503	CMP	N3-C2-N1	-11.85	119.82	128.89
2	A	501	CMP	N3-C2-N1	-11.70	119.93	128.89
2	B	504	CMP	N3-C2-N1	-11.62	120.00	128.89
2	B	503	CMP	C4'-O4'-C1'	-5.04	104.18	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	CMP	C4'-O4'-C1'	-4.75	104.50	109.72
2	B	504	CMP	O3'-C3'-C4'	-3.94	107.57	110.72
2	A	502	CMP	C4'-O4'-C1'	-3.50	105.88	109.72
2	B	504	CMP	C4'-O4'-C1'	-3.33	106.06	109.72
2	B	503	CMP	O3'-C3'-C4'	-3.21	108.16	110.72
2	B	503	CMP	O5'-P-O3'	-3.15	101.13	105.75
2	B	504	CMP	O4'-C1'-N9	-3.05	101.70	108.10
2	B	504	CMP	O5'-P-O3'	-2.87	101.54	105.75
2	A	501	CMP	C4-C5-N7	-2.55	107.13	109.48
2	A	502	CMP	O4'-C1'-N9	-2.46	102.94	108.10
2	B	503	CMP	C1'-N9-C4	-2.43	123.28	126.94
2	A	502	CMP	C5'-C4'-C3'	-2.41	107.26	112.62
2	A	502	CMP	O5'-P-O3'	-2.40	102.23	105.75
2	B	503	CMP	C2'-C1'-N9	-2.31	110.75	114.29
2	B	504	CMP	O4'-C4'-C3'	-2.22	99.75	104.86
2	A	502	CMP	C1'-N9-C4	-2.21	123.60	126.94
2	B	504	CMP	C5'-C4'-C3'	-2.19	107.75	112.62
2	A	501	CMP	C5'-C4'-C3'	-2.14	107.86	112.62
2	B	503	CMP	O2P-P-O1P	3.25	119.15	108.80
2	A	502	CMP	O2P-P-O1P	3.40	119.64	108.80
2	B	504	CMP	O2P-P-O1P	3.48	119.88	108.80
2	A	501	CMP	O2P-P-O1P	3.51	119.99	108.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CMP	2	0
2	A	502	CMP	1	0
2	B	503	CMP	2	0
2	B	504	CMP	1	0

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	383/398 (96%)	0.13	29 (7%)	17	18	9, 18, 48, 66	0
1	B	380/398 (95%)	0.17	17 (4%)	37	40	9, 19, 44, 66	0
All	All	763/796 (95%)	0.15	46 (6%)	25	28	9, 19, 47, 66	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	311	ASP	8.5
1	A	125	GLY	7.7
1	A	126	ASP	6.2
1	B	313	GLY	6.0
1	A	313	GLY	5.8
1	B	312	ASN	5.5
1	B	299	ARG	5.1
1	A	315	THR	5.1
1	A	269	SER	5.0
1	A	299	ARG	4.8
1	B	269	SER	4.4
1	A	311	ASP	4.0
1	A	309	THR	4.0
1	A	314	SER	4.0
1	B	208	ASP	4.0
1	B	309	THR	3.9
1	B	315	THR	3.9
1	A	270	LEU	3.6
1	A	312	ASN	3.6
1	B	375	ASP	3.5
1	A	127	ARG	3.5
1	B	314	SER	3.4
1	A	124	GLU	3.4
1	A	207	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	374	GLY	3.1
1	B	377	GLU	2.9
1	B	335	GLN	2.9
1	B	376	GLN	2.8
1	A	374	GLY	2.8
1	A	208	ASP	2.7
1	A	268	SER	2.6
1	B	187	GLU	2.6
1	A	300	ASP	2.5
1	A	375	ASP	2.5
1	A	187	GLU	2.5
1	A	129	LEU	2.4
1	B	297	ILE	2.3
1	A	122	ALA	2.3
1	A	210	LEU	2.3
1	A	376	GLN	2.3
1	A	310	GLN	2.2
1	A	213	GLU	2.2
1	A	373	ASN	2.1
1	A	77	SER	2.1
1	A	271	ASP	2.0
1	B	307	LYS	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	CMP	A	502	22/22	0.99	0.08	-0.24	9,11,14,15	0
2	CMP	B	504	22/22	0.98	0.07	-0.73	5,10,13,15	0
2	CMP	B	503	22/22	0.98	0.07	-0.87	7,11,13,17	0
2	CMP	A	501	22/22	0.98	0.07	-0.88	8,11,12,15	0

6.5 Other polymers (i)

There are no such residues in this entry.