wwPDB X-ray Structure Validation Summary Report (i)

Sep 12, 2023 – 09:14 AM EDT

PDB ID	:	4NF1
Title	:	Structure of N-acetyltransferase domain of X. fastidiosa NAGS/K without his-tag
Authors	:	Zhao, G.; Jin, Z.; Allewell, N.M.; Tuchman, M.; Shi, D.
Deposited on	:	2013-10-30
Resolution	:	1.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

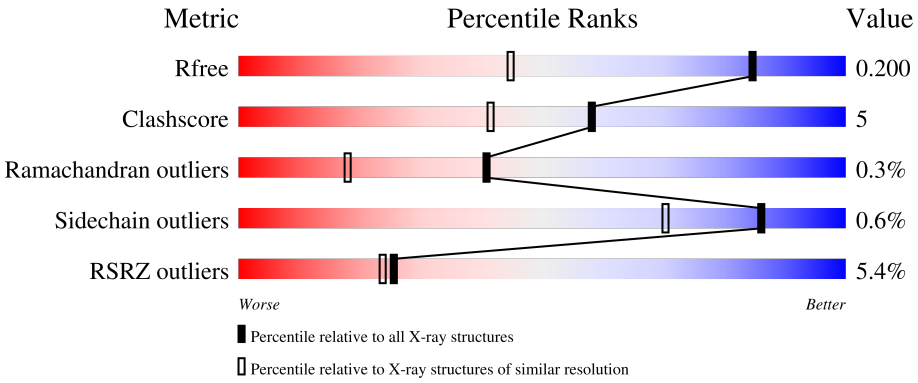
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	150	90% 7%
1	B	150	10% 89% 7%
1	C	150	91% 7%
1	D	150	5% 94%
1	E	150	92% 6%

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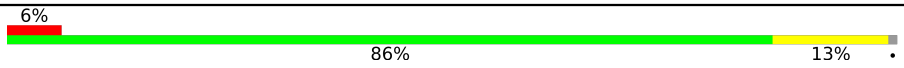
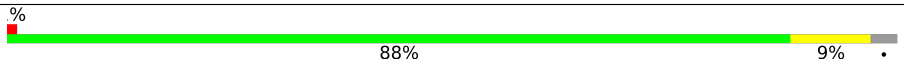
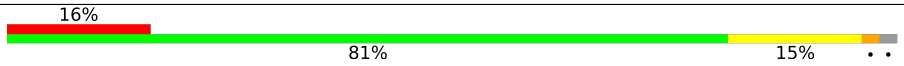
Mol	Chain	Length	Quality of chain
1	F	150	
1	G	150	
1	H	150	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11687 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 Acetylglutamate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	2	0
			1232	794	219	216	3			
1	B	146	Total	C	N	O	S	0	3	0
			1235	794	220	218	3			
1	C	147	Total	C	N	O	S	0	4	0
			1248	804	220	220	4			
1	D	149	Total	C	N	O	S	0	0	0
			1248	801	224	219	4			
1	E	147	Total	C	N	O	S	0	1	0
			1235	794	220	217	4			
1	F	148	Total	C	N	O	S	0	1	0
			1250	803	226	217	4			
1	G	146	Total	C	N	O	S	0	2	0
			1232	794	219	216	3			
1	H	147	Total	C	N	O	S	0	1	0
			1236	796	222	214	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	GLY	-	expression tag	UNP Q87EL2
A	290	SER	-	expression tag	UNP Q87EL2
A	291	HIS	-	expression tag	UNP Q87EL2
A	292	MET	-	expression tag	UNP Q87EL2
B	289	GLY	-	expression tag	UNP Q87EL2
B	290	SER	-	expression tag	UNP Q87EL2
B	291	HIS	-	expression tag	UNP Q87EL2
B	292	MET	-	expression tag	UNP Q87EL2
C	289	GLY	-	expression tag	UNP Q87EL2
C	290	SER	-	expression tag	UNP Q87EL2
C	291	HIS	-	expression tag	UNP Q87EL2
C	292	MET	-	expression tag	UNP Q87EL2
D	289	GLY	-	expression tag	UNP Q87EL2

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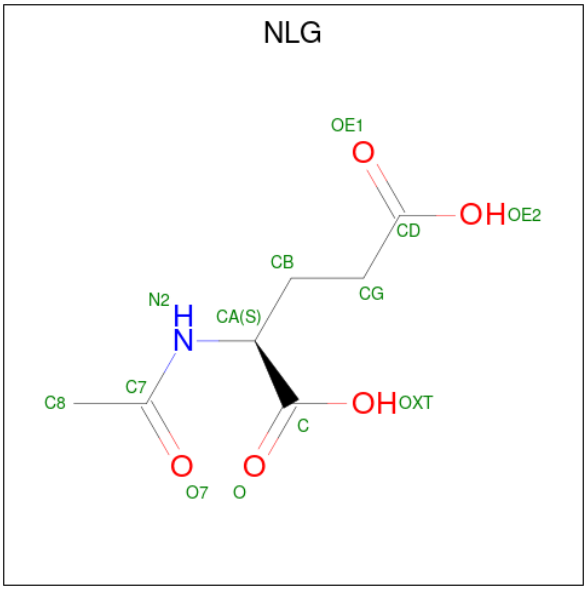
Chain	Residue	Modelled	Actual	Comment	Reference
D	290	SER	-	expression tag	UNP Q87EL2
D	291	HIS	-	expression tag	UNP Q87EL2
D	292	MET	-	expression tag	UNP Q87EL2
E	289	GLY	-	expression tag	UNP Q87EL2
E	290	SER	-	expression tag	UNP Q87EL2
E	291	HIS	-	expression tag	UNP Q87EL2
E	292	MET	-	expression tag	UNP Q87EL2
F	289	GLY	-	expression tag	UNP Q87EL2
F	290	SER	-	expression tag	UNP Q87EL2
F	291	HIS	-	expression tag	UNP Q87EL2
F	292	MET	-	expression tag	UNP Q87EL2
G	289	GLY	-	expression tag	UNP Q87EL2
G	290	SER	-	expression tag	UNP Q87EL2
G	291	HIS	-	expression tag	UNP Q87EL2
G	292	MET	-	expression tag	UNP Q87EL2
H	289	GLY	-	expression tag	UNP Q87EL2
H	290	SER	-	expression tag	UNP Q87EL2
H	291	HIS	-	expression tag	UNP Q87EL2
H	292	MET	-	expression tag	UNP Q87EL2

- Molecule 2 is N-ACETYL-L-GLUTAMATE (three-letter code: NLG) (formula: $C_7H_{11}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	1	5		
2	B	1	Total	C	N	O	0	0
			13	7	1	5		

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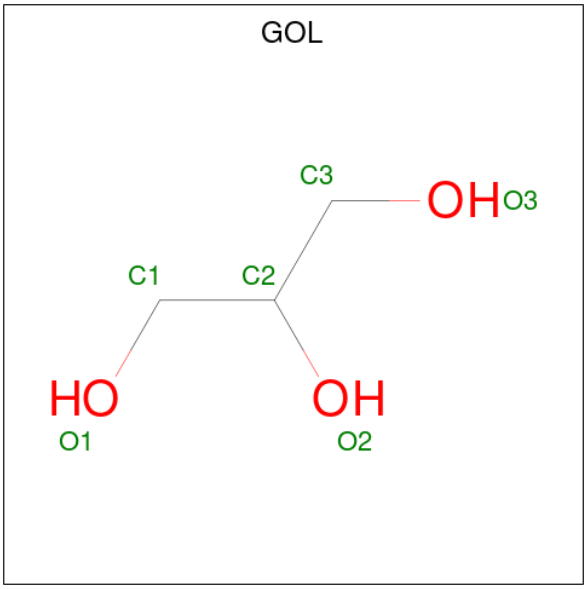
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 13 7 1 5	0	0
2	D	1	Total C N O 13 7 1 5	0	0
2	E	1	Total C N O 13 7 1 5	0	0
2	F	1	Total C N O 13 7 1 5	0	0
2	G	1	Total C N O 13 7 1 5	0	0
2	H	1	Total C N O 13 7 1 5	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total Cl 2 2	0	0
4	D	1	Total Cl 1 1	0	0
4	E	2	Total Cl 2 2	0	0
4	G	2	Total Cl 2 2	0	0

- Molecule 5 is water.

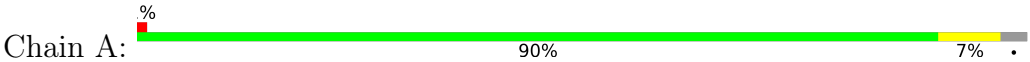
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	249	Total O 249 249	0	0
5	B	165	Total O 165 165	0	0
5	C	278	Total O 278 278	0	0
5	D	202	Total O 202 202	0	0
5	E	217	Total O 217 217	0	0
5	F	174	Total O 174 174	0	0
5	G	215	Total O 215 215	0	0
5	H	147	Total O 147 147	0	0

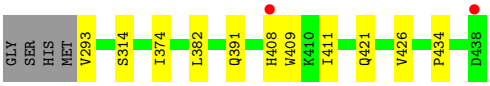
3 Residue-property plots (i)

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: Acetylglutamate kinase

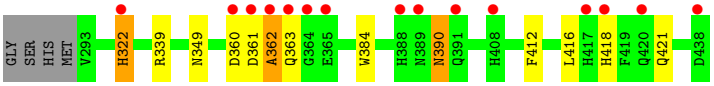
Chain A:





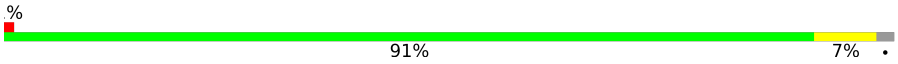
- Molecule 1: Acetylglutamate kinase

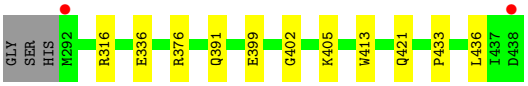
Chain B:



- Molecule 1: Acetylglutamate kinase

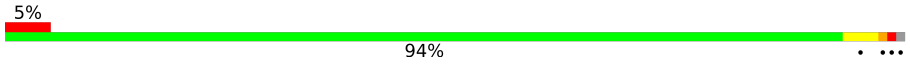
Chain C:

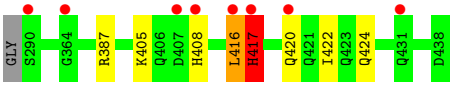




- Molecule 1: Acetylglutamate kinase

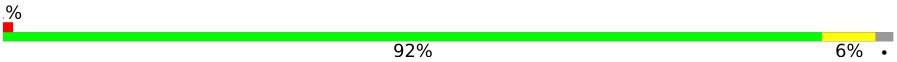
Chain D:

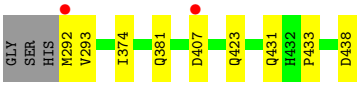




- Molecule 1: Acetylglutamate kinase

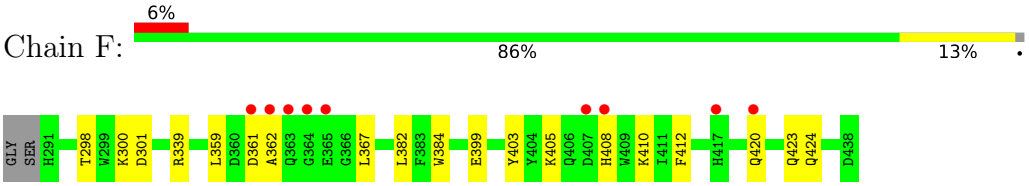
Chain E:





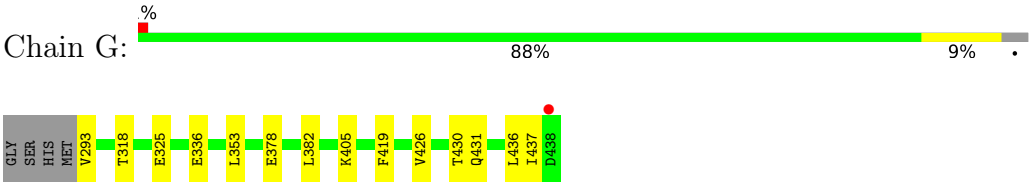
- Molecule 1: Acetylglutamate kinase

Chain F:



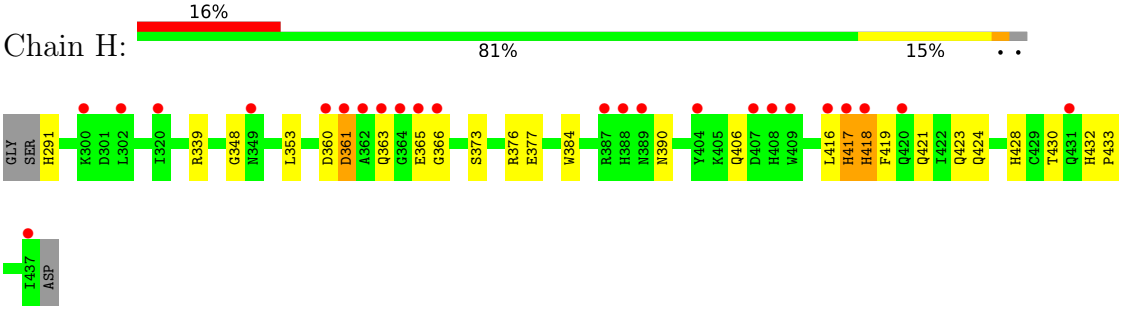
• Molecule 1: Acetylglutamate kinase

Chain G:



• Molecule 1: Acetylglutamate kinase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.87Å 123.35Å 76.66Å 90.00° 107.62° 90.00°	Depositor
Resolution (Å)	34.07 – 1.40 34.07 – 1.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (34.07-1.40) 90.5 (34.07-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.179 , 0.199 0.180 , 0.200	Depositor DCC
R_{free} test set	2000 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å^2)	14.2	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11687	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1236e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: NLG, GOL, 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	0.40	0/1277	0.58	0/1738
1	B	0.34	0/1283	0.54	0/1746
1	C	0.38	0/1299	0.53	0/1767
1	D	0.34	0/1288	0.53	0/1752
1	E	0.39	0/1277	0.54	0/1737
1	F	0.33	0/1293	0.49	0/1758
1	G	0.37	0/1277	0.52	0/1738
1	H	0.33	0/1279	0.52	0/1741
All	All	0.36	0/10273	0.53	0/13977

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	D	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	416	LEU	Peptide
1	D	417	HIS	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	1232	0	1193	15	0
1	B	1235	0	1193	9	0
1	C	1248	0	1211	10	0
1	D	1248	0	1198	10	1
1	E	1235	0	1191	7	1
1	F	1250	0	1206	15	0
1	G	1232	0	1193	13	0
1	H	1236	0	1194	21	1
2	A	13	0	9	0	0
2	B	13	0	9	0	0
2	C	13	0	9	1	0
2	D	13	0	9	0	0
2	E	13	0	9	0	0
2	F	13	0	9	0	0
2	G	13	0	9	1	0
2	H	13	0	9	0	0
3	A	6	0	8	2	0
3	G	6	0	8	0	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	1	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
5	A	249	0	0	8	2
5	B	165	0	0	5	3
5	C	278	0	0	7	0
5	D	202	0	0	3	1
5	E	217	0	0	3	0
5	F	174	0	0	7	1
5	G	215	0	0	3	0
5	H	147	0	0	10	0
All	All	11687	0	9667	94	5

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 5.

The worst 5 of 94 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:390:ASN:ND2	5:B:797:HOH:O	1.90	1.04
1:A:408:HIS:CD2	1:G:378:GLU:HB3	1.99	0.98
1:D:416:LEU:O	5:D:773:HOH:O	1.82	0.95
1:E:433:PRO:HG2	1:G:431:GLN:HB3	1.48	0.95
1:G:293:VAL:N	5:G:689:HOH:O	2.08	0.86

All (5) 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)
1:H:365:GLU:OE1	5:A:646:HOH:O[2_855]	1.90	0.30
1:D:424:GLN:NE2	5:B:855:HOH:O[1_454]	2.03	0.17
5:B:836:HOH:O	5:D:737:HOH:O[1_656]	2.07	0.13
5:B:816:HOH:O	5:F:762:HOH:O[2_746]	2.18	0.02
1:E:438:ASP:OD2	5:A:682:HOH:O[2_755]	2.19	0.01

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	146/150 (97%)	143 (98%)	3 (2%)	0	100 100
1	B	147/150 (98%)	139 (95%)	5 (3%)	3 (2%)	7 0
1	C	149/150 (99%)	146 (98%)	3 (2%)	0	100 100
1	D	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	22 5
1	E	146/150 (97%)	144 (99%)	2 (1%)	0	100 100
1	F	147/150 (98%)	144 (98%)	3 (2%)	0	100 100
1	G	146/150 (97%)	144 (99%)	2 (1%)	0	100 100
1	H	146/150 (97%)	140 (96%)	6 (4%)	0	100 100
All	All	1174/1200 (98%)	1142 (97%)	28 (2%)	4 (0%)	41 18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	ALA
1	B	363	GLN
1	D	417	HIS
1	B	390	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	131/132 (99%)	130 (99%)	1 (1%)	81	62
1	B	132/132 (100%)	131 (99%)	1 (1%)	81	62
1	C	134/132 (102%)	134 (100%)	0	100	100
1	D	132/132 (100%)	132 (100%)	0	100	100
1	E	131/132 (99%)	131 (100%)	0	100	100
1	F	132/132 (100%)	131 (99%)	1 (1%)	81	62
1	G	131/132 (99%)	131 (100%)	0	100	100
1	H	131/132 (99%)	128 (98%)	3 (2%)	50	18
All	All	1054/1056 (100%)	1048 (99%)	6 (1%)	86	70

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	361	ASP
1	H	417	HIS
1	H	418	HIS
1	B	322	HIS
1	A	382	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	420	GLN

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Mol	Chain	Res	Type
1	H	418	HIS
1	H	428	HIS
1	A	421	GLN
1	A	349	ASN

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 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

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	NLG	E	501	-	12,12,12	1.39	1 (8%)	15,15,15	1.21	2 (13%)
2	NLG	C	501	-	12,12,12	1.29	1 (8%)	15,15,15	1.38	2 (13%)
3	GOL	A	502	-	5,5,5	0.27	0	5,5,5	0.28	0
3	GOL	G	502	-	5,5,5	0.34	0	5,5,5	0.30	0
2	NLG	F	600	-	12,12,12	1.40	1 (8%)	15,15,15	1.33	1 (6%)
2	NLG	D	501	-	12,12,12	1.45	1 (8%)	15,15,15	1.20	1 (6%)
2	NLG	B	600	-	12,12,12	1.46	1 (8%)	15,15,15	1.12	1 (6%)
2	NLG	A	501	-	12,12,12	1.26	1 (8%)	15,15,15	1.48	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NLG	G	501	-	12,12,12	1.29	1 (8%)	15,15,15	1.37	2 (13%)
2	NLG	H	600	-	12,12,12	1.44	1 (8%)	15,15,15	1.27	1 (6%)

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	NLG	E	501	-	-	2/13/13/13	-
2	NLG	C	501	-	-	0/13/13/13	-
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	G	502	-	-	2/4/4/4	-
2	NLG	F	600	-	-	2/13/13/13	-
2	NLG	D	501	-	-	2/13/13/13	-
2	NLG	B	600	-	-	2/13/13/13	-
2	NLG	A	501	-	-	0/13/13/13	-
2	NLG	G	501	-	-	0/13/13/13	-
2	NLG	H	600	-	-	2/13/13/13	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	600	NLG	C7-N2	3.57	1.46	1.34
2	D	501	NLG	C7-N2	3.37	1.46	1.34
2	B	600	NLG	C7-N2	3.30	1.45	1.34
2	F	600	NLG	C7-N2	3.29	1.45	1.34
2	C	501	NLG	C7-N2	3.22	1.45	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	600	NLG	CG-CB-CA	3.76	120.18	113.16
2	A	501	NLG	OXT-C-O	-2.84	117.65	124.09
2	E	501	NLG	CG-CB-CA	2.79	118.37	113.16
2	H	600	NLG	CG-CB-CA	2.76	118.32	113.16
2	A	501	NLG	CB-CG-CD	2.72	119.71	112.51

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	502	GOL	O1-C1-C2-C3
3	G	502	GOL	O1-C1-C2-O2
2	D	501	NLG	OE2-CD-CG-CB
2	E	501	NLG	OE2-CD-CG-CB
2	F	600	NLG	OE2-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NLG	1	0
3	A	502	GOL	2	0
2	G	501	NLG	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

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	146/150 (97%)	0.06	2 (1%) 75 74	8, 14, 32, 39	0
1	B	146/150 (97%)	0.64	15 (10%) 6 6	12, 22, 51, 87	0
1	C	147/150 (98%)	0.06	2 (1%) 75 74	8, 15, 28, 53	0
1	D	149/150 (99%)	0.41	8 (5%) 25 24	12, 20, 44, 74	0
1	E	147/150 (98%)	0.10	2 (1%) 75 74	9, 18, 33, 54	0
1	F	148/150 (98%)	0.39	9 (6%) 21 19	11, 21, 48, 74	0
1	G	146/150 (97%)	0.10	1 (0%) 87 86	10, 17, 33, 56	0
1	H	147/150 (98%)	1.08	24 (16%) 1 1	15, 27, 64, 94	0
All	All	1176/1200 (98%)	0.35	63 (5%) 25 24	8, 19, 44, 94	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	ALA	19.4
1	H	365	GLU	15.1
1	H	364	GLY	11.3
1	H	417	HIS	9.5
1	D	417	HIS	9.2

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 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, 95^{th} 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
3	GOL	G	502	6/6	0.79	0.17	27,44,47,48	0
3	GOL	A	502	6/6	0.87	0.14	23,31,37,46	0
2	NLG	H	600	13/13	0.94	0.09	17,22,31,32	0
2	NLG	B	600	13/13	0.94	0.09	14,17,26,27	0
2	NLG	G	501	13/13	0.94	0.08	12,16,18,20	0
2	NLG	F	600	13/13	0.95	0.08	14,17,27,34	0
2	NLG	C	501	13/13	0.96	0.08	10,14,22,24	0
2	NLG	D	501	13/13	0.96	0.07	12,16,23,23	0
2	NLG	E	501	13/13	0.96	0.08	10,14,19,22	0
2	NLG	A	501	13/13	0.96	0.07	10,12,17,22	0
4	CL	D	502	1/1	0.98	0.07	27,27,27,27	0
4	CL	E	502	1/1	0.99	0.07	17,17,17,17	0
4	CL	E	503	1/1	0.99	0.05	27,27,27,27	0
4	CL	G	503	1/1	0.99	0.07	16,16,16,16	0
4	CL	C	502	1/1	1.00	0.06	15,15,15,15	0
4	CL	C	503	1/1	1.00	0.05	21,21,21,21	0
4	CL	A	503	1/1	1.00	0.07	13,13,13,13	0
4	CL	G	504	1/1	1.00	0.04	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.