Full wwPDB X-ray Structure Validation Report (i)

Jul 7, 2016 – 02:45 PM EDT

PDB ID	:	5IG4
Title	:	Crystal structure of N. vectensis CaMKII-A hub
Authors	:	Bhattacharyya, M.; Pappireddi, N.; Gee, C.L.; Barros, T.; Kuriyan, J.
Deposited on	:	2016-02-26
Resolution	:	2.35 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:

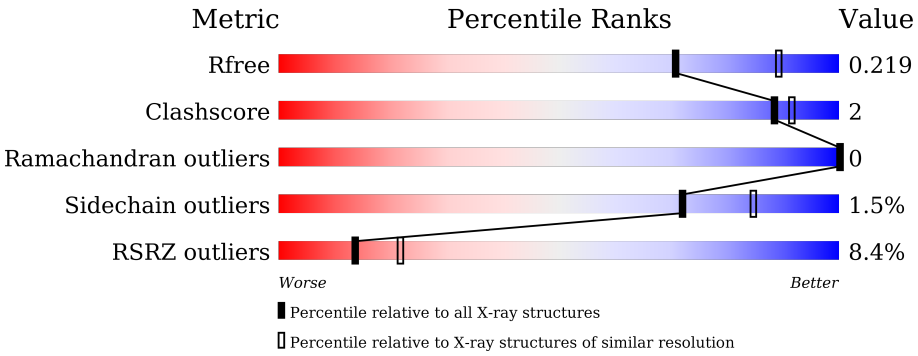
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 2.35 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.



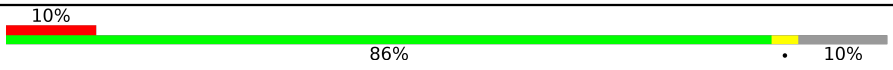
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	145	4% 84% • • 11%
1	B	145	8% 84% 6% 10%
1	C	145	6% 83% • • 12%
1	D	145	8% 80% 10% 10%
1	E	145	8% 80% 9% • 10%
1	F	145	10% 85% • • 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	145	

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
2	GOL	B	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14647 atoms, of which 7185 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 Predicted protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	129	Total	C	H	N	O	S	0	1	0
			2059	659	1021	179	196	4			
1	B	130	Total	C	H	N	O	S	0	0	0
			2059	657	1020	180	198	4			
1	C	128	Total	C	H	N	O	S	0	0	0
			2023	648	1001	175	195	4			
1	D	130	Total	C	H	N	O	S	0	2	0
			2081	664	1032	182	198	5			
1	E	131	Total	C	H	N	O	S	0	1	0
			2095	668	1040	184	199	4			
1	F	129	Total	C	H	N	O	S	0	3	0
			2079	666	1028	180	200	5			
1	G	130	Total	C	H	N	O	S	0	1	0
			2073	662	1027	182	198	4			

There are 21 discrepancies between the modelled and reference sequences:

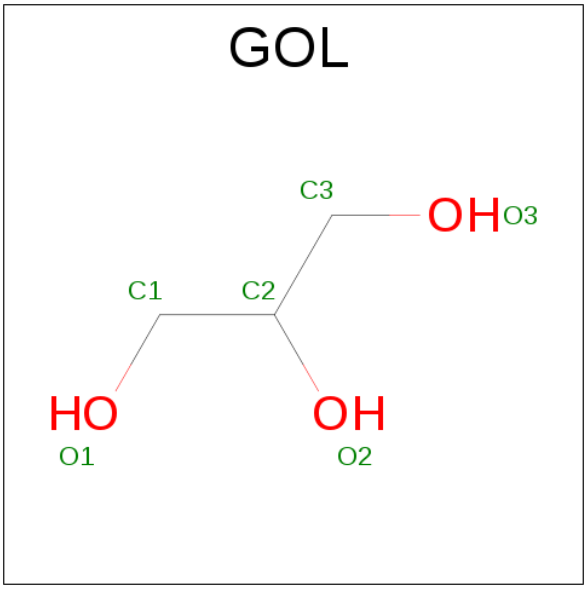
Chain	Residue	Modelled	Actual	Comment	Reference
A	330	GLY	-	expression tag	UNP A7T0H5
A	331	PRO	-	expression tag	UNP A7T0H5
A	332	HIS	-	expression tag	UNP A7T0H5
B	330	GLY	-	expression tag	UNP A7T0H5
B	331	PRO	-	expression tag	UNP A7T0H5
B	332	HIS	-	expression tag	UNP A7T0H5
C	330	GLY	-	expression tag	UNP A7T0H5
C	331	PRO	-	expression tag	UNP A7T0H5
C	332	HIS	-	expression tag	UNP A7T0H5
D	330	GLY	-	expression tag	UNP A7T0H5
D	331	PRO	-	expression tag	UNP A7T0H5
D	332	HIS	-	expression tag	UNP A7T0H5
E	330	GLY	-	expression tag	UNP A7T0H5
E	331	PRO	-	expression tag	UNP A7T0H5
E	332	HIS	-	expression tag	UNP A7T0H5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	330	GLY	-	expression tag	UNP A7T0H5
F	331	PRO	-	expression tag	UNP A7T0H5
F	332	HIS	-	expression tag	UNP A7T0H5
G	330	GLY	-	expression tag	UNP A7T0H5
G	331	PRO	-	expression tag	UNP A7T0H5
G	332	HIS	-	expression tag	UNP A7T0H5

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	20	Total	O	0	0
			20	20		
3	C	24	Total	O	0	0
			24	24		
3	D	18	Total	O	0	0
			18	18		

Continued on next page...

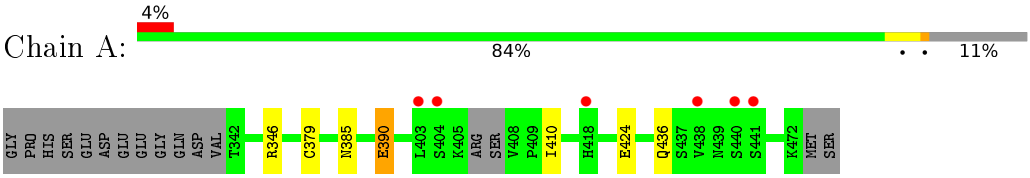
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	11	Total O 11 11	0	0
3	F	21	Total O 21 21	0	0
3	G	23	Total O 23 23	0	0

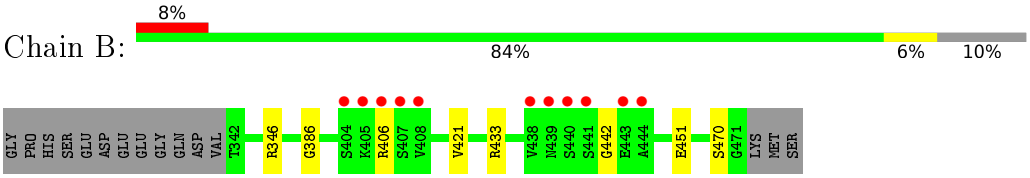
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

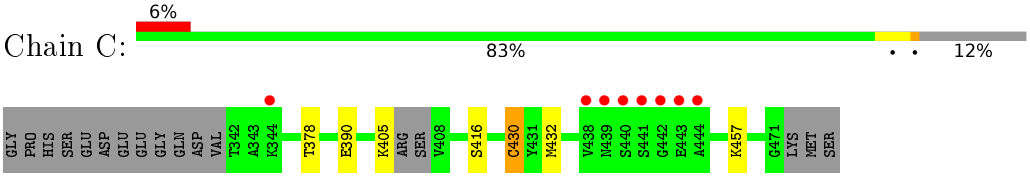
- Molecule 1: Predicted protein



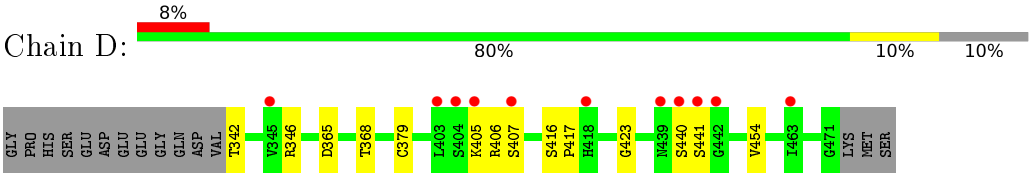
- Molecule 1: Predicted protein



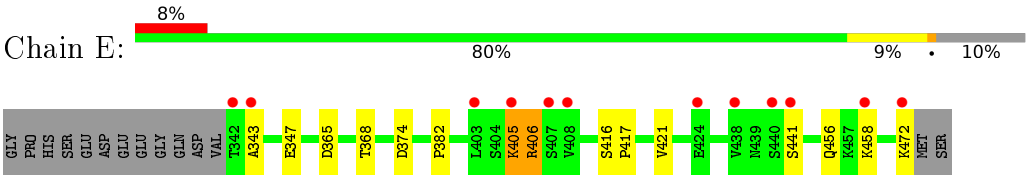
- Molecule 1: Predicted protein



- Molecule 1: Predicted protein

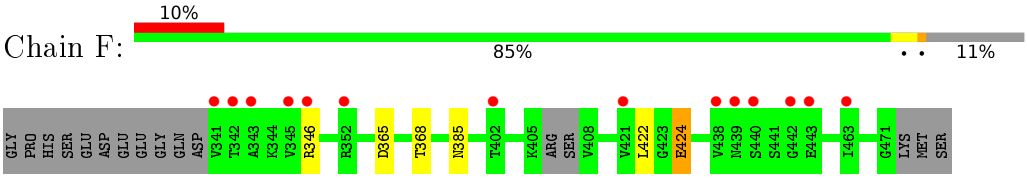


- Molecule 1: Predicted protein



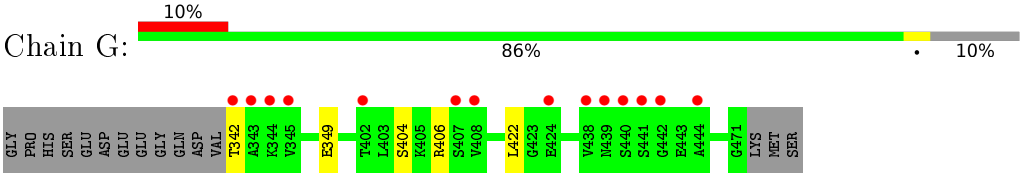
- Molecule 1: Predicted protein

Chain F:



- Molecule 1: Predicted protein

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	78.47Å 180.10Å 179.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.08 – 2.35 46.08 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.08-2.35) 99.3 (46.08-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.192 , 0.220 0.191 , 0.219	Depositor DCC
R_{free} test set	2602 reflections (4.92%)	DCC
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14647	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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

5.1 Standard geometry

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

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	0.47	0/1064	0.58	0/1441
1	B	0.43	0/1062	0.57	0/1440
1	C	0.48	1/1044 (0.1%)	0.56	0/1415
1	D	0.39	0/1079	0.55	0/1463
1	E	0.42	0/1082	0.53	0/1466
1	F	0.40	0/1077	0.52	0/1460
1	G	0.41	0/1073	0.55	0/1455
All	All	0.43	1/7481 (0.0%)	0.55	0/10140

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	430	CYS	CB-SG	-5.19	1.73	1.81

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	1038	1021	1021	4	0
1	B	1039	1020	1020	4	1
1	C	1022	1001	1001	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1049	1032	1032	10	0
1	E	1055	1040	1040	10	0
1	F	1051	1028	1026	3	0
1	G	1046	1027	1027	4	0
2	B	6	8	8	1	1
2	C	6	8	8	0	0
3	A	33	0	0	1	0
3	B	20	0	0	0	0
3	C	24	0	0	1	0
3	D	18	0	0	1	0
3	E	11	0	0	0	0
3	F	21	0	0	0	0
3	G	23	0	0	3	0
All	All	7462	7185	7183	36	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 (36) 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:E:406:ARG:NH1	1:E:406:ARG:O	2.03	0.91
1:E:374:ASP:OD2	1:E:458:LYS:NZ	2.09	0.85
1:B:470:SER:OG	2:B:501:GOL:O3	1.95	0.83
1:G:349:GLU:OE1	3:G:501:HOH:O	2.00	0.79
1:D:406:ARG:HB3	1:D:407:SER:HA	1.65	0.78
1:A:390:GLU:OE1	3:A:501:HOH:O	2.02	0.78
1:D:365:ASP:OD2	1:D:368:THR:OG1	2.01	0.76
1:D:406:ARG:CB	1:D:407:SER:HA	2.17	0.73
1:D:342:THR:N	3:D:501:HOH:O	2.20	0.72
1:D:346:ARG:NH2	1:D:423:GLY:O	2.27	0.66
1:G:404:SER:O	3:G:502:HOH:O	2.15	0.63
1:C:457:LYS:O	3:C:601:HOH:O	2.18	0.56
1:E:365:ASP:OD2	1:E:368:THR:OG1	2.17	0.55
1:C:416:SER:OG	1:C:432:MET:CE	2.56	0.54
1:F:346:ARG:NH2	1:F:424:GLU:O	2.39	0.49
1:B:442:GLY:HA3	1:E:405:LYS:HE2	1.93	0.49
1:D:440:SER:O	1:D:441:SER:OG	2.27	0.45
1:E:405:LYS:HG3	1:E:405:LYS:O	2.16	0.45
1:D:440:SER:O	1:D:441:SER:CB	2.64	0.45
1:A:346:ARG:HH12	1:A:424:GLU:HA	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ARG:HD3	1:B:451:GLU:OE2	2.17	0.44
1:C:378:THR:HG22	1:C:390:GLU:HG3	1.99	0.44
1:C:416:SER:OG	1:C:432:MET:HE2	2.16	0.44
1:E:456:GLN:NE2	1:F:422:LEU:HA	2.33	0.44
1:D:454:VAL:HG11	1:G:422:LEU:HD11	2.00	0.43
1:B:346:ARG:NH1	1:B:421:VAL:HG13	2.33	0.43
1:E:416:SER:N	1:E:417:PRO:CD	2.82	0.43
1:F:365:ASP:OD2	1:F:368:THR:OG1	2.13	0.43
1:E:343:ALA:O	1:E:347:GLU:HG3	2.19	0.43
1:E:421:VAL:HG13	1:E:421:VAL:O	2.18	0.43
1:A:410:ILE:HA	1:A:436:GLN:O	2.19	0.42
1:D:405:LYS:O	1:D:406:ARG:HG2	2.20	0.41
1:G:406:ARG:O	1:G:406:ARG:HG3	2.21	0.41
1:A:385:ASN:HB3	3:G:506:HOH:O	2.21	0.41
1:D:416:SER:N	1:D:417:PRO:CD	2.83	0.40
1:E:382:PRO:HB3	1:E:472:LYS:HG2	2.04	0.40

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)
1:B:386:GLY:H	2:B:501:GOL:HO1[3_657]	1.19	0.41

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	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
1	B	128/145 (88%)	126 (98%)	2 (2%)	0	100	100
1	C	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
1	D	130/145 (90%)	124 (95%)	6 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	130/145 (90%)	126 (97%)	4 (3%)	0	100	100
1	F	128/145 (88%)	127 (99%)	1 (1%)	0	100	100
1	G	129/145 (89%)	127 (98%)	2 (2%)	0	100	100
All	All	895/1015 (88%)	875 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	118/131 (90%)	116 (98%)	2 (2%)	68	82
1	B	118/131 (90%)	117 (99%)	1 (1%)	86	94
1	C	116/131 (88%)	114 (98%)	2 (2%)	68	82
1	D	120/131 (92%)	119 (99%)	1 (1%)	86	94
1	E	120/131 (92%)	117 (98%)	3 (2%)	55	70
1	F	120/131 (92%)	118 (98%)	2 (2%)	68	82
1	G	119/131 (91%)	118 (99%)	1 (1%)	86	94
All	All	831/917 (91%)	819 (99%)	12 (1%)	72	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	379	CYS
1	A	390	GLU
1	B	406	ARG
1	C	405	LYS
1	C	430	CYS
1	D	379	CYS
1	E	405	LYS
1	E	406	ARG
1	E	441	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	385	ASN
1	F	424	GLU
1	G	342	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

2 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	GOL	B	501	-	5,5,5	0.38	0	5,5,5	0.90	0
2	GOL	C	501	-	5,5,5	0.31	0	5,5,5	0.56	0

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	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	GOL	C	501	-	-	0/4/4/4	0/0/0/0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	GOL	1	1

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	129/145 (88%)	0.53	6 (4%)	35	50	29, 42, 80, 102	0
1	B	130/145 (89%)	0.67	11 (8%)	13	21	31, 47, 96, 105	0
1	C	128/145 (88%)	0.52	8 (6%)	23	35	30, 45, 91, 146	0
1	D	130/145 (89%)	0.66	11 (8%)	13	21	37, 56, 98, 120	0
1	E	131/145 (90%)	0.67	12 (9%)	11	18	39, 60, 99, 164	0
1	F	129/145 (88%)	0.64	14 (10%)	7	13	36, 52, 98, 123	0
1	G	130/145 (89%)	0.61	14 (10%)	8	13	35, 51, 93, 100	0
All	All	907/1015 (89%)	0.61	76 (8%)	14	22	29, 50, 97, 164	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	441	SER	7.8
1	F	341	VAL	7.1
1	F	342	THR	5.6
1	B	441	SER	5.5
1	B	444	ALA	5.2
1	B	438	VAL	4.8
1	E	342	THR	4.6
1	E	440	SER	4.6
1	E	472	LYS	4.6
1	G	407	SER	4.4
1	G	440	SER	4.4
1	D	407	SER	4.3
1	E	408	VAL	4.1
1	A	403	LEU	4.0
1	A	404	SER	3.9
1	B	404	SER	3.7
1	B	407	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	440	SER	3.7
1	C	442	GLY	3.6
1	C	438	VAL	3.5
1	F	439	ASN	3.5
1	C	440	SER	3.4
1	F	440	SER	3.4
1	G	343	ALA	3.3
1	F	345	VAL	3.3
1	B	443	GLU	3.2
1	F	442	GLY	3.2
1	G	345	VAL	3.2
1	F	352	ARG	3.2
1	G	424	GLU	3.1
1	D	405	LYS	3.1
1	G	442	GLY	3.1
1	E	441	SER	3.1
1	F	343	ALA	3.1
1	A	441	SER	3.0
1	E	407	SER	3.0
1	F	402	THR	3.0
1	C	439	ASN	2.9
1	A	418[A]	HIS	2.9
1	C	441	SER	2.8
1	C	344	LYS	2.8
1	D	404	SER	2.7
1	G	444	ALA	2.7
1	G	402	THR	2.7
1	D	440	SER	2.6
1	E	403	LEU	2.6
1	A	438	VAL	2.6
1	C	443	GLU	2.5
1	G	344	LYS	2.5
1	G	342	THR	2.5
1	E	438	VAL	2.5
1	F	438	VAL	2.5
1	E	405	LYS	2.5
1	F	346	ARG	2.5
1	F	421	VAL	2.5
1	G	408	VAL	2.5
1	G	438	VAL	2.5
1	G	441	SER	2.4
1	F	463	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	345	VAL	2.4
1	B	439	ASN	2.4
1	D	439	ASN	2.4
1	E	424	GLU	2.4
1	F	443	GLU	2.3
1	A	440	SER	2.3
1	D	403	LEU	2.2
1	D	442	GLY	2.2
1	B	405	LYS	2.2
1	B	406	ARG	2.2
1	D	418[A]	HIS	2.2
1	D	463	ILE	2.2
1	C	444	ALA	2.1
1	B	408	VAL	2.1
1	E	343	ALA	2.1
1	G	439	ASN	2.1
1	E	458	LYS	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

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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	B	501	6/6	0.89	0.21	2.65	42,52,69,83	0
2	GOL	C	501	6/6	0.92	0.21	1.22	36,57,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.