wwPDB X-ray Structure Validation Summary Report (i)

Jan 24, 2017 – 06:02 PM EST

PDB ID	:	1NKZ
Title	:	Crystal structure of LH2 B800-850 from Rps. acidophila at 2.0 Angstrom resolution
Authors	:	Papiz, M.Z.; Prince, S.M.; Howard, T.; Cogdell, R.J.; Isaacs, N.W.
Deposited on	:	2003-01-06
Resolution	:	2.00 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
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:

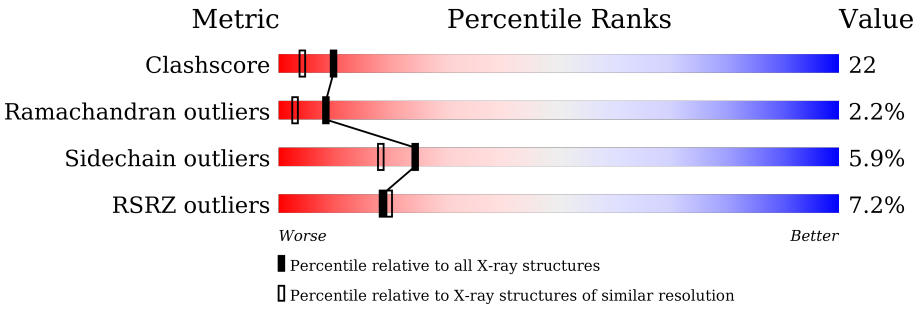
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	53	9% 74% 19% 6% •
1	C	53	9% 77% 17% 6%
1	E	53	11% 75% 17% 6% •
2	B	41	2% 83% 12% • •
2	D	41	2% 85% 10% • •
2	F	41	5% 88% 7% • •

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	RG1	A	404	-	-	-	X
3	RG1	B	401	-	-	-	X
3	RG1	C	403	-	-	-	X
3	RG1	C	405	-	-	-	X
3	RG1	E	406	-	-	-	X
4	BOG	A	507	X	X	-	X
4	BOG	C	504	X	X	-	X
4	BOG	C	508	X	X	-	X
4	BOG	E	505	X	-	-	X
4	BOG	E	506	X	X	-	X
4	BOG	E	509	X	X	-	X
6	BEN	C	510	-	-	-	X
6	BEN	E	511	-	-	-	X
6	BEN	E	512	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3461 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 Light-harvesting protein B-800/850, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	C	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	E	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			

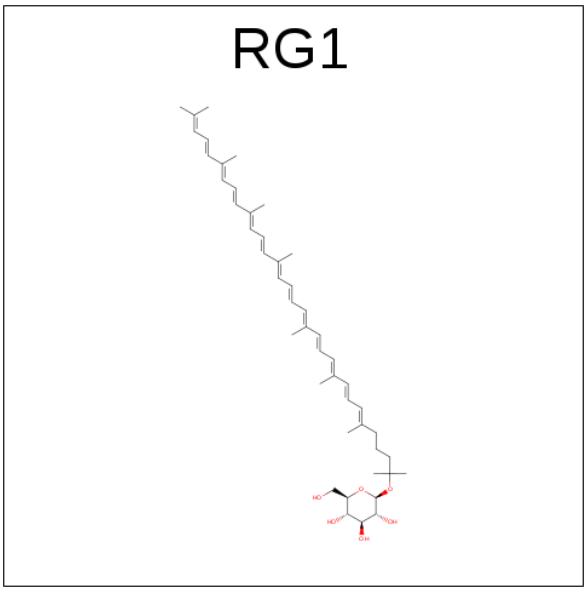
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
C	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
E	1	CXM	MET	MODIFIED RESIDUE	UNP P26789

- Molecule 2 is a protein called Light-harvesting protein B-800/850, beta chain.

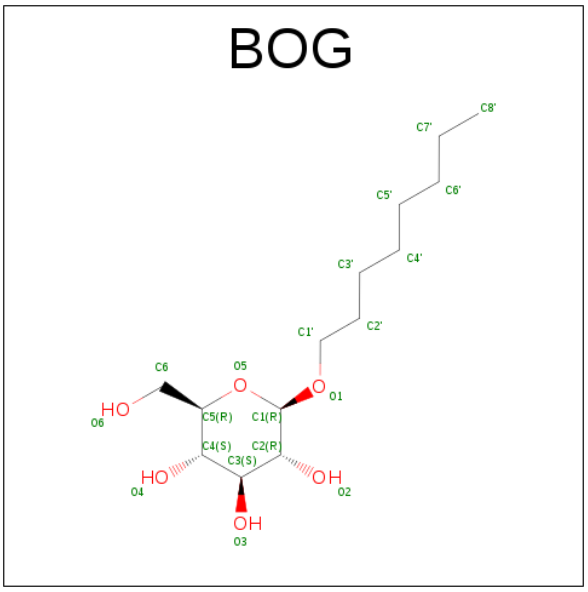
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	D	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	F	41	Total	C	N	O	0	0	0
			323	213	53	57			

- Molecule 3 is SUGAR (RHODOPIN B-D-GLUCOSIDE) (three-letter code: RG1) (formula: $C_{46}H_{66}O_6$).



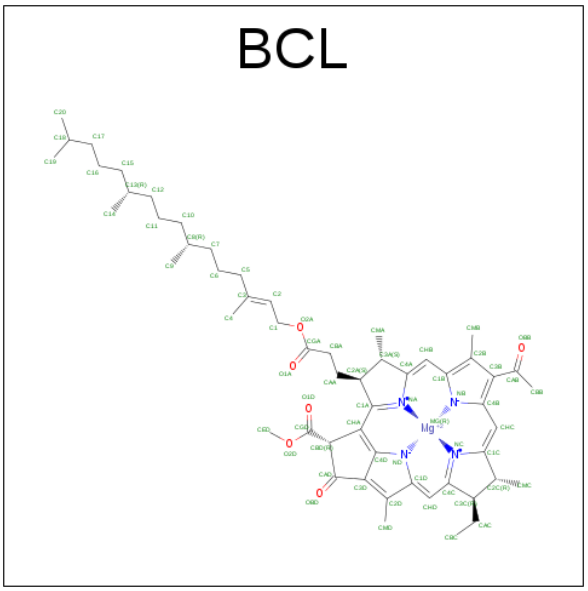
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 52 46 6	0	0
3	D	1	Total C O 52 46 6	0	0
3	C	1	Total C O 52 46 6	0	0
3	A	1	Total C O 52 46 6	10	0
3	C	1	Total C O 52 46 6	10	0
3	E	1	Total C O 52 46 6	10	0

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



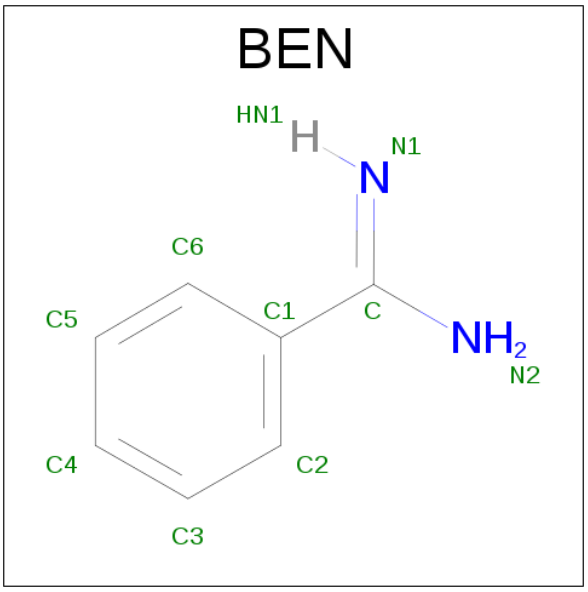
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 20 14 6	0	0
4	E	1	Total C O 20 14 6	0	0
4	E	1	Total C O 20 14 6	0	0
4	A	1	Total C O 20 14 6	0	0
4	C	1	Total C O 20 14 6	0	0
4	E	1	Total C O 20 14 6	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BENZAMIDINE (three-letter code: BEN) (formula: $C_7H_8N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N 9 7 2	0	0
6	E	1	Total C N 9 7 2	0	0
6	E	1	Total C N 9 7 2	0	0

- Molecule 7 is water.

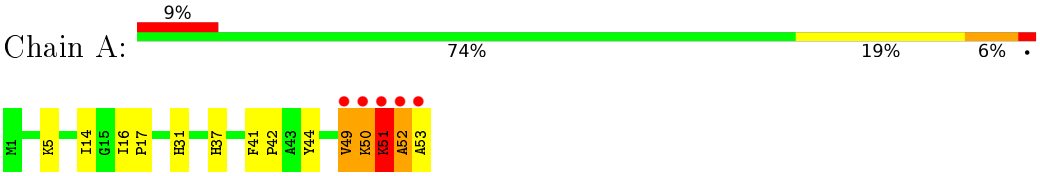
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	41	Total O 41 41	0	0
7	B	35	Total O 35 35	0	0
7	C	43	Total O 43 43	0	0
7	D	38	Total O 38 38	0	0
7	E	49	Total O 49 49	0	0
7	F	24	Total O 24 24	0	0

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.

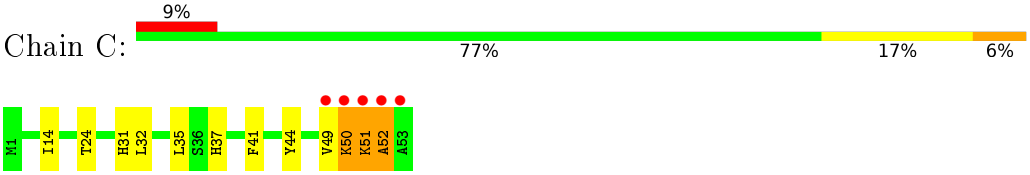
- Molecule 1: Light-harvesting protein B-800/850, alpha chain

Chain A:



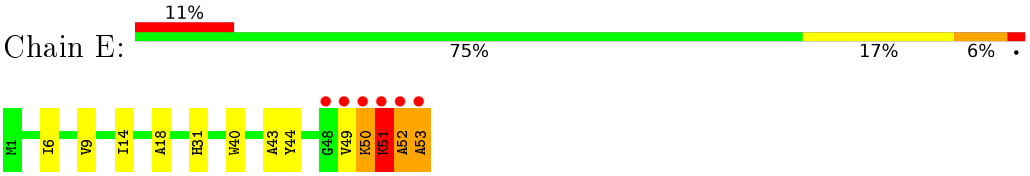
- Molecule 1: Light-harvesting protein B-800/850, alpha chain

Chain C:



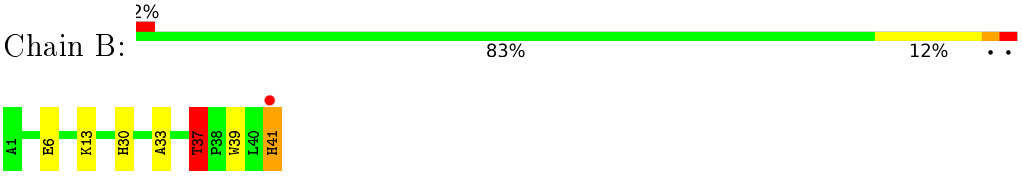
- Molecule 1: Light-harvesting protein B-800/850, alpha chain

Chain E:



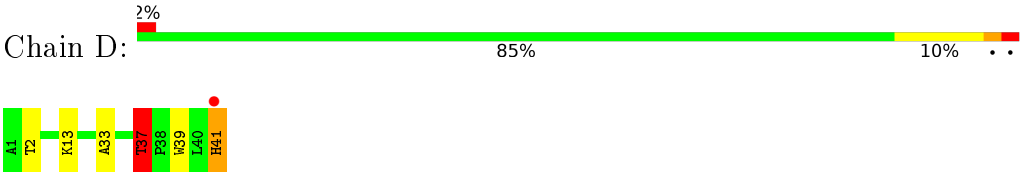
- Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain B:



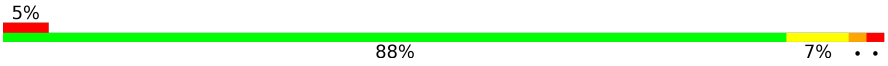
- Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain D:



- Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	117.05Å 117.05Å 298.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.00 31.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (8.00-2.00) 97.8 (31.99-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.17 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.169 , 0.190 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 68.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.001 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3461	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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: BCL, RG1, BEN, CXM, BOG

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	0.99	1/404 (0.2%)	0.68	0/556
1	C	0.51	0/404	0.68	0/556
1	E	1.18	1/404 (0.2%)	0.70	0/556
2	B	0.50	0/332	0.69	1/453 (0.2%)
2	D	0.58	0/332	0.71	1/453 (0.2%)
2	F	0.52	0/332	0.70	1/453 (0.2%)
All	All	0.78	2/2208 (0.1%)	0.69	3/3027 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	53	ALA	C-O	21.36	1.64	1.23
1	A	53	ALA	C-O	15.82	1.53	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	37	THR	N-CA-CB	-5.90	99.09	110.30
2	F	37	THR	N-CA-CB	-5.61	99.63	110.30
2	D	37	THR	N-CA-CB	-5.09	100.63	110.30

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	403	0	422	18	0
1	C	403	0	422	26	0
1	E	403	0	422	21	0
2	B	323	0	321	13	1
2	D	323	0	321	10	0
2	F	323	0	321	7	0
3	A	52	0	65	16	0
3	B	52	0	66	3	0
3	C	104	0	131	14	0
3	D	52	0	66	0	0
3	E	52	0	65	16	0
4	A	20	0	20	6	0
4	C	40	0	40	6	0
4	E	60	0	60	6	0
5	A	132	0	148	12	0
5	B	66	0	74	3	0
5	C	132	0	148	13	0
5	D	66	0	74	4	0
5	E	132	0	148	9	0
5	F	66	0	74	4	0
6	C	9	0	7	1	0
6	E	18	0	14	3	0
7	A	41	0	0	2	1
7	B	35	0	0	3	0
7	C	43	0	0	3	0
7	D	38	0	0	3	1
7	E	49	0	0	4	2
7	F	24	0	0	1	0
All	All	3461	0	3429	146	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 22.

The worst 5 of 146 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:53:ALA:O	1:E:53:ALA:C	1.63	1.35
1:E:9:VAL:HB	7:E:554:HOH:O	1.36	1.24
3:E:406:RG1:CM5	5:E:305:BCL:HMA3	1.84	1.08
3:A:404:RG1:CM5	5:A:301:BCL:HMA3	1.84	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:405:RG1:CM5	5:C:303:BCL:HMA3	1.91	1.01

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)
7:E:537:HOH:O	7:E:553:HOH:O[4_555]	1.95	0.25
7:A:542:HOH:O	7:A:542:HOH:O[12_555]	2.07	0.13
2:B:6:GLU:OE1	2:B:13:LYS:NZ[12_555]	2.12	0.08
7:D:426:HOH:O	7:D:436:HOH:O[12_555]	2.16	0.04
7:E:520:HOH:O	7:E:553:HOH:O[4_555]	2.16	0.04

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	51/53 (96%)	48 (94%)	1 (2%)	2 (4%)	4 1
1	C	51/53 (96%)	48 (94%)	1 (2%)	2 (4%)	4 1
1	E	51/53 (96%)	47 (92%)	2 (4%)	2 (4%)	4 1
2	B	39/41 (95%)	38 (97%)	1 (3%)	0	100 100
2	D	39/41 (95%)	38 (97%)	1 (3%)	0	100 100
2	F	39/41 (95%)	38 (97%)	1 (3%)	0	100 100
All	All	270/282 (96%)	257 (95%)	7 (3%)	6 (2%)	8 3

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ALA
1	C	52	ALA
1	E	52	ALA

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Mol	Chain	Res	Type
1	A	51	LYS
1	C	51	LYS

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	40/40 (100%)	37 (92%)	3 (8%)	17 11
1	C	40/40 (100%)	39 (98%)	1 (2%)	55 55
1	E	40/40 (100%)	38 (95%)	2 (5%)	30 24
2	B	33/33 (100%)	31 (94%)	2 (6%)	23 17
2	D	33/33 (100%)	30 (91%)	3 (9%)	12 6
2	F	33/33 (100%)	31 (94%)	2 (6%)	23 17
All	All	219/219 (100%)	206 (94%)	13 (6%)	24 18

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	50	LYS
2	D	2	THR
1	E	51	LYS
2	B	41	HIS
1	E	50	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	7	GLN
2	D	7	GLN
2	F	7	GLN
2	F	41	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)

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CXM	A	1	1,5	6,10,11	0.68	0	5,11,13	1.06	1 (20%)
1	CXM	C	1	1,5	6,10,11	0.46	0	5,11,13	0.87	0
1	CXM	E	1	1,5	6,10,11	0.46	0	5,11,13	0.96	1 (20%)

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
1	CXM	A	1	1,5	-	0/6/10/12	0/0/0/0
1	CXM	C	1	1,5	-	0/6/10/12	0/0/0/0
1	CXM	E	1	1,5	-	0/6/10/12	0/0/0/0

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	A	1	CXM	O-C-CA	-2.17	119.75	125.69
1	E	1	CXM	O-C-CA	-2.06	120.06	125.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\|>2$
5	BCL	A	301	1	55,74,74	2.47	13 (23%)	55,115,115	1.88	15 (27%)
5	BCL	A	307	1	55,74,74	2.46	13 (23%)	55,115,115	1.79	14 (25%)
3	RG1	A	404	-	52,52,52	1.83	6 (11%)	63,67,67	2.84	16 (25%)
4	BOG	A	507	-	20,20,20	5.41	14 (70%)	25,25,25	5.64	17 (68%)
5	BCL	B	302	2	55,74,74	2.43	12 (21%)	55,115,115	1.79	13 (23%)
3	RG1	B	401	-	52,52,52	1.55	5 (9%)	63,67,67	1.60	10 (15%)
5	BCL	C	303	1	55,74,74	2.50	13 (23%)	55,115,115	1.74	13 (23%)
5	BCL	C	308	1	55,74,74	2.43	13 (23%)	55,115,115	1.83	15 (27%)
3	RG1	C	403	-	52,52,52	1.34	3 (5%)	63,67,67	1.27	5 (7%)
3	RG1	C	405	-	52,52,52	1.84	6 (11%)	63,67,67	2.86	14 (22%)
4	BOG	C	504	-	20,20,20	5.39	14 (70%)	25,25,25	4.41	17 (68%)
4	BOG	C	508	-	20,20,20	5.38	14 (70%)	25,25,25	4.13	17 (68%)
6	BEN	C	510	-	9,9,9	1.48	1 (11%)	9,11,11	0.85	1 (11%)
5	BCL	D	304	2	55,74,74	2.49	12 (21%)	55,115,115	1.74	14 (25%)
3	RG1	D	402	-	52,52,52	1.38	4 (7%)	63,67,67	1.24	5 (7%)
5	BCL	E	305	1	55,74,74	2.48	12 (21%)	55,115,115	1.81	14 (25%)
5	BCL	E	309	1	55,74,74	2.50	12 (21%)	55,115,115	1.83	15 (27%)
3	RG1	E	406	-	52,52,52	1.80	6 (11%)	63,67,67	2.75	14 (22%)
4	BOG	E	505	-	20,20,20	5.39	14 (70%)	25,25,25	4.16	16 (64%)
4	BOG	E	506	-	20,20,20	5.40	14 (70%)	25,25,25	4.35	17 (68%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BOG	E	509	-	20,20,20	5.38	15 (75%)	25,25,25	4.61	17 (68%)
6	BEN	E	511	-	9,9,9	1.49	1 (11%)	9,11,11	0.79	0
6	BEN	E	512	-	9,9,9	1.55	1 (11%)	9,11,11	0.86	0
5	BCL	F	306	2	55,74,74	2.42	13 (23%)	55,115,115	1.79	14 (25%)

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
5	BCL	A	301	1	-	0/37/137/137	0/0/9/9
5	BCL	A	307	1	-	0/37/137/137	0/0/9/9
3	RG1	A	404	-	-	0/51/71/71	0/1/1/1
4	BOG	A	507	-	4/4/5/5	0/11/31/31	0/1/1/1
5	BCL	B	302	2	-	0/37/137/137	0/0/9/9
3	RG1	B	401	-	-	0/51/71/71	0/1/1/1
5	BCL	C	303	1	-	0/37/137/137	0/0/9/9
5	BCL	C	308	1	-	0/37/137/137	0/0/9/9
3	RG1	C	403	-	-	0/51/71/71	0/1/1/1
3	RG1	C	405	-	-	0/51/71/71	0/1/1/1
4	BOG	C	504	-	4/4/5/5	0/11/31/31	0/1/1/1
4	BOG	C	508	-	4/4/5/5	0/11/31/31	0/1/1/1
6	BEN	C	510	-	-	0/4/4/4	0/1/1/1
5	BCL	D	304	2	-	0/37/137/137	0/0/9/9
3	RG1	D	402	-	-	0/51/71/71	0/1/1/1
5	BCL	E	305	1	-	0/37/137/137	0/0/9/9
5	BCL	E	309	1	-	0/37/137/137	0/0/9/9
3	RG1	E	406	-	-	0/51/71/71	0/1/1/1
4	BOG	E	505	-	4/4/5/5	0/11/31/31	0/1/1/1
4	BOG	E	506	-	4/4/5/5	0/11/31/31	0/1/1/1
4	BOG	E	509	-	4/4/5/5	0/11/31/31	0/1/1/1
6	BEN	E	511	-	-	0/4/4/4	0/1/1/1
6	BEN	E	512	-	-	0/4/4/4	0/1/1/1
5	BCL	F	306	2	-	0/37/137/137	0/0/9/9

The worst 5 of 231 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	506	BOG	O1-C1	-9.37	1.23	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	507	BOG	O1-C1	-9.32	1.23	1.40
4	A	507	BOG	C4-C5	-9.30	1.32	1.53
4	C	504	BOG	O1-C1	-9.29	1.23	1.40
4	C	508	BOG	O1-C1	-9.29	1.23	1.40

The worst 5 of 293 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	405	RG1	C7-C6-C5	-11.32	113.80	127.69
3	A	404	RG1	C7-C6-C5	-11.15	114.01	127.69
3	E	406	RG1	C7-C6-C5	-10.92	114.29	127.69
4	E	506	BOG	O1-C1'-C2'	-9.96	80.98	109.63
4	C	504	BOG	O1-C1'-C2'	-9.08	83.49	109.63

5 of 24 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	504	BOG	C4
4	C	504	BOG	C3
4	C	504	BOG	C5
4	C	504	BOG	C2
4	E	506	BOG	C4

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	BCL	9	0
5	A	307	BCL	3	0
3	A	404	RG1	16	0
4	A	507	BOG	6	0
5	B	302	BCL	3	0
3	B	401	RG1	3	0
5	C	303	BCL	8	0
5	C	308	BCL	5	0
3	C	405	RG1	14	0
4	C	504	BOG	4	0
4	C	508	BOG	2	0
6	C	510	BEN	1	0
5	D	304	BCL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	305	BCL	6	0
5	E	309	BCL	3	0
3	E	406	RG1	16	0
4	E	505	BOG	2	0
4	E	506	BOG	3	0
4	E	509	BOG	1	0
6	E	511	BEN	1	0
6	E	512	BEN	2	0
5	F	306	BCL	4	0

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	52/53 (98%)	0.43	5 (9%)	10	11	14, 18, 50, 51	0
1	C	52/53 (98%)	0.35	5 (9%)	10	11	14, 18, 50, 51	0
1	E	52/53 (98%)	0.69	6 (11%)	6	7	14, 18, 50, 51	0
2	B	41/41 (100%)	-0.25	1 (2%)	62	63	16, 18, 22, 35	0
2	D	41/41 (100%)	-0.27	1 (2%)	62	63	16, 18, 23, 35	0
2	F	41/41 (100%)	-0.25	2 (4%)	33	35	16, 18, 23, 35	0
All	All	279/282 (98%)	0.16	20 (7%)	18	20	14, 18, 44, 51	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	52	ALA	13.8
1	E	51	LYS	13.6
1	A	51	LYS	10.7
1	E	49	VAL	9.9
1	A	49	VAL	9.5

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

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
1	CXM	E	1	11/12	0.97	0.13	-	13,16,20,20	0
1	CXM	C	1	11/12	0.94	0.11	-	14,17,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CXM	A	1	11/12	0.97	0.07	-	15,17,20,20	0

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, 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
4	BOG	A	507	20/20	0.31	0.57	23.12	88,104,108,108	0
6	BEN	E	512	9/9	0.65	0.37	22.08	76,79,80,80	0
6	BEN	C	510	9/9	0.68	0.36	19.34	73,76,78,79	0
4	BOG	E	509	20/20	0.28	0.39	14.95	81,100,105,106	0
4	BOG	E	505	20/20	0.44	0.46	14.78	99,111,116,116	0
4	BOG	E	506	20/20	0.50	0.45	13.63	89,102,105,105	0
4	BOG	C	508	20/20	0.35	0.37	12.30	79,96,102,104	0
4	BOG	C	504	20/20	0.49	0.46	10.90	86,101,103,104	0
6	BEN	E	511	9/9	0.62	0.28	10.62	77,80,83,83	0
3	RG1	B	401	52/52	0.81	0.20	2.48	13,16,29,31	0
3	RG1	C	403	52/52	0.80	0.19	2.00	13,16,29,31	0
3	RG1	C	405	52/52	0.43	0.63	1.58	39,57,63,63	52
3	RG1	D	402	52/52	0.87	0.17	1.45	13,16,28,31	0
3	RG1	A	404	52/52	0.54	0.56	1.44	40,57,63,63	52
3	RG1	E	406	52/52	0.53	0.56	0.80	40,57,63,64	52
5	BCL	A	301	66/66	0.96	0.12	0.46	13,16,22,24	0
5	BCL	E	309	66/66	0.90	0.13	0.43	11,16,37,43	0
5	BCL	C	303	66/66	0.96	0.12	0.42	13,16,22,23	0
5	BCL	A	307	66/66	0.91	0.12	0.21	11,17,38,43	0
5	BCL	C	308	66/66	0.91	0.12	0.12	11,16,38,43	0
5	BCL	E	305	66/66	0.96	0.10	0.03	13,17,21,24	0
5	BCL	F	306	66/66	0.95	0.10	0.01	13,16,29,36	0
5	BCL	D	304	66/66	0.95	0.12	-0.01	13,16,29,36	0
5	BCL	B	302	66/66	0.95	0.10	-0.02	12,16,29,36	0

6.5 Other polymers (i)

There are no such residues in this entry.