wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:37 AM GMT

PDB ID	:	2RG0
Title	:	Crystal structure of cellobiohydrolase from Melanocarpus albomyces complexed with cellotetraose
Authors	:	Parkkinen, T.; Koivula, A.; Vehmaanper, J.; Rouvinen, J.
Deposited on	:	2007-10-02
Resolution	:	2.10 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:

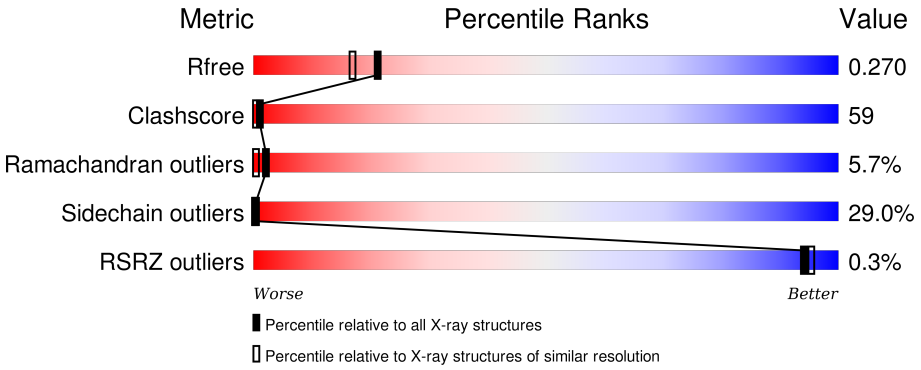
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	430	22% 55% 21%
1	B	430	21% 55% 22%
1	C	430	20% 59% 20%
1	D	430	23% 56% 19%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PCA	A	1	-	-	X	-
1	PCA	B	1	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13956 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.

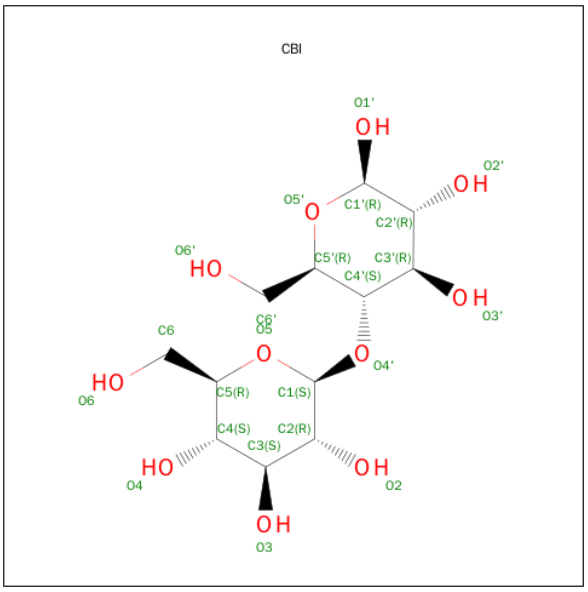
- Molecule 1 is a protein called Cellulose 1,4-beta-cellobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	B	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	C	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	D	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			

There are 4 discrepancies between the modelled and reference sequences:

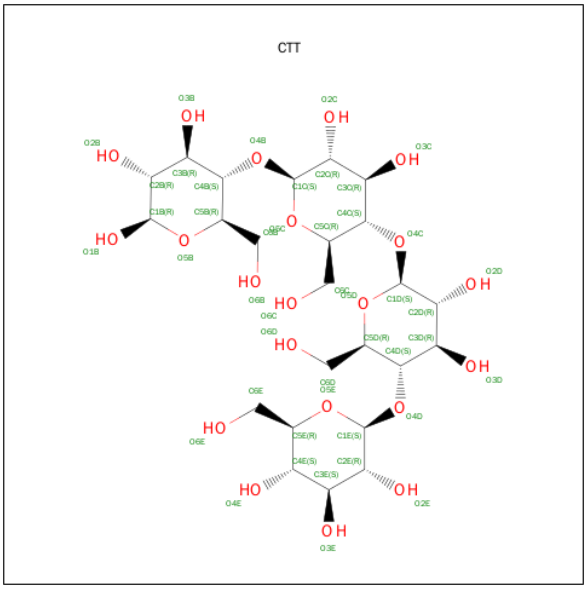
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
B	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
C	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
D	1	PCA	GLN	ENGINEERED	UNP Q8J0K6

- Molecule 2 is SUGAR (CELLOBIOSE) (three-letter code: CBI) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 23 12 11	0	0
2	A	1	Total C O 23 12 11	0	0
2	C	1	Total C O 23 12 11	0	0
2	D	1	Total C O 23 12 11	0	0
2	D	1	Total C O 23 12 11	0	0

- Molecule 3 is CELLOTETRAOSE (three-letter code: CTT) (formula: $C_{24}H_{42}O_{21}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 45 24 21	0	0

- Molecule 4 is water.

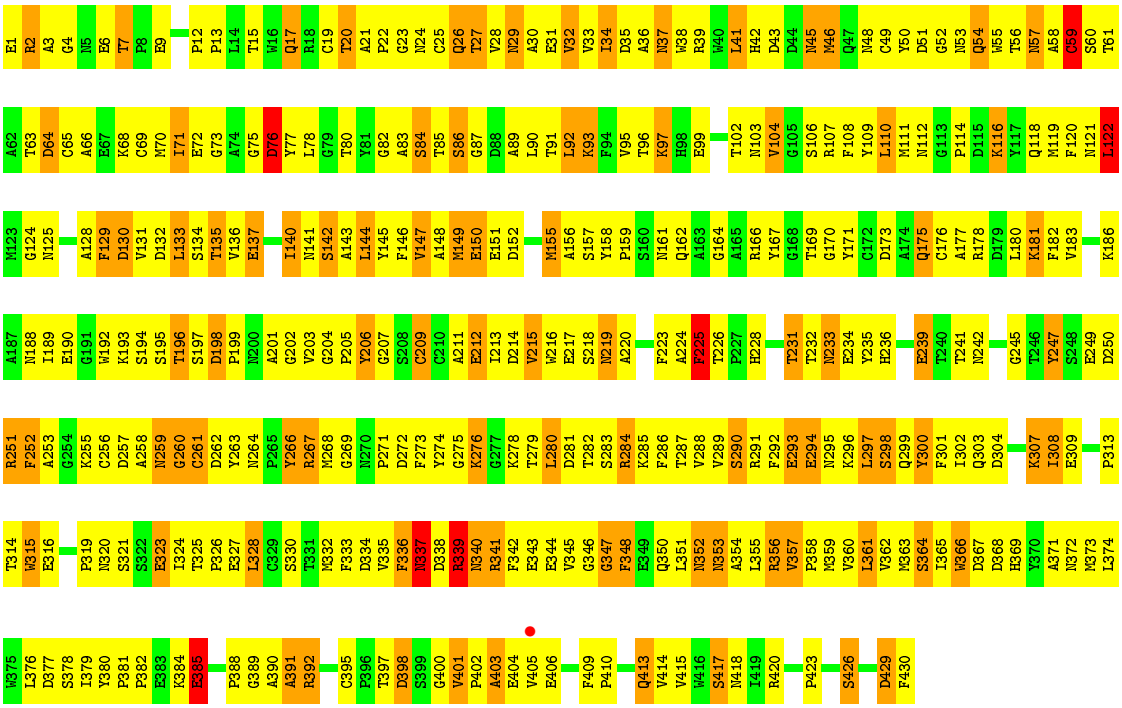
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	101	Total O 101 101	0	0
4	B	109	Total O 109 109	0	0
4	C	122	Total O 122 122	0	0
4	D	132	Total O 132 132	0	0

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.

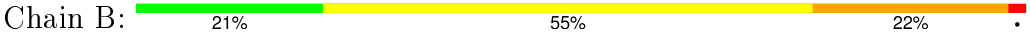
- Molecule 1: Cellulose 1,4-beta-cellobiosidase

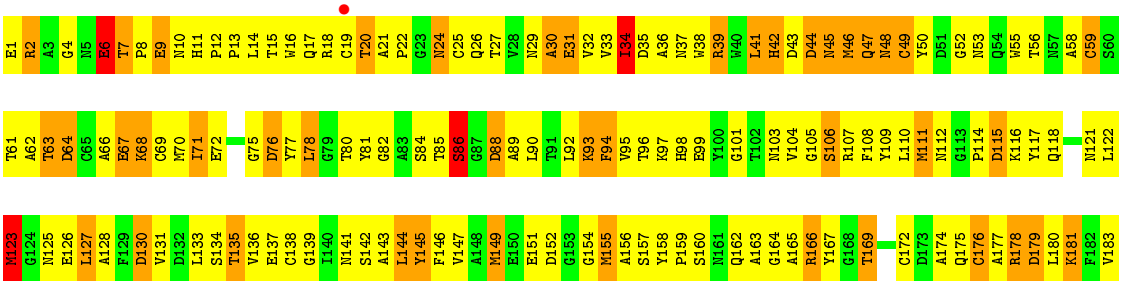
Chain A:

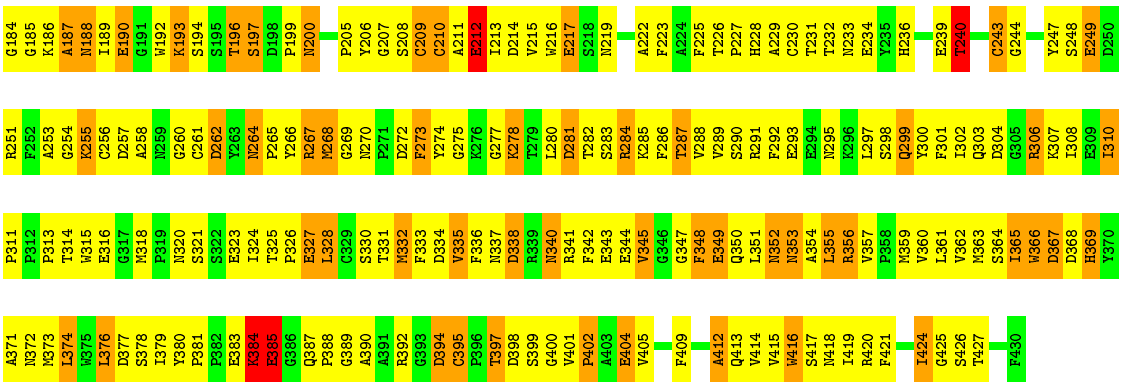


- Molecule 1: Cellulose 1,4-beta-cellobiosidase

Chain B:

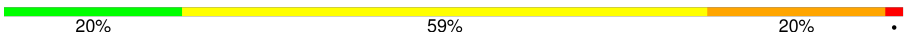


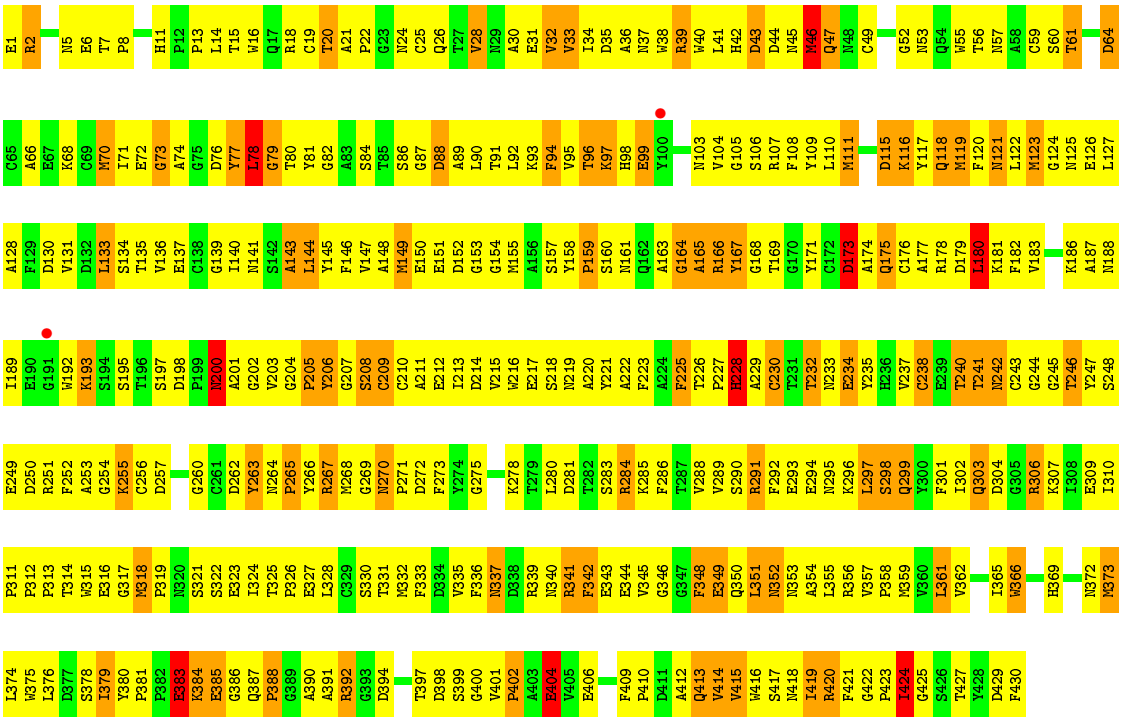




• Molecule 1: Cellulose 1,4-beta-cellobiosidase

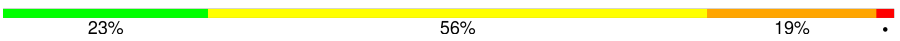
Chain C:

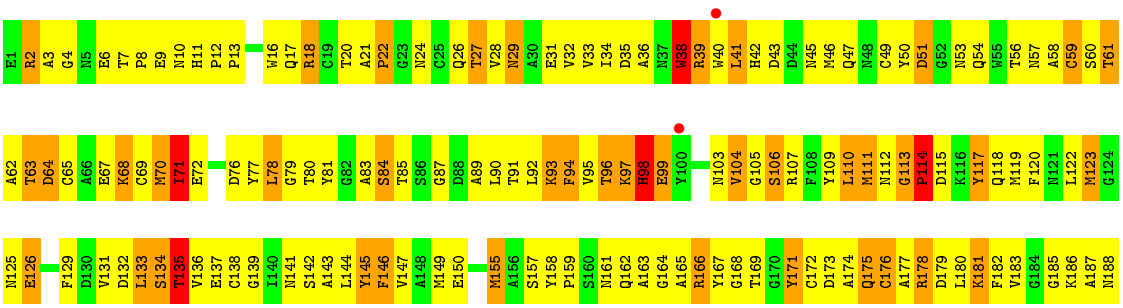


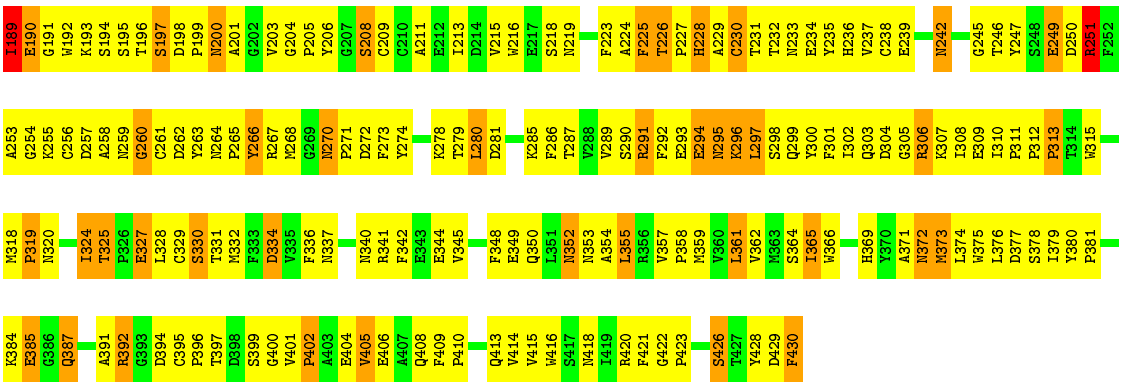


• Molecule 1: Cellulose 1,4-beta-cellobiosidase

Chain D:






I189 E190 G191 W192 K193 S194 S195 T196 S197 D198 P199 N200 A201 G202 V203 G204 P205 Y206 G207 S208 C209 C210 A211 E212 I213 D214 V215 W216 E217 S218 N219 F223 A224 F225 T226 P227 H228 A229 C230 T231 T232 N233 E234 Y235 H236 V237 C238 E239 N242 G245 T246 Y247 S248 E249 D250 R251 F252
A253 G254 K255 C256 D257 A258 N259 G260 C261 D262 Y263 N264 P265 Y266 R267 M268 G269 N270 P271 D272 F273 Y274 K278 T279 L280 D281 K285 F286 T287 V288 V289 S290 R291 F292 E293 E294 N295 K296 L297 S298 Q299 Y300 F301 I302 Q303 D304 G305 R306 K307 I308 E309 I310 P311 P312 P313 T314 W315
M318 P319 N320 I324 T325 P326 E327 L328 C329 S330 T331 M332 F333 D334 V335 F336 N337 N340 R341 F342 E343 E344 V345 F348 E349 Q350 L351 N352 N353 A354 L355 R356 V357 P358 M359 V360 L361 V362 M363 S364 I365 W366 H369 Y370 A371 N372 M373 L374 W375 L376 D377 S378 I379 Y380 P381
K384 E385 G386 Q387 A391 R392 G393 D394 C395 P396 T397 D398 S399 G400 V401 P402 A403 E404 V405 E406 A407 Q408 F409 P410 Q413 V414 V415 W416 S417 N418 I419 R420 F421 G422 P423 S426 Y427 Y428 D429 F430

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.98Å 94.81Å 190.43Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 24.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-2.10) 98.1 (24.62-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.211 , 0.282 0.211 , 0.270	Depositor DCC
R_{free} test set	5188 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	9.8	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 68.3	EDS
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 105275 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	13956	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTT, PCA, CBI

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	0.32	0/3416	0.95	3/4648 (0.1%)
1	B	0.33	0/3416	0.98	5/4648 (0.1%)
1	C	0.32	0/3416	0.93	2/4648 (0.0%)
1	D	0.33	0/3416	0.99	6/4648 (0.1%)
All	All	0.33	0/13664	0.96	16/18592 (0.1%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	251	ARG	CD-NE-CZ	8.88	136.04	123.60
1	B	366	TRP	C-N-CA	8.45	142.81	121.70
1	D	18	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	C	228	HIS	CA-CB-CG	6.30	124.31	113.60
1	B	42	HIS	C-N-CA	6.11	136.98	121.70

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	3333	0	3028	376	0
1	B	3333	0	3027	401	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3333	0	3028	399	0
1	D	3333	0	3028	360	0
2	A	46	0	44	11	0
2	C	23	0	22	3	0
2	D	46	0	44	11	0
3	B	45	0	42	9	0
4	A	101	0	0	12	0
4	B	109	0	0	11	0
4	C	122	0	0	12	0
4	D	132	0	0	12	0
All	All	13956	0	12263	1514	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

The worst 5 of 1514 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:HE3	1:D:6:GLU:HB3	1.39	1.04
1:B:37:ASN:HA	1:B:181:LYS:HE2	1.38	1.02
1:D:21:ALA:HB3	1:D:24:ASN:HD22	1.18	1.01
1:C:250:ASP:HB3	1:C:253:ALA:HB2	1.42	1.01
1:B:2:ARG:HA	1:B:162:GLN:HB2	1.40	0.99

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	428/430 (100%)	354 (83%)	57 (13%)	17 (4%)	4 1
1	B	428/430 (100%)	336 (78%)	64 (15%)	28 (6%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	428/430 (100%)	332 (78%)	69 (16%)	27 (6%)	2 0
1	D	428/430 (100%)	331 (77%)	71 (17%)	26 (6%)	2 0
All	All	1712/1720 (100%)	1353 (79%)	261 (15%)	98 (6%)	2 0

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	CYS
1	A	122	LEU
1	A	278	LYS
1	A	347	GLY
1	B	6	GLU

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	354/354 (100%)	240 (68%)	114 (32%)	0 0
1	B	354/354 (100%)	251 (71%)	103 (29%)	0 0
1	C	354/354 (100%)	255 (72%)	99 (28%)	0 0
1	D	354/354 (100%)	259 (73%)	95 (27%)	0 0
All	All	1416/1416 (100%)	1005 (71%)	411 (29%)	0 0

5 of 411 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	316	GLU
1	C	59	CYS
1	D	290	SER
1	B	332	MET
1	B	384	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	320	ASN
1	C	29	ASN
1	D	340	ASN
1	B	340	ASN
1	B	387	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)

4 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	PCA	A	1	1	7,8,9	1.88	1 (14%)	9,10,12	1.56	2 (22%)
1	PCA	B	1	1	7,8,9	1.74	1 (14%)	9,10,12	1.43	3 (33%)
1	PCA	C	1	1	7,8,9	1.77	1 (14%)	9,10,12	1.35	2 (22%)
1	PCA	D	1	1	7,8,9	1.81	1 (14%)	9,10,12	1.30	1 (11%)

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	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	PCA	CD-N	4.28	1.47	1.33
1	B	1	PCA	CD-N	4.31	1.48	1.33
1	D	1	PCA	CD-N	4.34	1.48	1.33
1	A	1	PCA	CD-N	4.45	1.48	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	PCA	OE-CD-CG	-2.66	120.87	126.81
1	B	1	PCA	CB-CA-C	-2.48	109.37	112.76
1	C	1	PCA	CB-CA-C	-2.16	109.81	112.76
1	A	1	PCA	CB-CA-C	-2.09	109.91	112.76
1	B	1	PCA	O-C-CA	-2.07	119.98	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	4	0
1	B	1	PCA	4	0
1	C	1	PCA	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	CBI	A	431	-	24,24,24	0.49	0	35,35,35	1.19	3 (8%)
2	CBI	A	432	-	24,24,24	0.44	0	35,35,35	1.17	4 (11%)
3	CTT	B	431	-	48,48,48	0.47	0	71,71,71	1.21	8 (11%)
2	CBI	C	431	-	24,24,24	0.46	0	35,35,35	1.13	3 (8%)
2	CBI	D	431	-	24,24,24	0.48	0	35,35,35	1.03	2 (5%)
2	CBI	D	432	-	24,24,24	0.46	0	35,35,35	1.27	2 (5%)

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	CBI	A	431	-	-	0/8/48/48	0/2/2/2
2	CBI	A	432	-	-	0/8/48/48	0/2/2/2
3	CTT	B	431	-	-	0/20/100/100	0/4/4/4
2	CBI	C	431	-	-	0/8/48/48	0/2/2/2
2	CBI	D	431	-	-	0/8/48/48	0/2/2/2
2	CBI	D	432	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	432	CBI	C1-O4'-C4'	-4.33	106.70	118.01
2	A	431	CBI	C1-O4'-C4'	-3.95	107.68	118.01
3	B	431	CTT	C1D-O4C-C4C	-3.35	109.25	118.01
3	B	431	CTT	C1E-O4D-C4D	-3.27	109.47	118.01
2	C	431	CBI	C1-O4'-C4'	-3.16	109.76	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	431	CBI	3	0
2	A	432	CBI	8	0
3	B	431	CTT	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	431	CBI	3	0
2	D	431	CBI	5	0
2	D	432	CBI	6	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	429/430 (99%)	-0.55	1 (0%)	95	96	12, 32, 53, 70	0
1	B	429/430 (99%)	-0.55	1 (0%)	95	96	11, 33, 55, 80	0
1	C	429/430 (99%)	-0.59	2 (0%)	91	93	10, 31, 53, 83	0
1	D	429/430 (99%)	-0.62	2 (0%)	91	93	10, 31, 49, 68	0
All	All	1716/1720 (99%)	-0.57	6 (0%)	94	95	10, 32, 53, 83	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	VAL	5.2
1	C	100	TYR	4.7
1	B	19	CYS	2.4
1	D	100	TYR	2.3
1	C	191	GLY	2.2

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	PCA	A	1	8/9	0.96	0.08	-	15,28,31,49	0
1	PCA	D	1	8/9	0.97	0.06	-	19,25,30,40	0
1	PCA	B	1	8/9	0.96	0.09	-	28,41,48,52	0
1	PCA	C	1	8/9	0.93	0.11	-	21,32,43,57	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
3	CTT	B	431	45/45	0.94	0.10	0.25	15,35,48,60	0
2	CBI	D	431	23/23	0.96	0.09	0.20	6,25,36,59	0
2	CBI	C	431	23/23	0.97	0.07	-0.42	17,22,37,50	0
2	CBI	A	431	23/23	0.95	0.08	-0.46	18,38,49,57	0
2	CBI	D	432	23/23	0.96	0.08	-0.47	7,30,42,51	0
2	CBI	A	432	23/23	0.97	0.08	-0.48	12,24,44,50	0

6.5 Other polymers (i)

There are no such residues in this entry.