wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:37 AM GMT

PDB ID	:	2RFZ
Title	:	Crystal structure of cellobiohydrolase from Melanocarpus albomyces complexed with cellotriose
Authors	:	Parkkinen, T.; Koivula, A.; Vehmaanper, J.; Rouvinen, J.
Deposited on	:	2007-10-02
Resolution	:	1.80 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:

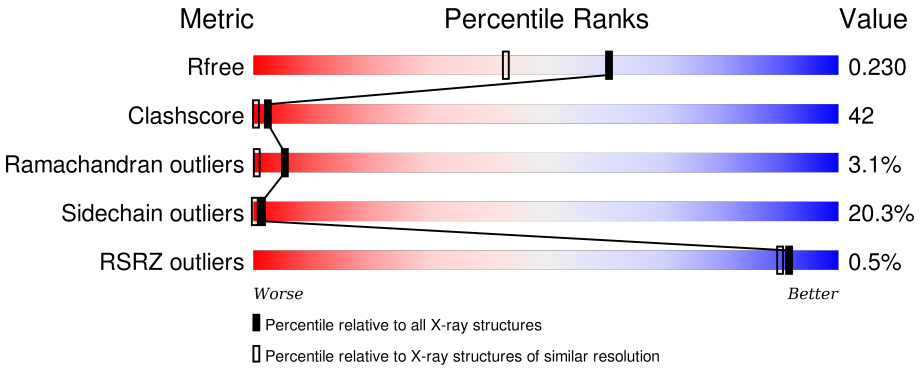
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	23% 56% 20%
1	B	430	33% 49% 17%
1	C	430	40% 47% 13%
1	D	430	43% 46% 10%

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	-
2	CTR	A	431	X	-	-	-
2	CTR	A	432	X	-	-	-
2	CTR	B	431	X	-	-	-
2	CTR	C	431	X	-	-	-
2	CTR	C	432	X	-	-	-
2	CTR	D	431	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14399 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.

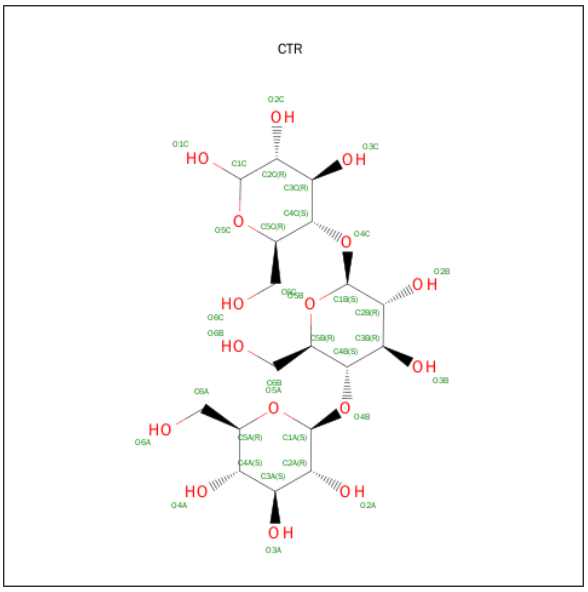
- Molecule 1 is a protein called Cellulose 1,4-beta-cellobiosidase.

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 (CELLOTRIOSE) (three-letter code: CTR) (formula: $C_{18}H_{32}O_{16}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 34 18 16	0	0
2	A	1	Total C O 34 18 16	0	0
2	B	1	Total C O 34 18 16	0	0
2	C	1	Total C O 34 18 16	0	0
2	C	1	Total C O 34 18 16	0	0
2	D	1	Total C O 34 18 16	0	0

- Molecule 3 is water.

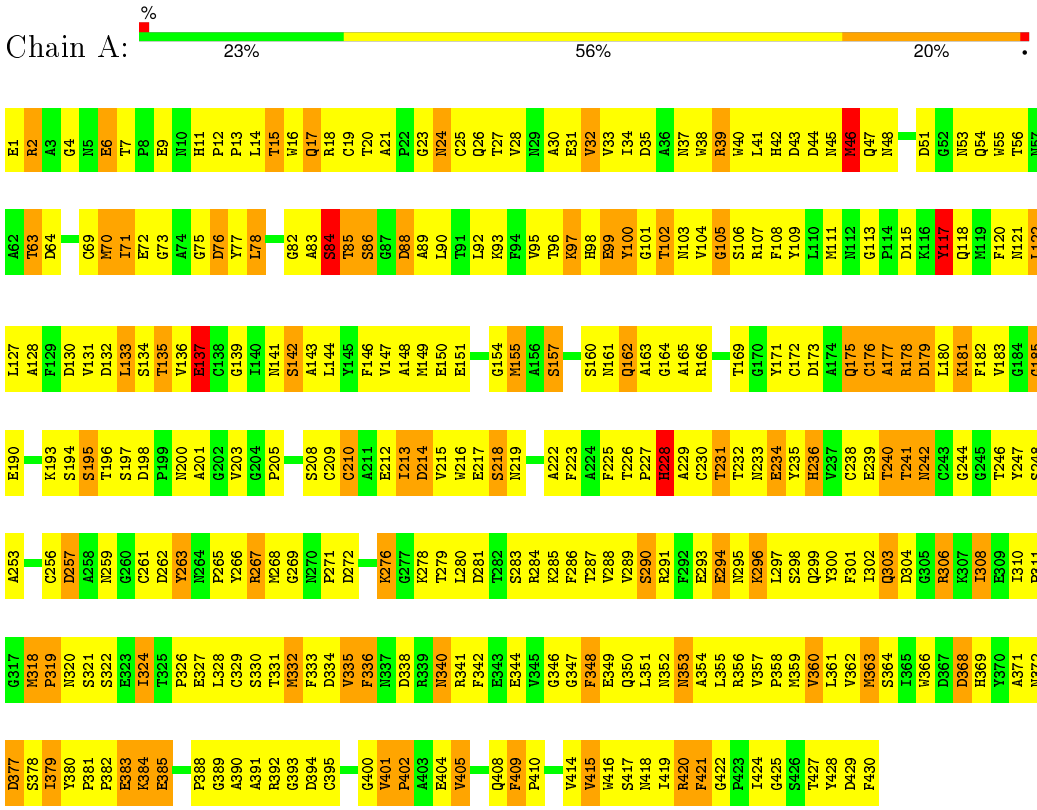
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	202	Total O 202 202	0	0
3	B	191	Total O 191 191	0	0
3	C	225	Total O 225 225	0	0
3	D	245	Total O 245 245	0	0

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.

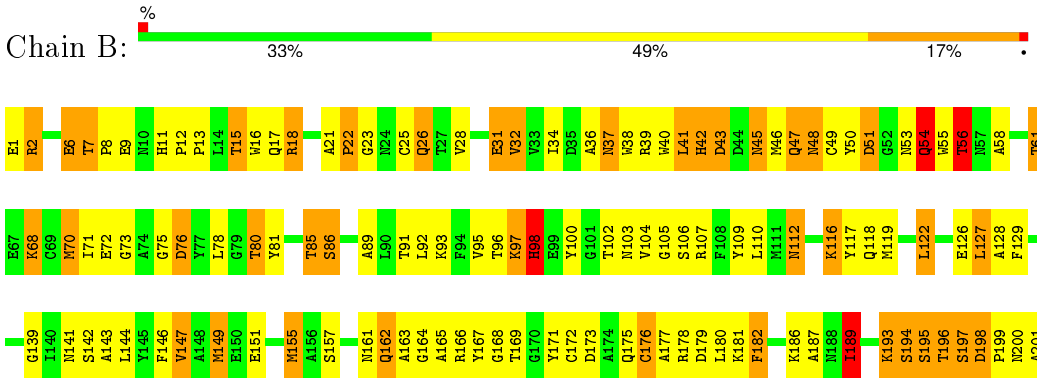
- Molecule 1: Cellulose 1,4-beta-cellobiosidase

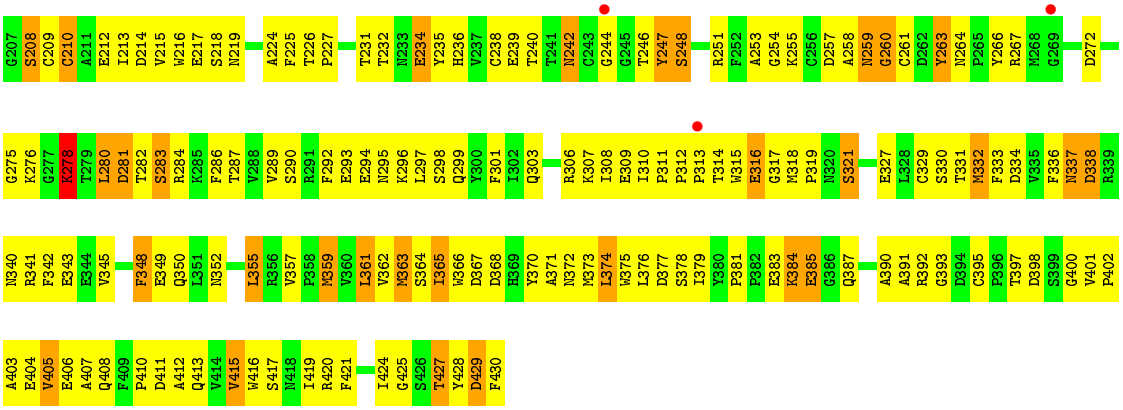
Chain A:



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

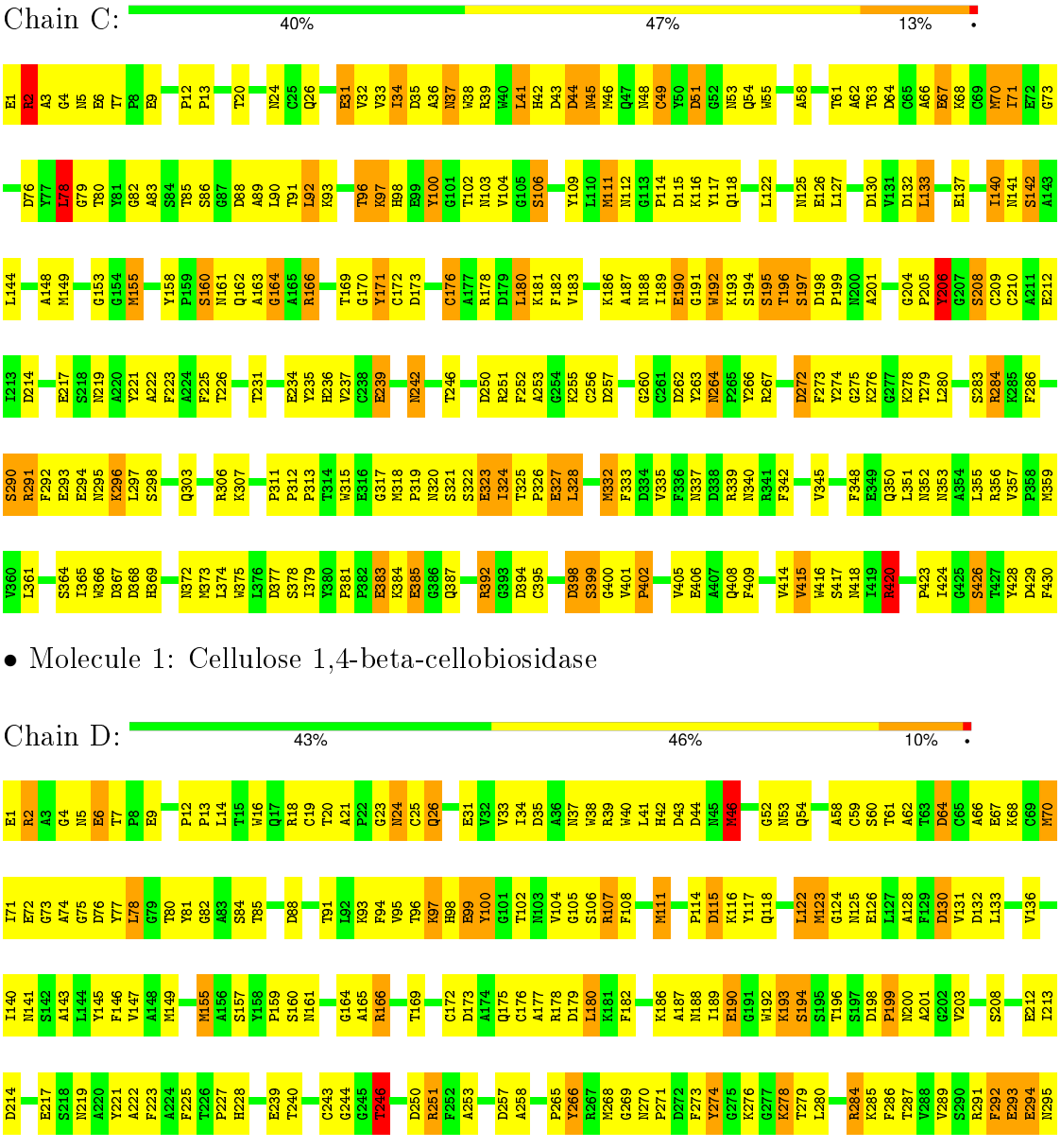
Chain B:





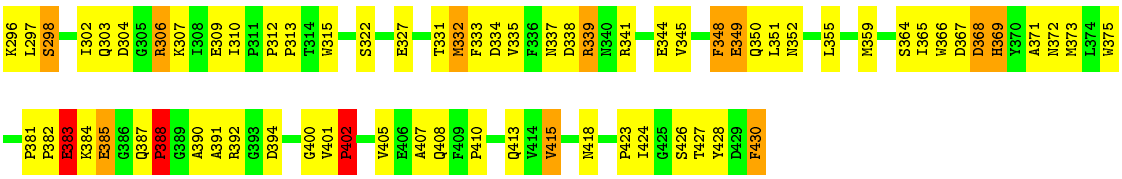
• Molecule 1: Cellulose 1,4-beta-cellobiosidase

Chain C:



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

Chain D:


K296
L297
S298
I302
Q303
D304
G305
R306
K307
I308
E309
I310
P311
P312
P313
T314
W315
S322
E327
T331
M332
F333
D334
V335
F336
N337
D338
R339
N340
R341
E344
V345
F348
E349
Q350
L351
N352
L355
M359
S364
I365
W366
D367
D368
H369
Y370
A371
N372
H373
L374
W375
P381
P382
E383
K384
E385
G386
Q387
P388
G389
A390
A391
R392
G393
D394
G400
V401
P402
V405
E406
A407
Q408
F409
P410
Q413
V414
V415
N418
P423
I424
G425
S426
T427
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	50.80Å 94.37Å 189.91Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 24.53 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.00-1.80) 96.6 (24.53-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.03 (at 1.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.261 , 0.237 0.190 , 0.230	Depositor DCC
R_{free} test set	8081 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	12.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 70.5	EDS
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Outliers	3 of 161992 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14399	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.69% 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: PCA, CTR

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	0.36	0/3416	1.09	11/4648 (0.2%)
1	B	0.36	0/3416	1.12	10/4648 (0.2%)
1	C	0.37	0/3416	1.16	10/4648 (0.2%)
1	D	0.38	0/3416	1.15	14/4648 (0.3%)
All	All	0.37	0/13664	1.13	45/18592 (0.2%)

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	58	ALA	C-N-CA	10.35	147.57	121.70
1	D	166	ARG	NE-CZ-NH1	-9.23	115.68	120.30
1	D	107	ARG	NE-CZ-NH1	-8.17	116.21	120.30
1	B	306	ARG	CD-NE-CZ	7.89	134.65	123.60
1	C	392	ARG	NE-CZ-NH2	-7.81	116.39	120.30

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	3333	0	3028	345	0
1	B	3333	0	3028	288	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3333	0	3028	239	0
1	D	3333	0	3027	239	0
2	A	68	0	64	15	0
2	B	34	0	32	5	0
2	C	68	0	64	9	0
2	D	34	0	32	5	0
3	A	202	0	0	18	0
3	B	191	0	0	15	0
3	C	225	0	0	19	0
3	D	245	0	0	19	0
All	All	14399	0	12303	1087	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 42.

The worst 5 of 1087 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:HD3	1:D:6:GLU:HG3	1.38	1.01
1:A:128:ALA:HB2	1:A:289:VAL:HG13	1.44	1.00
1:D:123:MET:HE2	1:D:294:GLU:H	1.25	0.98
1:C:298:SER:HB3	1:C:323:GLU:HG3	1.49	0.95
1:C:132:ASP:HB3	1:C:415:VAL:HG13	1.49	0.93

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%)	359 (84%)	54 (13%)	15 (4%)	4 0
1	B	428/430 (100%)	355 (83%)	56 (13%)	17 (4%)	4 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	428/430 (100%)	379 (89%)	37 (9%)	12 (3%)	6 1
1	D	428/430 (100%)	373 (87%)	46 (11%)	9 (2%)	9 1
All	All	1712/1720 (100%)	1466 (86%)	193 (11%)	53 (3%)	5 0

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	47	GLN
1	A	148	ALA
1	A	240	THR
1	A	384	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	354/354 (100%)	260 (73%)	94 (27%)	0 0
1	B	354/354 (100%)	274 (77%)	80 (23%)	1 0
1	C	354/354 (100%)	292 (82%)	62 (18%)	2 0
1	D	354/354 (100%)	303 (86%)	51 (14%)	4 0
All	All	1416/1416 (100%)	1129 (80%)	287 (20%)	1 0

5 of 287 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	157	SER
1	B	355	LEU
1	D	251	ARG
1	B	189	ILE
1	B	278	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	369	HIS
1	C	125	ASN
1	D	352	ASN
1	B	372	ASN
1	B	413	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	1.76	1 (14%)	9,10,12	1.45	2 (22%)
1	PCA	B	1	1	7,8,9	1.71	1 (14%)	9,10,12	1.50	3 (33%)
1	PCA	C	1	1	7,8,9	1.82	1 (14%)	9,10,12	1.88	2 (22%)
1	PCA	D	1	1	7,8,9	1.77	1 (14%)	9,10,12	1.70	3 (33%)

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	D	1	PCA	CD-N	4.16	1.47	1.33
1	B	1	PCA	CD-N	4.23	1.47	1.33
1	C	1	PCA	CD-N	4.34	1.48	1.33
1	A	1	PCA	CD-N	4.34	1.48	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	PCA	CB-CA-C	-3.32	108.22	112.76
1	D	1	PCA	OE-CD-CG	-3.29	119.46	126.81
1	C	1	PCA	OE-CD-CG	-3.27	119.51	126.81
1	B	1	PCA	OE-CD-CG	-2.87	120.40	126.81
1	A	1	PCA	O-C-CA	-2.78	118.09	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	5	0
1	B	1	PCA	2	0
1	C	1	PCA	2	0
1	D	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	CTR	A	431	-	36,36,36	0.56	0	53,53,53	1.40	8 (15%)
2	CTR	A	432	-	36,36,36	0.46	0	53,53,53	1.43	9 (16%)
2	CTR	B	431	-	36,36,36	0.51	0	53,53,53	1.10	5 (9%)
2	CTR	C	431	-	36,36,36	0.59	0	53,53,53	1.49	6 (11%)
2	CTR	C	432	-	36,36,36	0.50	0	53,53,53	1.32	6 (11%)
2	CTR	D	431	-	36,36,36	0.55	0	53,53,53	1.34	6 (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
2	CTR	A	431	-	1/1/15/15	0/14/74/74	0/3/3/3
2	CTR	A	432	-	1/1/15/15	0/14/74/74	0/3/3/3
2	CTR	B	431	-	1/1/15/15	0/14/74/74	0/3/3/3
2	CTR	C	431	-	1/1/15/15	0/14/74/74	0/3/3/3
2	CTR	C	432	-	1/1/15/15	0/14/74/74	0/3/3/3
2	CTR	D	431	-	1/1/15/15	0/14/74/74	0/3/3/3

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	432	CTR	C1A-O4B-C4B	-3.77	108.16	118.01
2	A	432	CTR	C1B-O5B-C5B	-3.59	106.78	113.75
2	B	431	CTR	C1B-O5B-C5B	-3.50	106.96	113.75
2	C	431	CTR	C1B-O4C-C4C	-3.49	108.89	118.01
2	C	432	CTR	C1A-O5A-C5A	-3.48	107.00	113.75

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	431	CTR	C1C
2	C	431	CTR	C1C
2	A	432	CTR	C1C
2	B	431	CTR	C1C
2	D	431	CTR	C1C

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	CTR	8	0
2	A	432	CTR	7	0
2	B	431	CTR	5	0
2	C	431	CTR	4	0
2	C	432	CTR	5	0
2	D	431	CTR	5	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%)	-0.13	4 (0%)	85	83	9, 29, 48, 80	0
1	B	429/430 (99%)	-0.17	4 (0%)	85	83	11, 28, 44, 61	0
1	C	429/430 (99%)	-0.50	0	100	100	6, 22, 37, 68	0
1	D	429/430 (99%)	-0.50	0	100	100	7, 20, 36, 58	0
All	All	1716/1720 (99%)	-0.33	8 (0%)	91	90	6, 25, 42, 80	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	GLY	2.7
1	B	66	ALA	2.6
1	B	269	GLY	2.6
1	A	61	THR	2.3
1	A	59	CYS	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	D	1	8/9	0.99	0.06	-	5,17,23,43	0
1	PCA	C	1	8/9	0.94	0.12	-	14,25,27,28	0
1	PCA	B	1	8/9	0.95	0.09	-	17,32,40,51	0
1	PCA	A	1	8/9	0.91	0.13	-	24,29,38,39	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
2	CTR	C	432	34/34	0.93	0.12	1.44	7,35,60,78	0
2	CTR	D	431	34/34	0.95	0.09	1.04	14,29,53,59	0
2	CTR	A	432	34/34	0.93	0.12	0.17	15,36,57,76	0
2	CTR	B	431	34/34	0.96	0.09	-0.12	9,29,47,66	0
2	CTR	A	431	34/34	0.95	0.09	-0.51	10,30,41,43	0
2	CTR	C	431	34/34	0.98	0.06	-0.96	7,18,31,65	0

6.5 Other polymers (i)

There are no such residues in this entry.