Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 08:45 AM EDT

PDB ID	:	6WNI
Title	:	Crystal structure of CldA, the first cyclomaltodextrin glucanotransferase with a three-domain ABC distribution
Authors	:	Magana-Cuevas, E.; Centeno-Leija, S.; Serrano-Posada, H.
Deposited on	:	2020-04-22
Resolution	:	1.66 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

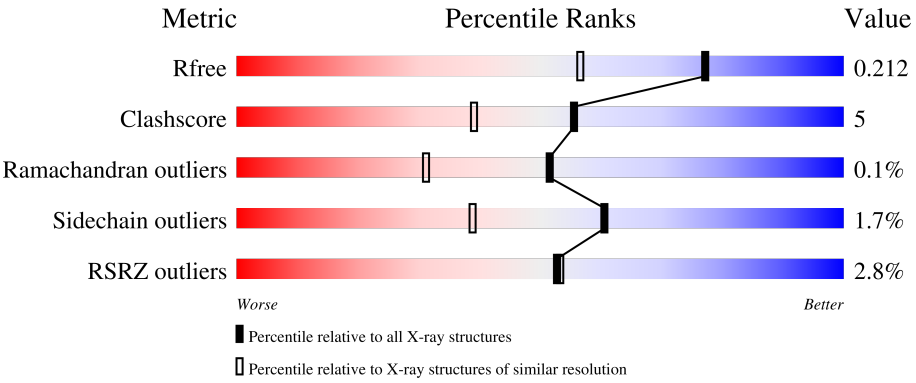
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	3% 85% 7% 8%
1	B	535	2% 86% 6% 8%

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
4	PEG	A	608	-	-	X	-
4	PEG	A	610	-	-	X	-
4	PEG	A	611	-	-	X	-
4	PEG	A	616	-	-	X	-
4	PEG	B	609	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9091 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 Cyclomaltodextrin glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	7	0
			4047	2588	672	774	13			
1	B	493	Total	C	N	O	S	0	4	0
			4019	2571	668	767	13			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	PRO	LEU	conflict	UNP U5CJP3
A	441	VAL	ILE	conflict	UNP U5CJP3
A	471	THR	ALA	conflict	UNP U5CJP3
A	507	ASP	GLY	conflict	UNP U5CJP3
A	509	THR	ALA	conflict	UNP U5CJP3
A	513	ASN	ASP	conflict	UNP U5CJP3
A	525	ALA	-	expression tag	UNP U5CJP3
A	526	ALA	-	expression tag	UNP U5CJP3
A	527	ALA	-	expression tag	UNP U5CJP3
A	528	LEU	-	expression tag	UNP U5CJP3
A	529	GLU	-	expression tag	UNP U5CJP3
A	530	HIS	-	expression tag	UNP U5CJP3
A	531	HIS	-	expression tag	UNP U5CJP3
A	532	HIS	-	expression tag	UNP U5CJP3
A	533	HIS	-	expression tag	UNP U5CJP3
A	534	HIS	-	expression tag	UNP U5CJP3
A	535	HIS	-	expression tag	UNP U5CJP3
B	106	PRO	LEU	conflict	UNP U5CJP3
B	441	VAL	ILE	conflict	UNP U5CJP3
B	471	THR	ALA	conflict	UNP U5CJP3
B	507	ASP	GLY	conflict	UNP U5CJP3
B	509	THR	ALA	conflict	UNP U5CJP3
B	513	ASN	ASP	conflict	UNP U5CJP3
B	525	ALA	-	expression tag	UNP U5CJP3
B	526	ALA	-	expression tag	UNP U5CJP3

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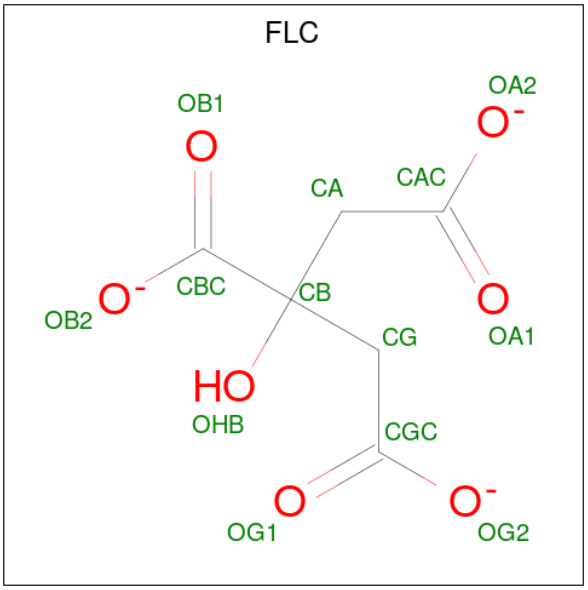
Chain	Residue	Modelled	Actual	Comment	Reference
B	527	ALA	-	expression tag	UNP U5CJP3
B	528	LEU	-	expression tag	UNP U5CJP3
B	529	GLU	-	expression tag	UNP U5CJP3
B	530	HIS	-	expression tag	UNP U5CJP3
B	531	HIS	-	expression tag	UNP U5CJP3
B	532	HIS	-	expression tag	UNP U5CJP3
B	533	HIS	-	expression tag	UNP U5CJP3
B	534	HIS	-	expression tag	UNP U5CJP3
B	535	HIS	-	expression tag	UNP U5CJP3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Ca 3 3	0	0
2	B	3	Total Ca 3 3	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0

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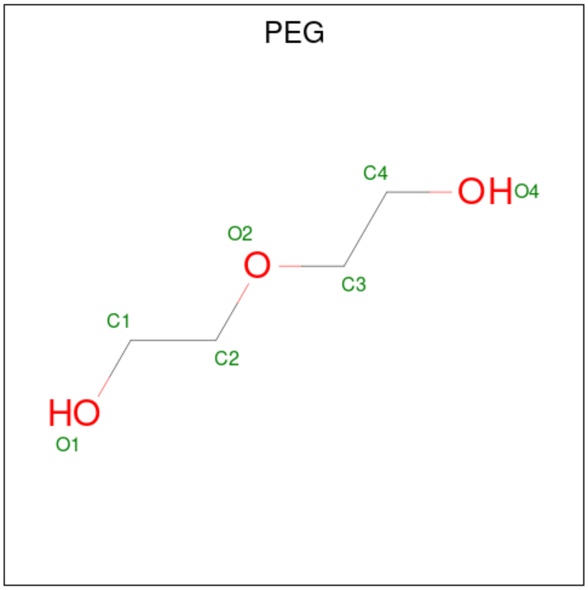
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

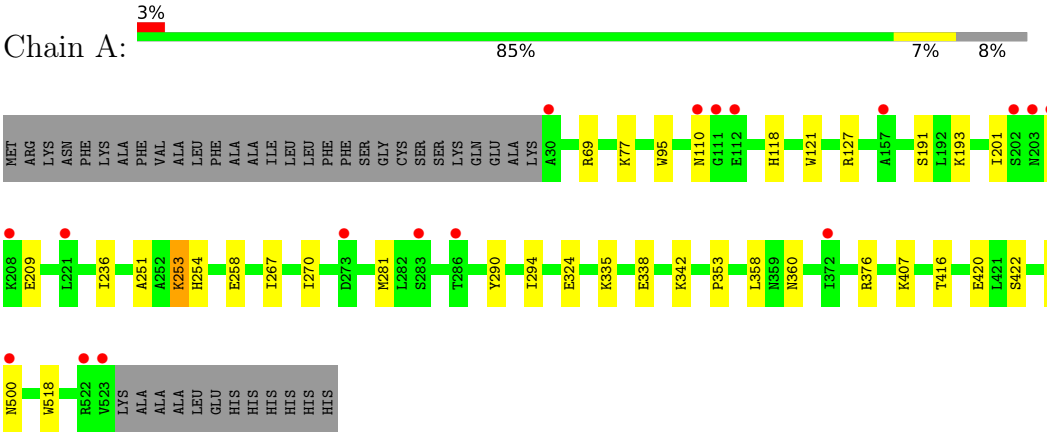
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	383	Total	O	0	0
			383	383		
5	B	465	Total	O	0	0
			465	465		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

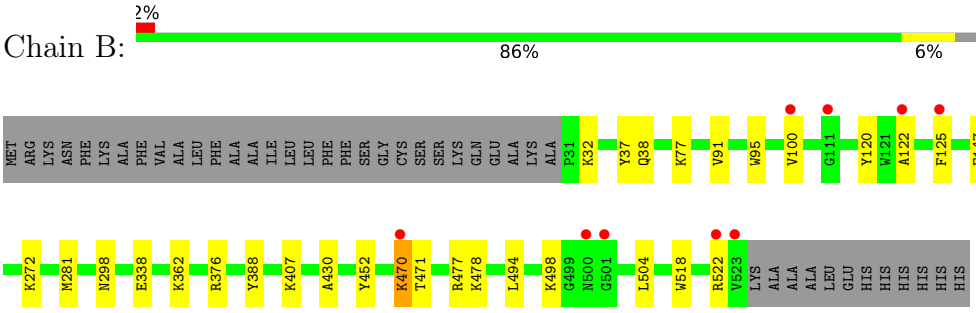
• Molecule 1: Cyclomaltodextrin glucanotransferase

Chain A:



• Molecule 1: Cyclomaltodextrin glucanotransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	66.44Å 66.44Å 209.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.50 – 1.66 28.50 – 1.66	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.50-1.66) 99.5 (28.50-1.66)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 1.66Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.188 , 0.212 0.188 , 0.212	Depositor DCC
R_{free} test set	6062 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.037 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9091	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6992e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CA, FLC

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	0.35	0/4150	0.55	0/5631
1	B	0.36	0/4122	0.55	0/5590
All	All	0.35	0/8272	0.55	0/11221

There are no bond length outliers.

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	4047	0	3916	35	0
1	B	4019	0	3895	30	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	13	0	5	0	0
3	B	39	0	15	1	0
4	A	84	0	120	34	0
4	B	35	0	50	14	0
5	A	383	0	0	23	4
5	B	465	0	0	7	4
All	All	9091	0	8001	83	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (83) 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)
4:B:610:PEG:O4	5:B:701:HOH:O	1.76	1.01
1:A:453:GLY:H	4:A:609:PEG:H22	1.29	0.95
4:A:612:PEG:O4	5:A:703:HOH:O	1.89	0.91
1:B:122:ALA:HB2	4:B:609:PEG:H31	1.53	0.91
4:A:616:PEG:C4	5:A:704:HOH:O	2.20	0.90
1:B:470:LYS:HG3	1:B:471:THR:H	1.39	0.88
4:A:616:PEG:O4	5:A:704:HOH:O	1.92	0.86
1:A:358:LEU:HD13	4:A:608:PEG:H22	1.60	0.83
4:A:608:PEG:O1	5:A:705:HOH:O	1.93	0.83
4:A:606:PEG:O1	5:A:706:HOH:O	2.03	0.76
1:A:353:PRO:HG2	4:A:608:PEG:H41	1.68	0.74
1:A:253:LYS:HD3	4:A:610:PEG:H32	1.71	0.71
1:A:251:ALA:HA	4:A:610:PEG:C2	2.23	0.68
1:A:251:ALA:HA	4:A:610:PEG:H22	1.74	0.68
1:B:157:ALA:HB3	4:B:609:PEG:H41	1.76	0.67
1:B:470:LYS:HG2	5:B:928:HOH:O	1.93	0.67
4:A:607:PEG:H12	5:A:761:HOH:O	1.95	0.67
1:A:121:TRP:CH2	4:A:611:PEG:H12	2.30	0.67
1:B:125:PHE:CE2	4:B:609:PEG:H12	2.32	0.65
1:B:122:ALA:CB	4:B:609:PEG:H31	2.26	0.64
1:A:338:GLU:OE2	5:A:707:HOH:O	2.15	0.64
1:A:118:HIS:HE2	4:A:611:PEG:H11	1.63	0.63
1:A:127:ARG:NH1	5:A:716:HOH:O	2.31	0.62
1:B:470:LYS:HG3	1:B:471:THR:N	2.13	0.62
4:B:608:PEG:O1	5:B:702:HOH:O	2.16	0.61
1:A:118:HIS:NE2	4:A:611:PEG:H11	2.16	0.60
1:A:253:LYS:HD3	4:A:610:PEG:H12	1.84	0.58
1:A:204:TRP:N	5:A:720:HOH:O	2.36	0.58
1:B:261:LYS:NZ	5:B:710:HOH:O	2.35	0.58
1:A:254:HIS:NE2	4:A:610:PEG:H42	2.19	0.58
1:A:453:GLY:N	4:A:609:PEG:H22	2.12	0.55
1:A:353:PRO:CG	4:A:608:PEG:H41	2.35	0.54
4:A:616:PEG:H32	5:A:942:HOH:O	2.09	0.52
4:A:614:PEG:H41	5:A:899:HOH:O	2.09	0.52
1:A:69:ARG:HG3	5:A:1019:HOH:O	2.09	0.51
1:B:120:TYR:C	4:B:609:PEG:H32	2.31	0.50
1:B:100:VAL:CG2	4:B:609:PEG:H21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:HIS:CD2	4:A:611:PEG:H11	2.47	0.49
1:A:77:LYS:NZ	5:A:711:HOH:O	2.25	0.49
4:A:615:PEG:H21	4:A:615:PEG:H42	1.56	0.48
1:B:157:ALA:H	4:B:609:PEG:C1	2.25	0.48
1:B:494:LEU:HB2	1:B:518:TRP:CE2	2.48	0.48
1:B:100:VAL:HG22	4:B:609:PEG:H21	1.95	0.48
1:B:147:GLU:HG3	5:B:955:HOH:O	2.14	0.47
1:A:324:GLU:H	1:A:324:GLU:CD	2.17	0.47
1:A:342:LYS:NZ	5:A:733:HOH:O	2.48	0.47
4:A:607:PEG:H11	5:A:842:HOH:O	2.15	0.47
1:A:420[B]:GLU:OE2	5:A:708:HOH:O	2.21	0.47
1:B:37:TYR:HB2	1:B:91:VAL:HG21	1.96	0.47
1:B:32[B]:LYS:HG3	3:B:606:FLC:CGC	2.45	0.46
1:B:362:LYS:HE3	1:B:388:TYR:CG	2.51	0.46
1:A:416:THR:O	1:A:420[B]:GLU:HG2	2.15	0.46
1:A:251:ALA:HA	4:A:610:PEG:H21	1.97	0.46
1:B:100:VAL:HG22	4:B:609:PEG:C2	2.46	0.46
1:A:353:PRO:CB	4:A:608:PEG:H41	2.46	0.46
4:A:610:PEG:H31	5:A:715:HOH:O	2.16	0.45
1:B:298:ASN:ND2	1:B:338:GLU:HG3	2.31	0.45
1:A:290:TYR:CZ	1:A:294:ILE:HD11	2.52	0.45
4:A:607:PEG:C1	5:A:761:HOH:O	2.61	0.45
1:A:290:TYR:CE1	1:A:294:ILE:HD11	2.52	0.45
1:B:478:LYS:HD3	1:B:498:LYS:HB2	1.99	0.45
1:B:407:LYS:HB2	1:B:407:LYS:HE3	1.62	0.45
4:A:605:PEG:O4	5:A:701:HOH:O	1.87	0.45
1:B:157:ALA:H	4:B:609:PEG:H11	1.83	0.44
4:A:616:PEG:H32	4:A:616:PEG:H11	1.33	0.44
1:A:191:SER:OG	4:A:614:PEG:H31	2.17	0.43
1:B:156:PHE:HA	4:B:609:PEG:O1	2.18	0.43
1:A:494:LEU:HB2	1:A:518:TRP:CE2	2.54	0.42
1:B:498:LYS:NZ	5:B:725:HOH:O	2.51	0.42
1:A:258:GLU:HB2	5:A:729:HOH:O	2.18	0.42
1:B:38:GLN:HG3	1:B:95:TRP:CD2	2.54	0.42
1:B:100:VAL:HG13	5:B:794:HOH:O	2.20	0.41
1:A:201:ILE:HG23	1:A:209:GLU:HG2	2.01	0.41
1:A:118:HIS:HE2	4:A:611:PEG:C1	2.31	0.41
1:A:236:ILE:HD12	1:A:236:ILE:HA	1.94	0.41
1:A:360:ASN:ND2	5:A:713:HOH:O	2.29	0.41
4:A:612:PEG:O1	5:A:709:HOH:O	2.22	0.41
1:A:267:ILE:O	1:A:270:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:LEU:HD23	1:B:504:LEU:HA	1.87	0.41
4:A:616:PEG:H11	5:A:942:HOH:O	2.20	0.41
1:B:430:ALA:HA	1:B:452:TYR:HB2	2.03	0.40
1:B:122:ALA:H	4:B:609:PEG:C3	2.34	0.40
1:B:272:LYS:HD2	1:B:272:LYS:N	2.36	0.40

All (4) 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)
5:A:1021:HOH:O	5:B:1000:HOH:O[3_455]	2.10	0.10
5:A:709:HOH:O	5:B:943:HOH:O[3_455]	2.16	0.04
5:A:1078:HOH:O	5:B:1159:HOH:O[1_445]	2.16	0.04
5:A:713:HOH:O	5:B:1085:HOH:O[3_455]	2.17	0.03

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	499/535 (93%)	483 (97%)	15 (3%)	1 (0%)	47 28
1	B	495/535 (92%)	477 (96%)	18 (4%)	0	100 100
All	All	994/1070 (93%)	960 (97%)	33 (3%)	1 (0%)	51 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	442/467 (95%)	433 (98%)	9 (2%)	55 32
1	B	439/467 (94%)	433 (99%)	6 (1%)	67 46
All	All	881/934 (94%)	866 (98%)	15 (2%)	60 39

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	110	ASN
1	A	193	LYS
1	A	253	LYS
1	A	281	MET
1	A	335	LYS
1	A	376	ARG
1	A	407	LYS
1	A	422	SER
1	B	77	LYS
1	B	281	MET
1	B	376	ARG
1	B	470	LYS
1	B	477	ARG
1	B	522	ARG

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 6 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PEG	A	607	-	6,6,6	0.16	0	5,5,5	0.09	0
4	PEG	A	614	-	6,6,6	0.15	0	5,5,5	0.09	0
4	PEG	A	605	-	6,6,6	0.16	0	5,5,5	0.16	0
3	FLC	B	605	-	12,12,12	1.39	3 (25%)	17,17,17	1.44	3 (17%)
4	PEG	A	611	-	6,6,6	0.18	0	5,5,5	0.06	0
3	FLC	B	604	-	12,12,12	1.69	4 (33%)	17,17,17	1.51	3 (17%)
4	PEG	A	608	-	6,6,6	0.13	0	5,5,5	0.09	0
4	PEG	A	610	-	6,6,6	0.13	0	5,5,5	0.09	0
4	PEG	A	609	-	6,6,6	0.11	0	5,5,5	0.08	0
4	PEG	A	606	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	A	615	-	6,6,6	0.15	0	5,5,5	0.14	0
4	PEG	B	611	-	6,6,6	0.10	0	5,5,5	0.09	0
4	PEG	A	613	-	6,6,6	0.13	0	5,5,5	0.12	0
4	PEG	B	608	-	6,6,6	0.12	0	5,5,5	0.15	0
3	FLC	A	604	-	12,12,12	1.61	3 (25%)	17,17,17	1.58	2 (11%)
4	PEG	A	612	-	6,6,6	0.11	0	5,5,5	0.10	0
4	PEG	B	610	-	6,6,6	0.11	0	5,5,5	0.11	0
4	PEG	B	607	-	6,6,6	0.11	0	5,5,5	0.07	0
3	FLC	B	606	-	12,12,12	1.17	1 (8%)	17,17,17	1.17	2 (11%)
4	PEG	A	616	-	6,6,6	0.12	0	5,5,5	0.08	0
4	PEG	B	609	-	6,6,6	0.25	0	5,5,5	0.07	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
4	PEG	A	607	-	-	2/4/4/4	-
4	PEG	A	614	-	-	4/4/4/4	-
4	PEG	A	605	-	-	2/4/4/4	-
3	FLC	B	605	-	-	5/16/16/16	-
4	PEG	A	611	-	-	2/4/4/4	-
3	FLC	B	604	-	-	3/16/16/16	-
4	PEG	A	608	-	-	2/4/4/4	-
4	PEG	A	610	-	-	3/4/4/4	-
4	PEG	A	609	-	-	2/4/4/4	-
4	PEG	A	606	-	-	1/4/4/4	-
4	PEG	A	615	-	-	2/4/4/4	-
4	PEG	B	611	-	-	1/4/4/4	-
4	PEG	A	613	-	-	3/4/4/4	-
4	PEG	B	608	-	-	0/4/4/4	-
3	FLC	A	604	-	-	3/16/16/16	-
4	PEG	A	612	-	-	1/4/4/4	-
4	PEG	B	610	-	-	2/4/4/4	-
4	PEG	B	607	-	-	3/4/4/4	-
3	FLC	B	606	-	-	0/16/16/16	-
4	PEG	A	616	-	-	4/4/4/4	-
4	PEG	B	609	-	-	3/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	604	FLC	OG2-CGC	-3.28	1.19	1.30
3	A	604	FLC	OG2-CGC	-3.20	1.20	1.30
3	A	604	FLC	OA2-CAC	-2.80	1.21	1.30
3	B	604	FLC	OB2-CBC	-2.70	1.20	1.30
3	B	605	FLC	OA2-CAC	-2.64	1.21	1.30
3	B	604	FLC	CB-CBC	2.62	1.56	1.53
3	B	604	FLC	OA2-CAC	-2.52	1.22	1.30
3	B	605	FLC	CB-CBC	2.40	1.55	1.53
3	A	604	FLC	CB-CBC	2.31	1.55	1.53
3	B	605	FLC	OG2-CGC	-2.24	1.23	1.30
3	B	606	FLC	OB2-CBC	-2.01	1.22	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	604	FLC	OB1-CBC-CB	-4.43	115.98	122.25
3	B	604	FLC	OB1-CBC-CB	-3.59	117.17	122.25
3	B	604	FLC	OB2-CBC-CB	3.46	119.05	113.05
3	A	604	FLC	OB2-CBC-CB	3.28	118.74	113.05
3	B	605	FLC	OB1-CBC-CB	-3.27	117.62	122.25
3	B	606	FLC	OB1-CBC-CB	-2.98	118.04	122.25
3	B	605	FLC	OB2-CBC-CB	2.41	117.23	113.05
3	B	604	FLC	CB-CG-CGC	2.31	119.41	113.81
3	B	605	FLC	CB-CA-CAC	2.26	119.28	113.81
3	B	606	FLC	OB2-CBC-CB	2.09	116.67	113.05

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	608	PEG	C4-C3-O2-C2
4	A	616	PEG	C1-C2-O2-C3
4	A	607	PEG	C1-C2-O2-C3
4	A	607	PEG	O2-C3-C4-O4
4	A	615	PEG	C4-C3-O2-C2
4	A	609	PEG	C4-C3-O2-C2
4	A	615	PEG	O2-C3-C4-O4
4	B	607	PEG	O1-C1-C2-O2
4	A	605	PEG	O2-C3-C4-O4
4	A	608	PEG	O1-C1-C2-O2
4	A	611	PEG	O1-C1-C2-O2
4	A	614	PEG	O1-C1-C2-O2
4	A	616	PEG	O1-C1-C2-O2
4	B	609	PEG	O1-C1-C2-O2
4	A	610	PEG	C1-C2-O2-C3
3	A	604	FLC	CAC-CA-CB-OHB
3	B	604	FLC	OHB-CB-CG-CGC
4	A	609	PEG	O2-C3-C4-O4
4	A	606	PEG	O1-C1-C2-O2
4	B	611	PEG	O2-C3-C4-O4
3	B	605	FLC	CB-CA-CAC-OA2
3	A	604	FLC	CAC-CA-CB-CG
3	B	605	FLC	CAC-CA-CB-CBC
3	B	605	FLC	CB-CA-CAC-OA1
4	A	605	PEG	O1-C1-C2-O2
4	A	612	PEG	O2-C3-C4-O4
4	B	609	PEG	O2-C3-C4-O4
4	A	613	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	A	613	PEG	C1-C2-O2-C3
4	B	607	PEG	C4-C3-O2-C2
4	A	611	PEG	C1-C2-O2-C3
4	B	607	PEG	C1-C2-O2-C3
4	A	610	PEG	O1-C1-C2-O2
4	B	610	PEG	O2-C3-C4-O4
4	A	614	PEG	C4-C3-O2-C2
3	B	605	FLC	CAC-CA-CB-CG
4	A	616	PEG	O2-C3-C4-O4
4	A	616	PEG	C4-C3-O2-C2
3	B	604	FLC	CA-CB-CG-CGC
3	B	605	FLC	CAC-CA-CB-OHB
4	A	614	PEG	C1-C2-O2-C3
4	B	610	PEG	C1-C2-O2-C3
4	B	609	PEG	C1-C2-O2-C3
3	A	604	FLC	CA-CB-CG-CGC
3	B	604	FLC	CAC-CA-CB-CG
4	A	610	PEG	C4-C3-O2-C2
4	A	613	PEG	O1-C1-C2-O2
4	A	614	PEG	O2-C3-C4-O4

There are no ring outliers.

15 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	607	PEG	3	0
4	A	614	PEG	2	0
4	A	605	PEG	1	0
4	A	611	PEG	5	0
4	A	608	PEG	5	0
4	A	610	PEG	7	0
4	A	609	PEG	2	0
4	A	606	PEG	1	0
4	A	615	PEG	1	0
4	B	608	PEG	1	0
4	A	612	PEG	2	0
4	B	610	PEG	1	0
3	B	606	FLC	1	0
4	A	616	PEG	5	0
4	B	609	PEG	12	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	494/535 (92%)	-0.01	18 (3%)	42	43	13, 22, 38, 62	0
1	B	493/535 (92%)	-0.11	10 (2%)	65	67	13, 21, 35, 62	0
All	All	987/1070 (92%)	-0.06	28 (2%)	53	53	13, 21, 37, 62	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	ALA	4.5
1	A	500	ASN	4.4
1	B	500	ASN	4.3
1	A	110	ASN	3.7
1	A	523	VAL	3.6
1	A	204	TRP	3.5
1	A	202	SER	3.1
1	A	111	GLY	3.0
1	B	523	VAL	3.0
1	B	470	LYS	2.8
1	B	125	PHE	2.6
1	B	522	ARG	2.5
1	A	203	ASN	2.5
1	A	273	ASP	2.5
1	B	100	VAL	2.5
1	A	286	THR	2.4
1	A	283	SER	2.4
1	A	522	ARG	2.3
1	A	112	GLU	2.3
1	B	122	ALA	2.3
1	B	111	GLY	2.2
1	B	202	SER	2.1
1	A	206	ASN	2.1
1	A	372	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	157	ALA	2.0
1	A	208	LYS	2.0
1	A	221	LEU	2.0
1	B	501	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	A	615	7/7	0.72	0.20	25,27,28,28	7
4	PEG	A	613	7/7	0.75	0.19	29,35,38,43	0
4	PEG	A	607	7/7	0.81	0.27	25,28,37,42	7
4	PEG	A	612	7/7	0.81	0.21	34,40,44,46	0
4	PEG	A	614	7/7	0.82	0.13	27,29,33,36	0
4	PEG	B	607	7/7	0.82	0.17	33,39,46,47	0
4	PEG	A	611	7/7	0.84	0.13	18,22,28,29	7
3	FLC	B	606	13/13	0.84	0.13	25,32,35,37	13
4	PEG	A	605	7/7	0.86	0.12	25,29,38,39	0
4	PEG	A	610	7/7	0.86	0.12	24,25,36,45	7
2	CA	B	602	1/1	0.87	0.09	18,18,18,18	0
4	PEG	B	608	7/7	0.87	0.16	37,39,42,44	0
2	CA	A	601	1/1	0.88	0.08	22,22,22,22	0
4	PEG	A	609	7/7	0.88	0.27	35,37,46,48	0
4	PEG	A	616	7/7	0.89	0.20	37,42,46,49	0
4	PEG	A	608	7/7	0.89	0.16	14,18,21,25	7
3	FLC	B	605	13/13	0.89	0.12	31,34,37,39	13
4	PEG	B	610	7/7	0.90	0.17	30,34,40,44	0
4	PEG	B	611	7/7	0.91	0.18	34,43,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	B	609	7/7	0.92	0.20	13,18,21,25	7
2	CA	B	603	1/1	0.92	0.08	19,19,19,19	0
4	PEG	A	606	7/7	0.92	0.09	26,32,36,43	0
3	FLC	A	604	13/13	0.93	0.08	20,25,30,30	0
3	FLC	B	604	13/13	0.94	0.07	22,23,31,32	0
2	CA	B	601	1/1	0.98	0.06	18,18,18,18	0
2	CA	A	602	1/1	0.99	0.06	17,17,17,17	0
2	CA	A	603	1/1	1.00	0.05	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.