Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:56 AM GMT

PDB ID	:	3K8L
Title	:	Crystal structure of SusG-D498N mutant with maltoheptaose
Authors	:	Koropatkin, N.M.; Smith, T.J.
Deposited on	:	2009-10-14
Resolution	:	2.30 Å(reported)

The following versions of software and data (see references (i)) 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 2.30 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	Percentile Ranks	Value
Rfree		0.213
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		2.1%
RSRZ outliers		1.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
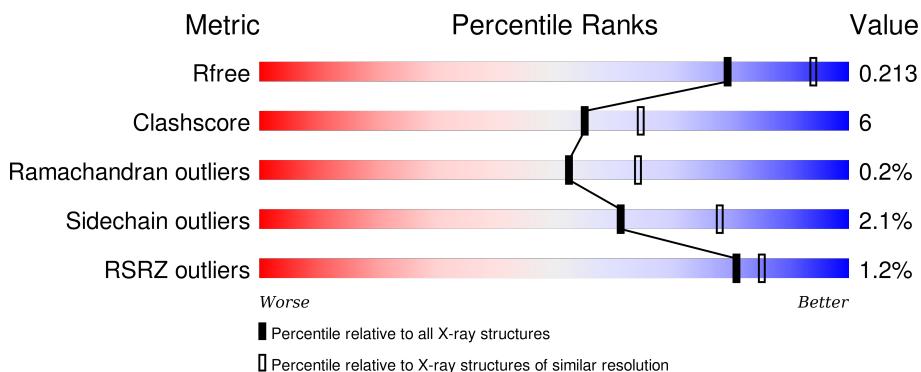
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	669	85% 12% • •
1	B	669	2% 82% 14% • •
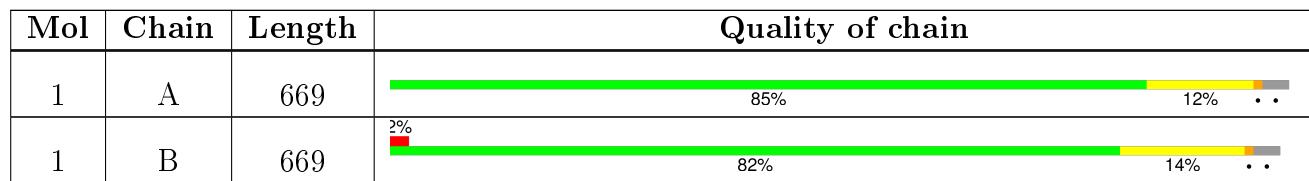
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CEY	A	730	-	-	-	X
4	CEY	B	830	-	-	-	X
4	CEY	B	840	-	-	-	X
5	GLC	A	740	-	-	-	X
6	EDO	A	900	-	-	-	X
6	EDO	A	930	-	-	-	X
6	EDO	B	920	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11264 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 Alpha-amylase, susG.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total 5169	C 3288	N 836	O 1029	S 16	0	0	0
1	B	646	Total 5146	C 3277	N 832	O 1021	S 16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	ASN	ASP	ENGINEERED	UNP Q8A1G3
B	498	ASN	ASP	ENGINEERED	UNP Q8A1G3

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

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

- Molecule 3 is ALPHA-D-GLUCOPYRANOSYL-(1->4)-ALPHA-D-GLUCOPYRANOSYL-(1->4)-ALPHA-D-GLUCOPYRANOSYL-(1->4)-ALPHA-D-GLUCOPYRANOSYL-(1->4)-ALPHA-D-GLUCOPYRANOSE (three-letter code: CEX) (formula: $C_{30}H_{52}O_{26}$).
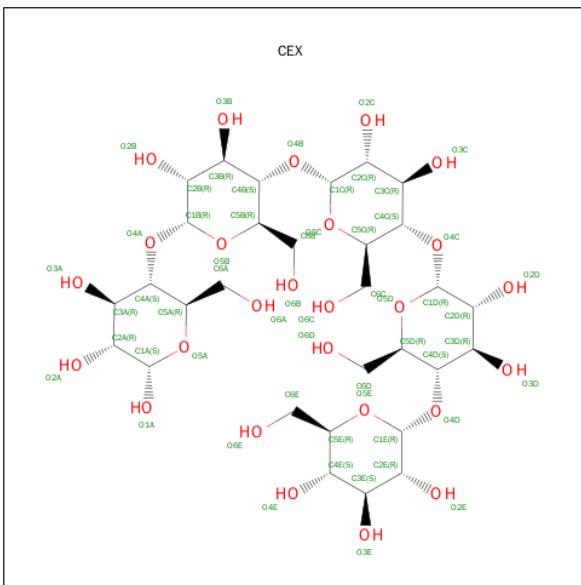
CEX

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	1	0
			56	30	26		
3	B	1	Total	C	O	0	0
			56	30	26		

- Molecule 4 is ALPHA-D-GLUCOPYRANOSYL-(1->4)-ALPHA-D-GLUCOPYRANOSYL-(1->4)-ALPHA-D-GLUCOPYRANOSYL-(1->4)-ALPHA-D-GLUCOPYRANOSYL-(1->4)-ALPHA-D-GLUCOPYRANOSYL-(1->4)-ALPHA-D-GLUCOPYRANOSE (three-letter code: CEY) (formula: $C_{36}H_{62}O_{31}$).


CEY
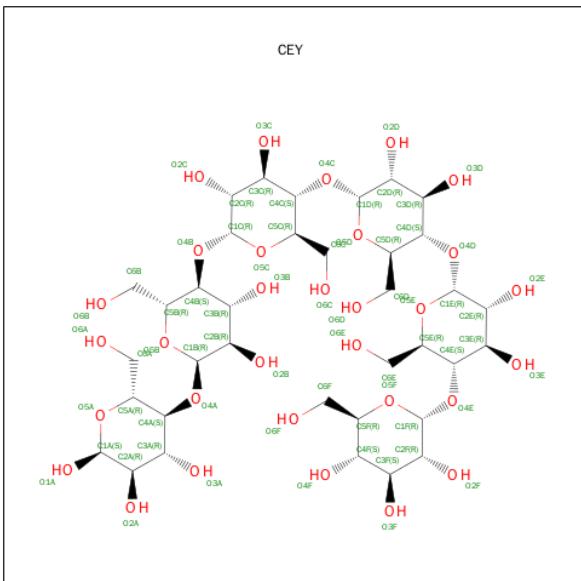
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 67	C 36	O 31	0	0
4	B	1	Total 67	C 36	O 31	0	0
4	B	1	Total 67	C 36	O 31	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	7	Total 78	C 42	O 36	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
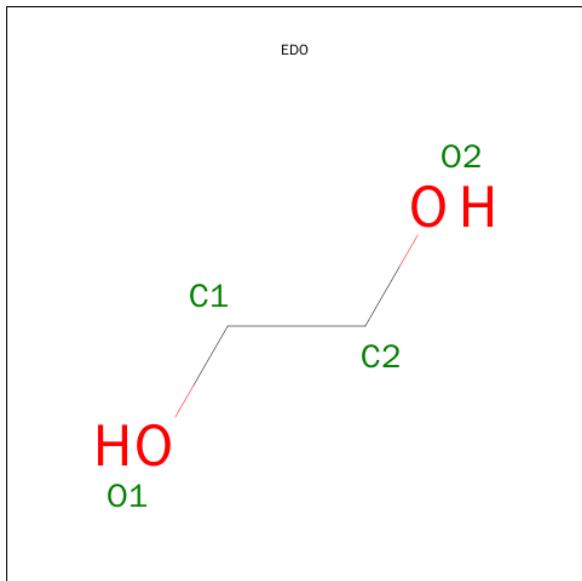
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	342	Total 342	O 342	0	0
7	B	196	Total 196	O 196	0	0

3 Residue-property plots ⓘ

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: Alpha-amylase, susG
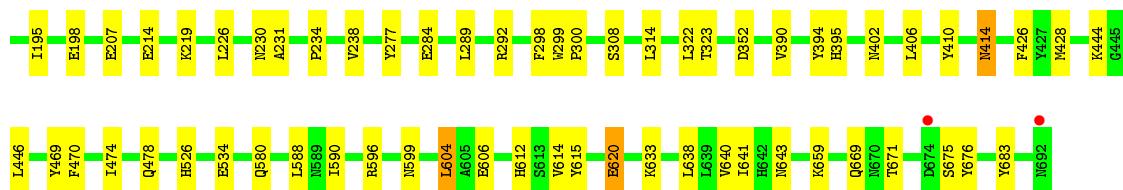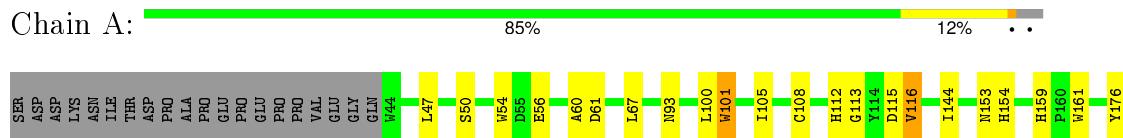
- Molecule 1: Alpha-amylase, susG
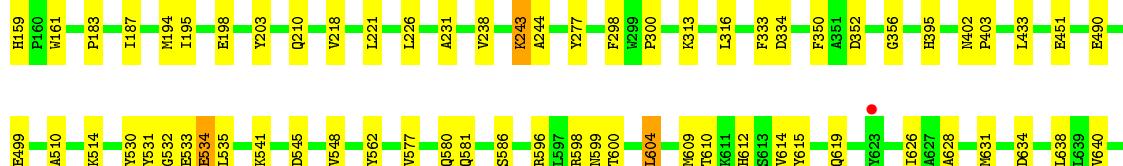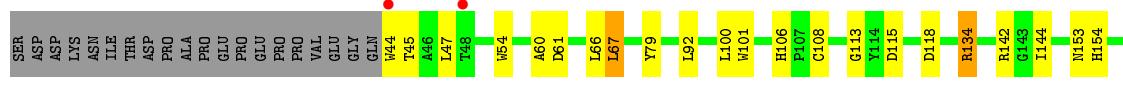
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	128.04Å 128.04Å 130.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 45.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-2.30) 92.2 (45.69-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	6.22 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.184 , 0.216 0.183 , 0.213	Depositor DCC
R_{free} test set	8826 reflections (11.14%)	DCC
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.3	EDS
Estimated twinning fraction	0.018 for -h,-l,-k 0.005 for -h,l,k 0.006 for l,-k,h 0.019 for -l,-k,-h 0.032 for h,-k,-l	Xtriage
L-test for twinning [2]	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Outliers	0 of 98588 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11264	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, CA, GLC, EDO, CEY, CEX

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	0/5308	0.60	0/7214
1	B	0.33	0/5284	0.56	0/7181
All	All	0.34	0/10592	0.58	0/14395

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 (i)

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	5169	0	4872	55	0
1	B	5146	0	4856	71	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	56	0	52	1	0
3	B	56	0	52	1	0
4	A	67	0	62	2	0
4	B	134	0	124	2	0
5	A	78	0	66	1	0
6	A	12	0	18	2	0
6	B	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	342	0	0	3	0
7	B	196	0	0	2	0
All	All	11264	0	10108	131	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 6.

All (131) 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:394:TYR:H	1:A:402:ASN:HD21	1.04	0.93
1:B:159:HIS:HD2	1:B:161:TRP:H	1.16	0.92
1:A:159:HIS:HD2	1:A:161:TRP:H	1.14	0.92
1:A:153:ASN:HD22	1:A:154:HIS:HD2	1.16	0.88
1:B:153:ASN:HD22	1:B:154:HIS:HD2	1.19	0.88
1:B:313:LYS:HG2	1:B:334:ASP:HA	1.59	0.85
1:A:612:HIS:HD2	1:A:615:TYR:H	1.27	0.82
1:B:596:ARG:O	1:B:600:THR:HG23	1.80	0.82
1:B:243:LYS:HE2	1:B:244:ALA:H	1.47	0.79
1:B:609:MET:HB2	1:B:631:MET:HE1	1.64	0.79
1:A:604:LEU:HD13	1:A:638:LEU:HD12	1.65	0.79
1:A:238:VAL:HG21	1:A:314:LEU:HD21	1.65	0.79
1:B:54:TRP:CD1	1:B:600:THR:HG22	2.17	0.78
1:A:159:HIS:CD2	1:A:161:TRP:H	2.01	0.78
1:B:604:LEU:HD13	1:B:638:LEU:HD12	1.71	0.73
1:A:153:ASN:HD22	1:A:154:HIS:CD2	2.06	0.70
1:B:153:ASN:HD22	1:B:154:HIS:CD2	2.07	0.70
1:B:60:ALA:H	1:B:599:ASN:HD22	1.38	0.70
1:A:61:ASP:OD2	1:A:526:HIS:HD2	1.77	0.68
1:A:414:ASN:ND2	1:A:426:PHE:H	1.92	0.67
1:B:183:PRO:O	1:B:187:ILE:HG12	1.95	0.66
1:B:67:LEU:HD22	1:B:531:TYR:HE2	1.59	0.66
1:A:238:VAL:CG2	1:A:314:LEU:HD21	2.26	0.65
1:B:243:LYS:HE2	1:B:244:ALA:N	2.11	0.65
1:A:198:GLU:OE1	1:A:395:HIS:HD2	1.80	0.65
4:A:730:CEY:H6BA	4:A:730:CEY:H5C	1.78	0.64
1:B:153:ASN:ND2	1:B:154:HIS:HD2	1.93	0.64
1:B:159:HIS:CD2	1:B:161:TRP:H	2.07	0.63
1:A:60:ALA:H	1:A:599:ASN:HD22	1.43	0.63
4:B:840:CEY:H5D	4:B:840:CEY:H6C	1.80	0.62
1:B:609:MET:CB	1:B:631:MET:HE1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HD21	1:A:669:GLN:HB3	1.82	0.62
1:A:394:TYR:H	1:A:402:ASN:ND2	1.87	0.61
1:B:612:HIS:CD2	1:B:614:VAL:H	2.18	0.61
1:A:219:LYS:HG2	1:A:284:GLU:HG3	1.81	0.61
1:B:67:LEU:HD22	1:B:531:TYR:CE2	2.36	0.60
1:A:410:TYR:HD2	1:A:428:MET:HE2	1.67	0.59
1:A:671:THR:HA	1:A:675:SER:O	2.03	0.59
1:B:577:VAL:O	1:B:581:GLN:HG3	2.03	0.59
1:B:612:HIS:HD2	1:B:615:TYR:H	1.50	0.58
1:B:433:LEU:HD23	4:B:840:CEY:O4B	2.03	0.57
1:B:298:PHE:O	1:B:300:PRO:HD3	2.04	0.57
1:B:60:ALA:H	1:B:599:ASN:ND2	2.03	0.57
1:A:428:MET:HE3	1:A:446:LEU:CD2	2.35	0.57
1:B:609:MET:HB2	1:B:631:MET:CE	2.35	0.56
1:B:198:GLU:OE1	1:B:395:HIS:HD2	1.89	0.56
1:B:598:ARG:NH1	7:B:875:HOH:O	2.26	0.55
1:B:238:VAL:HG13	1:B:316:LEU:HD23	1.88	0.54
1:B:221:LEU:HD11	1:B:244:ALA:HB2	1.89	0.54
1:B:226:LEU:HB2	1:B:277:TYR:HB2	1.89	0.53
1:A:50:SER:O	1:A:659:LYS:HE2	2.08	0.53
1:B:499:GLU:HA	1:B:541:LYS:HD2	1.90	0.53
1:B:100:LEU:HD13	1:B:144:ILE:CG2	2.39	0.53
1:A:596:ARG:HD3	7:A:967:HOH:O	2.08	0.53
3:A:720:CEX:H6CA	3:A:720:CEX:H5D	1.90	0.53
1:B:106:HIS:HB3	1:B:118:ASP:O	2.10	0.52
1:B:142:ARG:HG3	1:B:142:ARG:HH11	1.75	0.51
1:B:619:GLN:NE2	1:B:619:GLN:HA	2.27	0.50
1:A:234:PRO:HB2	1:A:322:LEU:HD12	1.92	0.50
1:A:580:GLN:NE2	1:A:588:LEU:H	2.10	0.50
1:A:640:VAL:O	1:A:641:ILE:HD13	2.11	0.50
1:B:626:ILE:N	1:B:626:ILE:HD12	2.27	0.50
1:B:92:LEU:HD13	1:B:100:LEU:HD21	1.94	0.50
1:A:469:TYR:OH	1:A:620:GLU:HG3	2.12	0.49
1:B:609:MET:CA	1:B:631:MET:HE1	2.42	0.49
1:A:54:TRP:CE2	1:A:56:GLU:HA	2.48	0.49
1:B:66:LEU:C	1:B:66:LEU:HD12	2.33	0.49
1:B:667:THR:HG22	1:B:680:LEU:HD23	1.94	0.48
1:B:108:CYS:SG	1:B:113:GLY:HA2	2.53	0.48
1:A:390:VAL:HB	1:A:406:LEU:HD11	1.95	0.48
1:A:470:PHE:O	1:A:474:ILE:HG12	2.14	0.48
1:B:45:THR:HG22	1:B:669:GLN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TYR:CD2	1:A:428:MET:HE2	2.49	0.48
1:B:218:VAL:HG21	1:B:333:PHE:CD1	2.49	0.47
1:A:612:HIS:CD2	1:A:614:VAL:H	2.31	0.47
1:B:79:TYR:CE1	1:B:562:TYR:HB2	2.49	0.47
1:B:612:HIS:HD2	1:B:615:TYR:N	2.12	0.47
1:A:444:LYS:HE3	1:B:634:ASP:OD2	2.14	0.47
1:A:176:TYR:OH	6:A:900:EDO:H11	2.15	0.47
1:A:633:LYS:HG2	7:B:701:HOH:O	2.14	0.47
1:A:112:HIS:HE2	6:A:930:EDO:H11	1.79	0.47
1:B:194:MET:HE3	1:B:356:GLY:H	1.81	0.46
1:B:643:ASN:O	1:B:683:TYR:HA	2.15	0.46
1:A:606:GLU:OE2	1:A:633:LYS:HE3	2.16	0.46
1:A:195:ILE:HG12	1:A:395:HIS:HB2	1.98	0.46
1:B:115:ASP:HB3	1:B:350:PHE:CE1	2.50	0.46
1:B:134:ARG:HB3	1:B:134:ARG:HH11	1.80	0.46
1:B:402:ASN:HB2	1:B:403:PRO:HD3	1.98	0.46
1:B:668:GLN:HB2	1:B:679:LYS:HB3	1.97	0.45
3:B:820:CEX:H5D	3:B:820:CEX:H6CA	1.98	0.45
1:B:451:GLU:OE1	1:B:490:GLU:OE2	2.34	0.45
1:B:668:GLN:OE1	1:B:679:LYS:HD3	2.17	0.45
1:B:656:LYS:O	1:B:656:LYS:HG3	2.17	0.45
1:B:510:ALA:O	1:B:514:LYS:HG3	2.17	0.44
1:B:100:LEU:HD13	1:B:144:ILE:HG21	1.98	0.44
1:A:474:ILE:O	1:A:478:GLN:HG3	2.17	0.44
5:A:743:GLC:H5	5:A:744:GLC:C6	2.48	0.44
1:A:292:ARG:HD2	1:A:299:TRP:CH2	2.52	0.44
1:A:54:TRP:CD2	1:A:56:GLU:HA	2.52	0.44
1:B:44:TRP:CE3	1:B:670:ASN:HB2	2.52	0.44
1:B:580:GLN:NE2	1:B:586:SER:HB2	2.33	0.44
1:A:116:VAL:HG13	7:A:753:HOH:O	2.17	0.44
1:B:47:LEU:HD12	1:B:667:THR:HB	2.00	0.44
1:B:183:PRO:HB2	1:B:203:TYR:CE1	2.53	0.43
1:B:203:TYR:OH	6:B:920:EDO:H21	2.18	0.43
1:A:580:GLN:HB3	1:A:580:GLN:HE21	1.65	0.43
1:A:643:ASN:O	1:A:683:TYR:HA	2.17	0.43
1:A:108:CYS:SG	1:A:113:GLY:HA2	2.58	0.43
1:A:226:LEU:HB2	1:A:277:TYR:HB2	2.01	0.43
1:A:100:LEU:HD13	1:A:144:ILE:HG21	2.01	0.43
1:B:530:TYR:O	1:B:533:GLU:HG2	2.19	0.43
1:B:195:ILE:HG12	1:B:395:HIS:HB2	2.00	0.42
1:A:105:ILE:HG12	1:A:105:ILE:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:ALA:HA	1:B:640:VAL:O	2.19	0.42
1:B:535:LEU:HD11	1:B:577:VAL:HG23	2.02	0.42
1:B:545:ASP:O	1:B:548:VAL:HG22	2.20	0.42
4:A:730:CEY:H5B	4:A:730:CEY:H6A	2.01	0.42
1:A:308:SER:HA	1:A:323:THR:HG21	2.02	0.42
1:A:633:LYS:HD2	7:A:831:HOH:O	2.19	0.42
1:B:101:TRP:CD1	1:B:101:TRP:C	2.92	0.42
1:A:207:GLU:OE1	1:A:395:HIS:HE1	2.02	0.41
1:A:298:PHE:O	1:A:300:PRO:HD3	2.20	0.41
1:A:428:MET:HE3	1:A:446:LEU:HD21	2.02	0.41
1:B:609:MET:HG2	1:B:610:THR:N	2.35	0.41
1:A:612:HIS:CD2	1:A:615:TYR:H	2.19	0.41
1:B:532:GLY:N	1:B:534:GLU:OE2	2.54	0.41
1:A:101:TRP:CD1	1:A:101:TRP:C	2.93	0.41
1:B:54:TRP:HD1	1:B:600:THR:HG22	1.76	0.40
1:A:60:ALA:HB3	1:A:599:ASN:ND2	2.37	0.40
1:B:115:ASP:HB3	1:B:350:PHE:HE1	1.87	0.40
1:A:669:GLN:OE1	1:A:676:TYR:HE1	2.04	0.40

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	647/669 (97%)	621 (96%)	25 (4%)	1 (0%)	52	64
1	B	642/669 (96%)	603 (94%)	38 (6%)	1 (0%)	52	64
All	All	1289/1338 (96%)	1224 (95%)	63 (5%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ALA
1	B	231	ALA

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	550/568 (97%)	536 (98%)	14 (2%)	55	73
1	B	547/568 (96%)	538 (98%)	9 (2%)	70	84
All	All	1097/1136 (97%)	1074 (98%)	23 (2%)	61	78

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	93	ASN
1	A	101	TRP
1	A	115	ASP
1	A	116	VAL
1	A	214	GLU
1	A	230	ASN
1	A	289	LEU
1	A	352	ASP
1	A	414	ASN
1	A	534	GLU
1	A	590	ILE
1	A	604	LEU
1	A	620	GLU
1	B	61	ASP
1	B	67	LEU
1	B	134	ARG
1	B	210	GLN
1	B	243	LYS
1	B	352	ASP
1	B	534	GLU
1	B	604	LEU

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Mol	Chain	Res	Type
1	B	678	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	94	GLN
1	A	106	HIS
1	A	154	HIS
1	A	159	HIS
1	A	230	ASN
1	A	274	ASN
1	A	324	ASN
1	A	337	GLN
1	A	395	HIS
1	A	402	ASN
1	A	414	ASN
1	A	526	HIS
1	A	543	ASN
1	A	561	ASN
1	A	573	ASN
1	A	580	GLN
1	A	581	GLN
1	A	589	ASN
1	A	599	ASN
1	A	608	ASN
1	A	612	HIS
1	A	669	GLN
1	B	94	GLN
1	B	106	HIS
1	B	154	HIS
1	B	159	HIS
1	B	395	HIS
1	B	422	HIS
1	B	543	ASN
1	B	561	ASN
1	B	580	GLN
1	B	581	GLN
1	B	589	ASN
1	B	599	ASN
1	B	612	HIS
1	B	619	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)

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

5.5 Carbohydrates (i)

7 carbohydrates 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	GLC	A	740	5	11,11,12	1.21	1 (9%)	14,15,17	0.73	0
5	GLC	A	741	5	11,11,12	1.47	2 (18%)	14,15,17	1.18	2 (14%)
5	GLC	A	742	5	11,11,12	1.30	3 (27%)	14,15,17	0.73	0
5	GLC	A	743	5	11,11,12	1.20	1 (9%)	14,15,17	1.09	0
5	GLC	A	744	5	11,11,12	1.13	0	14,15,17	0.71	0
5	GLC	A	745	5	11,11,12	0.87	0	14,15,17	0.88	0
5	BGC	A	746	5	12,12,12	0.95	0	17,17,17	0.82	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
5	GLC	A	740	5	-	0/2/19/22	0/1/1/1
5	GLC	A	741	5	-	0/2/19/22	0/1/1/1
5	GLC	A	742	5	-	0/2/19/22	0/1/1/1
5	GLC	A	743	5	-	0/2/19/22	0/1/1/1
5	GLC	A	744	5	-	0/2/19/22	0/1/1/1
5	GLC	A	745	5	-	0/2/19/22	0/1/1/1
5	BGC	A	746	5	-	0/2/22/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	742	GLC	O5-C5	2.02	1.47	1.43
5	A	740	GLC	C2-C3	2.06	1.55	1.52
5	A	742	GLC	C4-C5	2.11	1.57	1.53
5	A	741	GLC	C4-C3	2.21	1.58	1.52
5	A	742	GLC	O5-C1	2.29	1.47	1.43
5	A	741	GLC	O4-C4	2.33	1.48	1.43
5	A	743	GLC	O5-C1	2.72	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	741	GLC	C1-C2-C3	-2.08	107.09	109.54
5	A	741	GLC	O4-C4-C3	2.04	114.93	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	743	GLC	1	0
5	A	744	GLC	1	0

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	#$|Z| > 2$
3	CEX	A	720	-	60,60,60	0.99	4 (6%)	89,89,89	0.84	1 (1%)
4	CEY	A	730	-	72,72,72	1.02	4 (5%)	107,107,107	0.84	2 (1%)
6	EDO	A	900	-	3,3,3	0.73	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	EDO	A	910	-	3,3,3	0.66	0	2,2,2	0.46	0
6	EDO	A	930	-	3,3,3	0.74	0	2,2,2	0.44	0
3	CEX	B	820	-	60,60,60	1.00	3 (5%)	89,89,89	0.83	1 (1%)
4	CEY	B	830	-	72,72,72	1.19	7 (9%)	107,107,107	0.88	2 (1%)
4	CEY	B	840	-	72,72,72	1.08	4 (5%)	107,107,107	0.94	3 (2%)
6	EDO	B	920	-	3,3,3	0.77	0	2,2,2	0.41	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
3	CEX	A	720	-	-	0/26/126/126	0/5/5/5
4	CEY	A	730	-	-	0/32/152/152	0/6/6/6
6	EDO	A	900	-	-	0/1/1/1	0/0/0/0
6	EDO	A	910	-	-	0/1/1/1	0/0/0/0
6	EDO	A	930	-	-	0/1/1/1	0/0/0/0
3	CEX	B	820	-	-	0/26/126/126	0/5/5/5
4	CEY	B	830	-	-	0/32/152/152	0/6/6/6
4	CEY	B	840	-	-	0/32/152/152	0/6/6/6
6	EDO	B	920	-	-	0/1/1/1	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	730	CEY	O5F-C1F	2.00	1.47	1.41
4	B	830	CEY	O4A-C4A	2.01	1.48	1.43
4	B	840	CEY	O5E-C1E	2.01	1.47	1.41
3	B	820	CEX	O5C-C1C	2.04	1.47	1.41
4	A	730	CEY	O5D-C1D	2.04	1.47	1.41
3	A	720	CEX	O5D-C1D	2.06	1.47	1.41
3	A	720	CEX	O5A-C1A	2.07	1.47	1.43
4	B	830	CEY	O5E-C1E	2.08	1.47	1.41
4	B	840	CEY	O5A-C1A	2.09	1.47	1.43
4	A	730	CEY	O5B-C1B	2.10	1.47	1.41
3	A	720	CEX	O5B-C1B	2.10	1.47	1.41
3	B	820	CEX	O5E-C1E	2.13	1.47	1.41
4	B	830	CEY	O5D-C1D	2.16	1.47	1.41
4	B	830	CEY	O4A-C1B	2.19	1.47	1.41
4	B	830	CEY	O5F-C1F	2.19	1.47	1.41
3	A	720	CEX	O5E-C1E	2.20	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	820	CEX	O5D-C1D	2.22	1.47	1.41
4	B	840	CEY	O5D-C1D	2.24	1.47	1.41
4	B	830	CEY	C1A-C2A	2.28	1.57	1.52
4	B	830	CEY	O5C-C1C	2.38	1.47	1.41
4	A	730	CEY	O4A-C1B	2.46	1.48	1.41
4	B	840	CEY	O4C-C1D	3.09	1.50	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	840	CEY	C1B-O4A-C4A	-4.21	107.00	118.01
4	B	840	CEY	C1C-O4B-C4B	-3.46	108.96	118.01
4	A	730	CEY	C1F-O4E-C4E	-3.12	109.86	118.01
4	B	830	CEY	C1F-O4E-C4E	-3.12	109.86	118.01
4	B	840	CEY	C1F-O4E-C4E	-2.94	110.32	118.01
4	B	830	CEY	C1E-O4D-C4D	-2.38	111.78	118.01
3	B	820	CEX	C1E-O4D-C4D	-2.34	111.89	118.01
3	A	720	CEX	C1C-O4B-C4B	-2.11	112.49	118.01
4	A	730	CEY	C1E-O4D-C4D	-2.04	112.69	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	720	CEX	1	0
4	A	730	CEY	2	0
6	A	900	EDO	1	0
6	A	930	EDO	1	0
3	B	820	CEX	1	0
4	B	840	CEY	2	0
6	B	920	EDO	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	649/669 (97%)	-0.44	2 (0%)	94	96	15, 26, 44, 67	0
1	B	646/669 (96%)	-0.13	14 (2%)	65	73	20, 37, 54, 69	0
All	All	1295/1338 (96%)	-0.28	16 (1%)	81	85	15, 31, 52, 69	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	675	SER	3.5
1	A	692	ASN	3.5
1	B	674	ASP	3.3
1	B	677	THR	3.0
1	B	646	GLY	2.8
1	B	647	THR	2.8
1	B	671	THR	2.7
1	A	674	ASP	2.5
1	B	648	ALA	2.4
1	B	243	LYS	2.3
1	B	650	GLN	2.1
1	B	623	TYR	2.1
1	B	48	THR	2.1
1	B	678	LEU	2.1
1	B	676	TYR	2.0
1	B	44	TRP	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)

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, 95th 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
5	GLC	A	740	11/12	0.78	0.20	4.23	47,51,52,53	0
5	GLC	A	743	11/12	0.94	0.14	0.52	21,23,25,26	0
5	GLC	A	742	11/12	0.95	0.14	0.43	22,23,29,34	0
5	GLC	A	744	11/12	0.96	0.14	0.40	24,27,29,35	0
5	GLC	A	741	11/12	0.82	0.16	-	40,43,51,52	0
5	BGC	A	746	12/12	0.84	0.19	-	48,58,60,61	0
5	GLC	A	745	11/12	0.96	0.12	-	35,40,43,45	0

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, 95th 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
6	EDO	A	930	4/4	0.89	0.22	13.48	53,57,57,59	0
6	EDO	B	920	4/4	0.84	0.24	9.19	53,53,54,55	0
6	EDO	A	900	4/4	0.92	0.18	5.13	45,46,47,49	0
4	CEY	A	730	67/67	0.91	0.14	4.79	30,50,65,68	0
4	CEY	B	830	67/67	0.80	0.21	2.86	51,63,75,76	0
4	CEY	B	840	67/67	0.83	0.19	2.23	32,47,70,72	0
6	EDO	A	910	4/4	0.93	0.14	1.05	41,42,43,43	0
2	CA	A	700	1/1	0.98	0.10	1.03	31,31,31,31	0
3	CEX	A	720	56/56	0.90	0.13	0.55	27,41,65,66	1
3	CEX	B	820	56/56	0.93	0.14	0.44	22,43,70,71	0
2	CA	B	800	1/1	0.97	0.09	-0.85	37,37,37,37	0
2	CA	B	810	1/1	0.99	0.08	-2.11	29,29,29,29	0
2	CA	A	710	1/1	0.99	0.07	-3.81	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.