Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:46 AM GMT

PDB ID	:	2EBS
Title	:	Crystal Structure Anaalysis of Oligoxyloglucan reducing-end-specific cellobiohydrolase (OXG-RCBH) D465N Mutant Complexed with a Xyloglucan Heptasaccharide
Authors	:	Yaoi, K.; Kondo, H.; Hiyoshi, A.; Noro, N.; Sugimoto, H.; Miyazaki, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-02-09
Resolution	:	2.40 Å(reported)

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

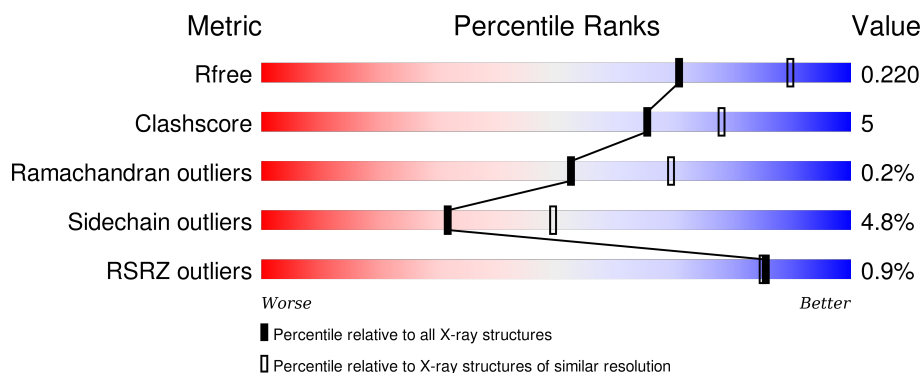|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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		0.220
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		4.8%
RSRZ outliers		0.9%

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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	789	2% 87% 10% ··
1	B	789	84% 12% ··

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12931 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 Oligoxyloglucan reducing end-specific cellobiohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	770	Total 5853	C 3699	N 993	O 1142	S 19	0	0	0
1	B	771	Total 5856	C 3702	N 995	O 1140	S 19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	465	ASN	ASP	ENGINEERED	UNP Q8J0D2
B	465	ASN	ASP	ENGINEERED	UNP Q8J0D2

- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	7	Total 72	C 39	O 33	0	0
2	B	7	Total 72	C 39	O 33	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	510	Total 510	O 510	0	0
3	B	568	Total 568	O 568	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: Oligoxyloglucan reducing end-specific cellobiohydrolase
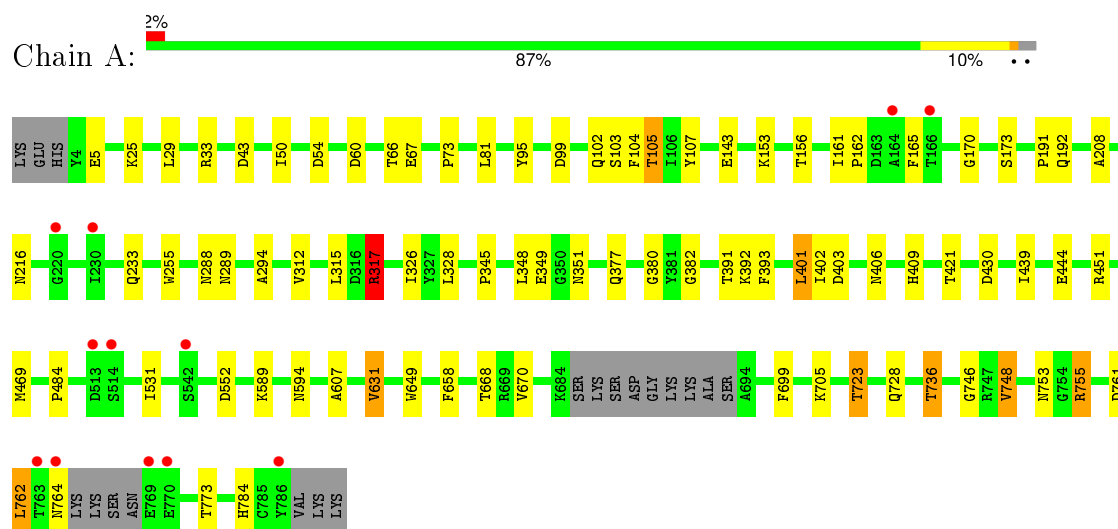
- Molecule 1: Oligoxyloglucan reducing end-specific cellobiohydrolase
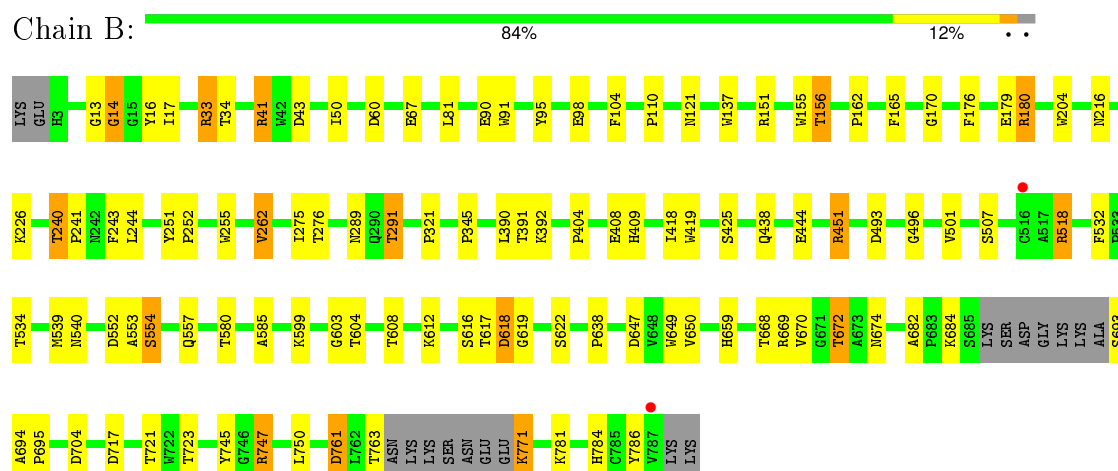
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.97Å 147.51Å 212.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 39.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (20.00-2.40) 95.0 (39.14-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.79 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.159 , 0.219 0.161 , 0.220	Depositor DCC
R_{free} test set	3641 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 72179 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12931	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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, XYS

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	0.63	0/6032	0.71	1/8248 (0.0%)
1	B	0.66	0/6036	0.72	6/8254 (0.1%)
All	All	0.64	0/12068	0.72	7/16502 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	14	GLY	N-CA-C	-10.34	87.26	113.10
1	A	317	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	151	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	33	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	B	33	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	451	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	244	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	13	GLY	Peptide

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	5853	0	5492	44	0
1	B	5856	0	5500	71	0
2	A	72	0	60	1	0
2	B	72	0	60	1	0
3	A	510	0	0	8	0
3	B	568	0	0	17	0
All	All	12931	0	11112	114	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 5.

All (114) 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:216:ASN:HB2	3:A:1295:HOH:O	1.59	1.00
1:B:612:LYS:HG3	3:B:1232:HOH:O	1.62	0.99
1:B:216:ASN:HB2	3:B:1336:HOH:O	1.66	0.95
1:A:736:THR:HG21	3:A:934:HOH:O	1.67	0.94
1:B:669:ARG:HD3	3:B:1344:HOH:O	1.72	0.88
1:A:43:ASP:HB2	1:A:50:ILE:HD11	1.58	0.85
1:B:289:ASN:HB2	3:B:1276:HOH:O	1.80	0.79
1:A:43:ASP:HB2	1:A:50:ILE:CD1	2.14	0.77
1:A:105:THR:HG22	3:A:1223:HOH:O	1.87	0.74
1:B:747:ARG:HD3	1:B:761:ASP:OD1	1.87	0.74
1:B:647:ASP:OD1	1:B:659:HIS:HE1	1.70	0.73
1:A:649:TRP:HZ3	1:A:670:VAL:HG21	1.55	0.71
1:A:631:VAL:HG13	1:A:658:PHE:CZ	2.26	0.70
1:B:771:LYS:N	3:B:865:HOH:O	2.25	0.70
1:A:60:ASP:OD1	1:A:784:HIS:HD2	1.75	0.69
1:A:294:ALA:O	1:A:317:ARG:HD3	1.94	0.68
1:B:518:ARG:HD3	1:B:539:MET:O	1.95	0.67
1:B:60:ASP:OD1	1:B:784:HIS:HD2	1.79	0.66
1:B:557:GLN:NE2	1:B:603:GLY:HA2	2.12	0.65
1:B:345:PRO:HG2	1:B:390:LEU:HD21	1.79	0.65
1:B:262:VAL:HG22	1:B:275:ILE:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:ASP:OD2	1:B:721:THR:HB	1.98	0.63
1:B:672:THR:HG22	3:B:1175:HOH:O	1.99	0.63
1:B:240:THR:CG2	3:B:950:HOH:O	2.47	0.62
1:B:156:THR:HG22	3:B:938:HOH:O	2.00	0.61
1:B:291:THR:HG23	1:B:321:PRO:O	2.02	0.60
1:B:391:THR:HG22	1:B:392:LYS:O	2.02	0.60
1:B:240:THR:HG22	1:B:243:PHE:H	1.65	0.60
1:B:674:ASN:ND2	3:B:1201:HOH:O	2.34	0.60
1:A:54:ASP:OD1	1:A:755:ARG:HD3	2.02	0.60
1:B:557:GLN:HE22	1:B:603:GLY:HA2	1.67	0.60
1:A:351:ASN:ND2	3:A:859:HOH:O	2.34	0.59
1:A:444:GLU:HG2	1:A:444:GLU:O	2.03	0.59
1:A:107:TYR:CZ	1:A:153:LYS:HG2	2.39	0.58
1:A:631:VAL:HG13	1:A:658:PHE:HZ	1.69	0.57
1:B:553:ALA:O	1:B:554:SER:CB	2.53	0.56
1:B:649:TRP:HZ3	1:B:670:VAL:HG21	1.72	0.54
1:B:608:THR:HG23	1:B:638:PRO:HG3	1.89	0.53
1:B:60:ASP:OD1	1:B:784:HIS:CD2	2.60	0.52
1:B:781:LYS:HE3	3:B:1351:HOH:O	2.10	0.52
1:B:638:PRO:HB3	1:B:650:VAL:HG22	1.91	0.52
1:B:43:ASP:HB2	1:B:50:ILE:HD12	1.91	0.52
1:A:649:TRP:CZ3	1:A:670:VAL:HG21	2.42	0.51
1:B:98:GLU:HA	1:B:98:GLU:OE1	2.10	0.51
1:A:401:LEU:HD22	1:A:402:ILE:O	2.11	0.50
1:B:180:ARG:HD3	3:B:1022:HOH:O	2.09	0.50
1:B:585:ALA:O	1:B:622:SER:HA	2.11	0.50
1:B:672:THR:HG23	1:B:704:ASP:O	2.12	0.50
1:B:162:PRO:HD3	1:B:204:TRP:HB2	1.94	0.50
1:B:451:ARG:HD2	1:B:493:ASP:HA	1.94	0.49
1:A:377:GLN:HG2	1:A:382:GLY:HA2	1.93	0.49
1:A:723:THR:HG22	3:A:1219:HOH:O	2.11	0.49
1:B:618:ASP:OD2	1:B:622:SER:OG	2.20	0.49
1:B:240:THR:HG23	1:B:241:PRO:HD2	1.95	0.49
1:B:17:ILE:HG13	1:B:418:ILE:HG13	1.95	0.48
1:A:345:PRO:HG2	1:A:348:LEU:HD11	1.95	0.48
1:B:404:PRO:HA	3:B:1363:HOH:O	2.12	0.48
1:B:694:ALA:HB1	1:B:695:PRO:HD2	1.95	0.48
1:B:90:GLU:HG3	1:B:91:TRP:HD1	1.79	0.48
1:A:380:GLY:HA2	3:A:1189:HOH:O	2.13	0.47
1:A:326:ILE:HD12	1:A:393:PHE:HE2	1.79	0.47
1:A:746:GLY:HA3	1:A:762:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ASP:HB3	1:A:406:ASN:O	2.14	0.47
1:B:682:ALA:HB3	1:B:745:TYR:HA	1.97	0.47
1:A:255:TRP:CD1	2:A:795:XYS:H51	2.50	0.47
1:B:262:VAL:HG13	1:B:276:THR:HA	1.96	0.46
1:B:540:ASN:HB2	3:B:1241:HOH:O	2.16	0.46
1:B:617:THR:O	1:B:617:THR:HG22	2.15	0.46
1:B:747:ARG:NH1	1:B:761:ASP:OD2	2.48	0.46
1:A:33:ARG:HB2	1:A:66:THR:HB	1.98	0.46
1:B:95:TYR:HB3	1:B:104:PHE:CD1	2.50	0.45
1:B:251:TYR:CG	1:B:252:PRO:HD2	2.51	0.45
1:A:25:LYS:HD2	1:A:73:PRO:O	2.16	0.45
1:B:110:PRO:HG3	1:B:155:TRP:HB2	1.98	0.45
1:A:99:ASP:HB2	1:A:102:GLN:HE21	1.82	0.45
1:A:439:ILE:HG13	1:A:439:ILE:O	2.17	0.45
1:B:16:TYR:OH	1:B:121:ASN:HB3	2.17	0.45
1:B:444:GLU:O	1:B:444:GLU:HG2	2.17	0.45
1:B:156:THR:CG2	3:B:938:HOH:O	2.60	0.45
1:A:161:ILE:HA	1:A:162:PRO:HD3	1.78	0.45
1:B:604:THR:HA	1:B:616:SER:O	2.16	0.44
1:B:240:THR:HG23	3:B:950:HOH:O	2.13	0.44
1:A:43:ASP:HB2	1:A:50:ILE:HD12	1.96	0.44
1:A:43:ASP:CB	1:A:50:ILE:HD11	2.38	0.44
1:B:41:ARG:NH2	3:B:1153:HOH:O	2.51	0.44
1:B:81:LEU:HB2	1:B:95:TYR:HB2	2.01	0.43
1:B:496:GLY:HA3	1:B:599:LYS:O	2.17	0.43
1:B:43:ASP:HB2	1:B:50:ILE:CD1	2.49	0.43
1:A:165:PHE:O	1:A:170:GLY:HA2	2.19	0.43
1:B:255:TRP:CD1	2:B:795:XYS:H51	2.53	0.43
1:A:699:PHE:CE2	1:A:748:VAL:HG22	2.54	0.43
1:A:409:HIS:HA	1:A:421:THR:O	2.18	0.43
1:A:191:PRO:HD3	1:A:233:GLN:OE1	2.18	0.43
1:A:103:SER:HA	1:A:773:THR:O	2.19	0.43
1:B:391:THR:HG21	1:B:419:TRP:HZ2	1.84	0.42
1:A:736:THR:HG22	3:A:874:HOH:O	2.18	0.42
1:B:137:TRP:CD1	1:B:176:PHE:HZ	2.38	0.42
1:A:728:GLN:HG2	3:A:1192:HOH:O	2.18	0.42
1:B:672:THR:CG2	3:B:1175:HOH:O	2.63	0.42
1:A:484:PRO:HD3	1:A:531:ILE:HG12	2.02	0.42
1:A:60:ASP:OD1	1:A:784:HIS:CD2	2.65	0.41
1:A:391:THR:HG22	1:A:392:LYS:O	2.20	0.41
1:B:409:HIS:CE1	1:B:438:GLN:HE22	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:TRP:CZ3	1:B:670:VAL:HG21	2.53	0.41
1:B:251:TYR:CD1	1:B:252:PRO:HD2	2.55	0.41
1:B:34:THR:HB	1:B:444:GLU:OE2	2.21	0.41
1:B:165:PHE:O	1:B:170:GLY:HA2	2.21	0.41
1:A:95:TYR:HB3	1:A:104:PHE:CD1	2.56	0.41
1:A:594:ASN:O	1:A:607:ALA:HA	2.21	0.41
1:B:408:GLU:OE1	1:B:425:SER:HB2	2.20	0.41
1:B:557:GLN:NE2	1:B:619:GLY:HA3	2.36	0.40
1:A:208:ALA:HB2	1:B:180:ARG:NH2	2.35	0.40
1:B:91:TRP:CG	1:B:786:TYR:HB2	2.56	0.40
1:B:532:PHE:HB3	1:B:534:THR:O	2.21	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	764/789 (97%)	730 (96%)	33 (4%)	1 (0%)	56 74
1	B	765/789 (97%)	731 (96%)	32 (4%)	2 (0%)	46 63
All	All	1529/1578 (97%)	1461 (96%)	65 (4%)	3 (0%)	52 69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	B	554	SER
1	B	14	GLY

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	608/625 (97%)	576 (95%)	32 (5%)	28	44
1	B	609/625 (97%)	583 (96%)	26 (4%)	35	55
All	All	1217/1250 (97%)	1159 (95%)	58 (5%)	31	49

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	29	LEU
1	A	67	GLU
1	A	81	LEU
1	A	105	THR
1	A	143	GLU
1	A	156	THR
1	A	173	SER
1	A	192	GLN
1	A	288	ASN
1	A	312	VAL
1	A	315	LEU
1	A	317	ARG
1	A	328	LEU
1	A	349	GLU
1	A	401	LEU
1	A	430	ASP
1	A	451	ARG
1	A	469	MET
1	A	552	ASP
1	A	589	LYS
1	A	631	VAL
1	A	668	THR
1	A	705	LYS
1	A	723	THR
1	A	736	THR
1	A	748	VAL

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Mol	Chain	Res	Type
1	A	753	ASN
1	A	755	ARG
1	A	761	ASP
1	A	762	LEU
1	A	764	ASN
1	B	33	ARG
1	B	41	ARG
1	B	67	GLU
1	B	156	THR
1	B	179	GLU
1	B	180	ARG
1	B	226	LYS
1	B	240	THR
1	B	262	VAL
1	B	291	THR
1	B	501	VAL
1	B	507	SER
1	B	518	ARG
1	B	552	ASP
1	B	580	THR
1	B	618	ASP
1	B	668	THR
1	B	672	THR
1	B	684	LYS
1	B	693	SER
1	B	723	THR
1	B	747	ARG
1	B	750	LEU
1	B	761	ASP
1	B	763	THR
1	B	771	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	192	GLN
1	A	198	HIS
1	A	242	ASN
1	A	465	ASN
1	A	753	ASN
1	A	784	HIS

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Mol	Chain	Res	Type
1	B	3	HIS
1	B	216	ASN
1	B	288	ASN
1	B	438	GLN
1	B	465	ASN
1	B	557	GLN
1	B	659	HIS
1	B	674	ASN
1	B	718	ASN
1	B	728	GLN
1	B	784	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

14 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
2	BGC	A	790	2	11,11,12	0.74	0	14,15,17	1.07	1 (7%)
2	XYS	A	791	2	9,9,10	1.29	1 (11%)	12,12,14	1.59	1 (8%)
2	BGC	A	792	2	11,11,12	0.63	0	14,15,17	2.67	4 (28%)
2	XYS	A	793	2	9,9,10	1.39	1 (11%)	12,12,14	1.73	2 (16%)
2	BGC	A	794	2	11,11,12	0.70	0	14,15,17	1.18	2 (14%)
2	XYS	A	795	2	9,9,10	1.31	1 (11%)	12,12,14	1.42	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	BGC	A	796	2	12,12,12	0.53	0	17,17,17	1.08	3 (17%)
2	BGC	B	790	2	11,11,12	0.85	1 (9%)	14,15,17	1.05	1 (7%)
2	XYS	B	791	2	9,9,10	1.11	1 (11%)	12,12,14	1.87	4 (33%)
2	BGC	B	792	2	11,11,12	0.72	0	14,15,17	3.05	3 (21%)
2	XYS	B	793	2	9,9,10	1.25	1 (11%)	12,12,14	0.77	0
2	BGC	B	794	2	11,11,12	0.67	0	14,15,17	0.81	0
2	XYS	B	795	2	9,9,10	1.16	1 (11%)	12,12,14	1.63	2 (16%)
2	BGC	B	796	2	12,12,12	0.52	0	17,17,17	1.32	1 (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	BGC	A	790	2	-	0/2/19/22	0/1/1/1
2	XYS	A	791	2	-	0/0/14/17	0/1/1/1
2	BGC	A	792	2	-	0/2/19/22	0/1/1/1
2	XYS	A	793	2	-	0/0/14/17	0/1/1/1
2	BGC	A	794	2	-	0/2/19/22	0/1/1/1
2	XYS	A	795	2	-	0/0/14/17	0/1/1/1
2	BGC	A	796	2	-	0/2/22/22	0/1/1/1
2	BGC	B	790	2	-	0/2/19/22	0/1/1/1
2	XYS	B	791	2	-	0/0/14/17	0/1/1/1
2	BGC	B	792	2	-	0/2/19/22	0/1/1/1
2	XYS	B	793	2	-	0/0/14/17	0/1/1/1
2	BGC	B	794	2	-	0/2/19/22	0/1/1/1
2	XYS	B	795	2	-	0/0/14/17	0/1/1/1
2	BGC	B	796	2	-	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)
2	A	793	XYS	O5-C1	-3.56	1.36	1.42
2	A	795	XYS	O5-C1	-3.34	1.36	1.42
2	B	793	XYS	O5-C1	-3.26	1.36	1.42
2	B	795	XYS	O5-C1	-3.01	1.37	1.42
2	A	791	XYS	O5-C1	-2.79	1.37	1.42
2	B	791	XYS	O5-C1	-2.17	1.38	1.42
2	B	790	BGC	O2-C2	-2.01	1.38	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	793	XYS	C4-C3-C2	-4.09	107.20	111.24
2	A	795	XYS	C4-C3-C2	-3.58	107.70	111.24
2	B	796	BGC	C1-C2-C3	-3.44	105.31	110.43
2	B	791	XYS	O4-C4-C3	-2.32	105.46	110.12
2	A	796	BGC	C1-C2-C3	-2.19	107.17	110.43
2	A	796	BGC	O4-C4-C3	-2.14	105.53	110.34
2	A	792	BGC	C3-C4-C5	-2.04	106.64	110.20
2	A	794	BGC	C1-C2-C3	2.02	111.93	109.54
2	A	796	BGC	O5-C5-C6	2.08	111.61	106.36
2	B	795	XYS	C5-C4-C3	2.11	112.04	109.54
2	A	795	XYS	C5-O5-C1	2.16	115.06	111.57
2	B	790	BGC	C1-C2-C3	2.18	112.12	109.54
2	A	790	BGC	C1-O5-C5	2.25	115.10	112.25
2	B	791	XYS	C5-O5-C1	2.31	115.30	111.57
2	A	794	BGC	C1-O5-C5	2.49	115.40	112.25
2	B	791	XYS	O5-C5-C4	2.69	115.34	110.31
2	A	792	BGC	C1-C2-C3	2.84	112.90	109.54
2	A	793	XYS	C5-O5-C1	3.10	116.56	111.57
2	B	792	BGC	O5-C1-C2	3.78	117.00	110.86
2	B	791	XYS	C5-C4-C3	3.95	114.22	109.54
2	B	795	XYS	C5-O5-C1	4.26	118.44	111.57
2	A	791	XYS	C5-C4-C3	4.42	114.78	109.54
2	A	792	BGC	O5-C1-C2	4.54	118.23	110.86
2	B	792	BGC	C1-C2-C3	5.57	116.13	109.54
2	A	792	BGC	C1-O5-C5	7.84	122.20	112.25
2	B	792	BGC	C1-O5-C5	9.00	123.67	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	795	XYS	1	0
2	B	795	XYS	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	770/789 (97%)	-0.40	12 (1%)	74	74	12, 22, 32, 51	0
1	B	771/789 (97%)	-0.56	2 (0%)	94	94	10, 20, 33, 44	0
All	All	1541/1578 (97%)	-0.48	14 (0%)	85	85	10, 21, 33, 51	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	770	GLU	3.5
1	A	764	ASN	3.3
1	A	763	THR	3.0
1	A	166	THR	2.8
1	A	514	SER	2.8
1	B	787	VAL	2.4
1	A	164	ALA	2.3
1	A	513	ASP	2.3
1	A	230	ILE	2.3
1	B	516	CYS	2.2
1	A	769	GLU	2.0
1	A	220	GLY	2.0
1	A	542	SER	2.0
1	A	786	TYR	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
2	BGC	A	792	11/12	0.96	0.15	0.13	18,20,21,22	0
2	BGC	B	796	12/12	0.98	0.10	-0.32	15,17,20,20	0
2	BGC	A	796	12/12	0.97	0.09	-0.74	13,17,19,20	0
2	BGC	B	792	11/12	0.97	0.12	-0.86	14,17,20,20	0
2	BGC	A	790	11/12	0.97	0.10	-0.86	20,21,27,34	0
2	BGC	A	794	11/12	0.97	0.10	-1.20	17,18,20,20	0
2	BGC	B	790	11/12	0.97	0.10	-1.80	14,20,25,29	0
2	BGC	B	794	11/12	0.98	0.09	-2.67	19,19,21,21	0
2	XYS	A	793	9/10	0.98	0.10	-	16,18,19,19	0
2	XYS	B	791	9/10	0.85	0.18	-	28,33,36,36	0
2	XYS	A	791	9/10	0.85	0.17	-	43,44,45,47	0
2	XYS	B	795	9/10	0.98	0.09	-	20,21,23,23	0
2	XYS	A	795	9/10	0.98	0.09	-	19,21,22,22	0
2	XYS	B	793	9/10	0.97	0.10	-	14,15,16,18	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.