Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:41 PM GMT

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PDB ID	:	4A5T
Title	:	STRUCTURAL BASIS FOR THE CONFORMATIONAL MODULATION
Authors	:	Xue, Y.; Bodin, C.; Olsson, K.
Deposited on	:	2011-10-28
Resolution	:	3.49 Å(reported)

1 Overall quality at a glance ⓘ

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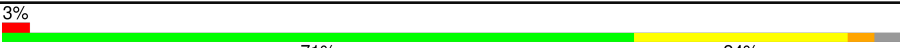*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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.
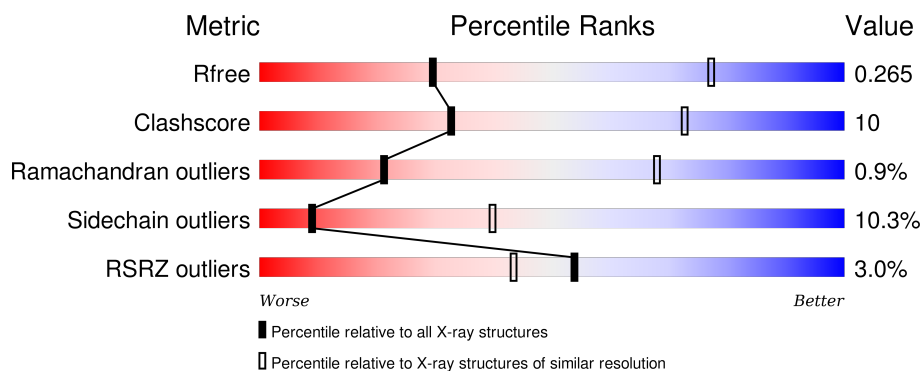
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	S	791	3% red; 71% green; 24% yellow; orange dot; grey dot

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6073 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 PLASMINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	S	767	6026	3742	1075	1151	58	0	0	0

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	S	3	45	25	2	18	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	S	2	2	2	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: PLASMINOGEN
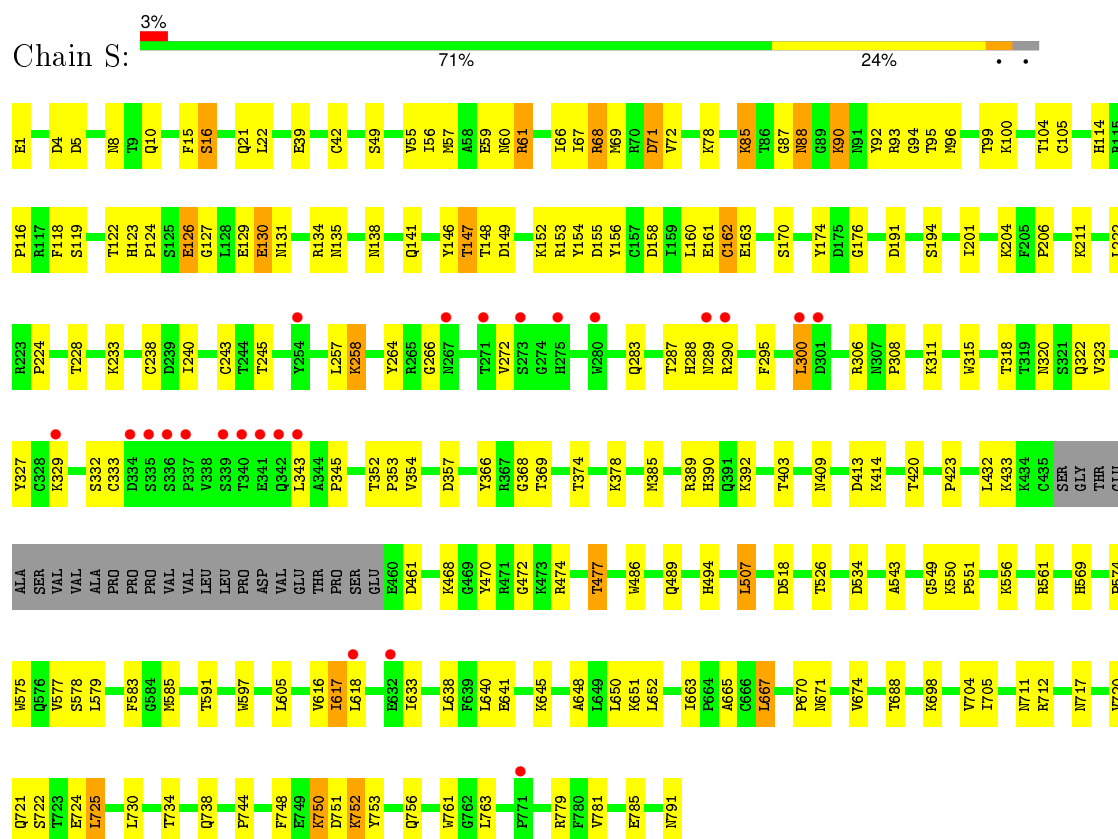
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	118.46Å 118.46Å 179.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.80 – 3.49 49.41 – 3.49	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.80-3.49) 95.3 (49.41-3.49)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.97 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.208 , 0.250 0.229 , 0.265	Depositor DCC
R_{free} test set	809 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	75.3	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.43$, $<L^2> = 0.26$	Xtriage
Outliers	0 of 16059 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6073	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: SIA, GAL, NGA, CL

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	S	0.39	0/6199	0.69	0/8428

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	S	6026	0	5690	121	0
2	S	45	0	38	2	0
3	S	2	0	0	2	0
All	All	6073	0	5728	123	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 10.

All (123) 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:S:409:ASN:HD21	1:S:413:ASP:H	1.14	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:206:PRO:HB2	1:S:423:PRO:HD2	1.54	0.90
1:S:224:PRO:HD2	1:S:240:ILE:HD13	1.55	0.86
1:S:147:THR:HG23	1:S:149:ASP:H	1.42	0.85
1:S:354:VAL:HG21	1:S:753:TYR:HE2	1.42	0.84
1:S:320:ASN:HB3	1:S:323:VAL:HG22	1.61	0.83
1:S:206:PRO:HB2	1:S:423:PRO:CD	2.09	0.81
1:S:99:THR:HG21	1:S:155:ASP:HB3	1.66	0.76
1:S:283:GLN:HE22	1:S:288:HIS:H	1.33	0.76
1:S:711:ASN:HD21	1:S:720:VAL:H	1.34	0.75
1:S:105:CYS:O	1:S:148:THR:HG23	1.87	0.75
1:S:354:VAL:HG21	1:S:753:TYR:CE2	2.22	0.74
1:S:147:THR:CG2	1:S:149:ASP:H	2.00	0.73
1:S:390:HIS:HD2	1:S:392:LYS:H	1.37	0.73
1:S:318:THR:OG1	1:S:323:VAL:HG23	1.91	0.70
1:S:597:TRP:CZ2	1:S:651:LYS:HD2	2.27	0.69
1:S:222:LEU:HD22	1:S:295:PHE:CZ	2.27	0.69
1:S:671:ASN:HD22	1:S:779:ARG:HD2	1.59	0.68
1:S:489:GLN:HE22	1:S:494:HIS:H	1.41	0.68
1:S:385:MET:HB3	1:S:389:ARG:HG2	1.78	0.65
1:S:90:LYS:HG2	1:S:138:ASN:HD22	1.62	0.64
1:S:114:HIS:CE1	1:S:153:ARG:HA	2.33	0.63
1:S:671:ASN:ND2	1:S:779:ARG:HD2	2.14	0.62
1:S:122:THR:HG22	1:S:123:HIS:CE1	2.35	0.62
1:S:311:LYS:HD3	1:S:315:TRP:NE1	2.14	0.61
1:S:160:LEU:N	1:S:160:LEU:HD12	2.16	0.61
1:S:352:THR:HG23	1:S:748:PHE:HE2	1.68	0.59
1:S:238:CYS:HB2	1:S:240:ILE:HD11	1.86	0.58
1:S:122:THR:C	1:S:124:PRO:HD3	2.24	0.58
1:S:141:GLN:HB2	1:S:156:TYR:CE2	2.38	0.57
1:S:222:LEU:CD2	1:S:295:PHE:CZ	2.87	0.57
1:S:641:GLU:O	1:S:645:LYS:HA	2.05	0.57
1:S:147:THR:CG2	1:S:149:ASP:HB3	2.36	0.56
1:S:272:VAL:HG22	1:S:329:LYS:HB2	1.86	0.56
1:S:222:LEU:CD2	1:S:295:PHE:HZ	2.20	0.55
1:S:550:LYS:HG3	1:S:752:LYS:HB3	1.89	0.55
1:S:68:ARG:HB3	3:S:1001:CL:CL	2.45	0.54
1:S:409:ASN:ND2	1:S:413:ASP:H	1.94	0.54
1:S:122:THR:CG2	1:S:123:HIS:CE1	2.90	0.53
1:S:1:GLU:HB3	1:S:4:ASP:HB2	1.90	0.53
1:S:272:VAL:HG23	1:S:327:TYR:O	2.09	0.53
1:S:781:VAL:O	1:S:785:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:123:HIS:HB3	1:S:126:GLU:HG2	1.91	0.53
1:S:85:LYS:O	1:S:162:CYS:HB2	2.09	0.52
1:S:92:TYR:CZ	1:S:94:GLY:HA3	2.45	0.51
1:S:409:ASN:HD21	1:S:413:ASP:N	1.95	0.51
1:S:21:GLN:HG3	1:S:55:VAL:HG22	1.92	0.51
1:S:605:LEU:HD13	1:S:638:LEU:HG	1.93	0.51
1:S:357:ASP:HB3	1:S:432:LEU:HD21	1.92	0.51
1:S:288:HIS:HD2	1:S:290:ARG:H	1.59	0.50
1:S:257:LEU:HB3	1:S:332:SER:HA	1.93	0.50
1:S:633:ILE:HG21	1:S:652:LEU:HB3	1.94	0.50
1:S:705:ILE:HD12	1:S:730:LEU:HD11	1.92	0.50
1:S:651:LYS:NZ	1:S:791:ASN:O	2.45	0.49
1:S:118:PHE:CD1	1:S:123:HIS:CE1	3.00	0.49
1:S:674:VAL:HG11	1:S:704:VAL:HG21	1.94	0.49
1:S:320:ASN:HB3	1:S:323:VAL:CG2	2.40	0.49
1:S:725:LEU:C	1:S:725:LEU:HD23	2.32	0.49
1:S:160:LEU:CD1	1:S:160:LEU:N	2.75	0.48
1:S:152:LYS:HD2	1:S:154:TYR:O	2.14	0.47
1:S:116:PRO:HB3	1:S:146:TYR:CE2	2.48	0.47
1:S:489:GLN:NE2	1:S:494:HIS:H	2.09	0.47
1:S:734:THR:HG21	1:S:738:GLN:HE22	1.80	0.47
1:S:127:GLY:O	1:S:129:GLU:HG2	2.15	0.47
1:S:578:SER:HB3	1:S:617:ILE:HG22	1.97	0.47
1:S:354:VAL:HG11	1:S:551:PRO:HD2	1.95	0.47
1:S:670:PRO:HA	1:S:781:VAL:CG1	2.45	0.47
1:S:549:GLY:HA2	1:S:575:TRP:CZ3	2.49	0.47
1:S:42:CYS:SG	1:S:56:ILE:HG23	2.56	0.46
1:S:222:LEU:HD11	1:S:289:ASN:HB3	1.97	0.46
1:S:147:THR:HG22	1:S:149:ASP:O	2.16	0.46
1:S:390:HIS:HD2	1:S:392:LYS:N	2.08	0.45
1:S:323:VAL:O	1:S:323:VAL:HG23	2.16	0.45
1:S:138:ASN:O	1:S:138:ASN:CG	2.55	0.45
1:S:118:PHE:HD1	1:S:123:HIS:CE1	2.34	0.45
1:S:300:LEU:HD11	1:S:308:PRO:HB3	1.98	0.45
1:S:390:HIS:CD2	1:S:392:LYS:H	2.27	0.45
1:S:138:ASN:O	1:S:138:ASN:OD1	2.34	0.45
1:S:352:THR:HA	1:S:353:PRO:HD3	1.94	0.45
1:S:591:THR:OG1	1:S:744:PRO:HB3	2.17	0.44
1:S:477:THR:OG1	1:S:534:ASP:HB3	2.17	0.44
1:S:88:ASN:OD1	1:S:135:ASN:ND2	2.51	0.44
2:S:899:SIA:H8	2:S:899:SIA:H32	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:577:VAL:HG22	1:S:618:LEU:CD2	2.48	0.44
1:S:174:TYR:CZ	1:S:176:GLY:HA3	2.52	0.44
1:S:470:TYR:CZ	1:S:472:GLY:HA3	2.52	0.44
1:S:206:PRO:CB	1:S:423:PRO:HD2	2.36	0.44
1:S:104:THR:HG22	1:S:105:CYS:O	2.18	0.44
1:S:147:THR:CG2	1:S:149:ASP:N	2.76	0.43
1:S:366:TYR:CZ	1:S:368:GLY:HA3	2.53	0.43
1:S:61:ARG:HB3	1:S:66:ILE:HD11	2.00	0.43
1:S:670:PRO:HA	1:S:781:VAL:HG11	2.01	0.43
1:S:577:VAL:CG1	1:S:616:VAL:HG13	2.48	0.43
1:S:574:PRO:HB2	1:S:663:ILE:H	1.83	0.43
1:S:153:ARG:NH2	3:S:1002:CL:CL	2.82	0.43
1:S:577:VAL:HG13	1:S:616:VAL:HG13	1.99	0.43
1:S:264:TYR:CZ	1:S:266:GLY:HA3	2.54	0.43
1:S:756:GLN:HA	1:S:756:GLN:HE21	1.84	0.43
1:S:258:LYS:HG2	1:S:333:CYS:SG	2.59	0.43
1:S:575:TRP:CG	1:S:665:ALA:HB2	2.53	0.42
1:S:461:ASP:O	1:S:474:ARG:NH1	2.52	0.42
1:S:551:PRO:HD3	1:S:575:TRP:CH2	2.55	0.42
1:S:413:ASP:OD1	1:S:414:LYS:N	2.37	0.42
1:S:616:VAL:HG11	1:S:652:LEU:HD21	2.02	0.42
2:S:899:SIA:H4	2:S:899:SIA:H112	2.00	0.42
1:S:71:ASP:OD1	1:S:72:VAL:N	2.53	0.42
1:S:16:SER:HB2	1:S:59:GLU:CD	2.40	0.42
1:S:711:ASN:ND2	1:S:720:VAL:H	2.10	0.42
1:S:93:ARG:HE	1:S:134:ARG:HD2	1.84	0.42
1:S:201:ILE:HG23	1:S:204:LYS:HG3	2.02	0.41
1:S:147:THR:HG21	1:S:149:ASP:HB3	2.01	0.41
1:S:288:HIS:HD2	1:S:290:ARG:N	2.19	0.41
1:S:667:LEU:HD12	1:S:667:LEU:HA	1.89	0.41
1:S:640:LEU:HD23	1:S:648:ALA:HB2	2.02	0.41
1:S:722:SER:C	1:S:724:GLU:H	2.23	0.41
1:S:90:LYS:HD2	1:S:90:LYS:HA	1.72	0.41
1:S:486:TRP:CD2	1:S:507:LEU:HG	2.56	0.41
1:S:357:ASP:HB3	1:S:432:LEU:CD2	2.50	0.40
1:S:318:THR:HG1	1:S:323:VAL:HG23	1.85	0.40
1:S:129:GLU:H	1:S:129:GLU:HG2	1.69	0.40
1:S:130:GLU:HB3	1:S:131:ASN:H	1.72	0.40
1:S:283:GLN:NE2	1:S:287:THR:HA	2.37	0.40
1:S:579:LEU:HD21	1:S:650:LEU:CD1	2.52	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	S	763/791 (96%)	700 (92%)	56 (7%)	7 (1%)	21 68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	717	ASN
1	S	163	GLU
1	S	750	LYS
1	S	345	PRO
1	S	761	TRP
1	S	87	GLY
1	S	543	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	S	673/694 (97%)	604 (90%)	69 (10%)	9 40

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	5	ASP
1	S	8	ASN
1	S	10	GLN
1	S	15	PHE

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Mol	Chain	Res	Type
1	S	16	SER
1	S	22	LEU
1	S	39	GLU
1	S	49	SER
1	S	57	MET
1	S	60	ASN
1	S	61	ARG
1	S	67	ILE
1	S	68	ARG
1	S	69	MET
1	S	71	ASP
1	S	78	LYS
1	S	85	LYS
1	S	88	ASN
1	S	90	LYS
1	S	95	THR
1	S	96	MET
1	S	100	LYS
1	S	119	SER
1	S	126	GLU
1	S	130	GLU
1	S	147	THR
1	S	158	ASP
1	S	161	GLU
1	S	162	CYS
1	S	170	SER
1	S	191	ASP
1	S	194	SER
1	S	211	LYS
1	S	228	THR
1	S	233	LYS
1	S	243	CYS
1	S	245	THR
1	S	258	LYS
1	S	300	LEU
1	S	306	ARG
1	S	322	GLN
1	S	343	LEU
1	S	369	THR
1	S	374	THR
1	S	378	LYS
1	S	403	THR

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Mol	Chain	Res	Type
1	S	420	THR
1	S	433	LYS
1	S	468	LYS
1	S	477	THR
1	S	507	LEU
1	S	518	ASP
1	S	526	THR
1	S	556	LYS
1	S	561	ARG
1	S	569	HIS
1	S	583	PHE
1	S	585	MET
1	S	617	ILE
1	S	667	LEU
1	S	688	THR
1	S	698	LYS
1	S	712	ARG
1	S	721	GLN
1	S	725	LEU
1	S	750	LYS
1	S	751	ASP
1	S	752	LYS
1	S	763	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	10	GLN
1	S	91	ASN
1	S	114	HIS
1	S	138	ASN
1	S	196	HIS
1	S	267	ASN
1	S	283	GLN
1	S	288	HIS
1	S	360	HIS
1	S	390	HIS
1	S	409	ASN
1	S	431	ASN
1	S	484	GLN
1	S	489	GLN
1	S	492	HIS

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Mol	Chain	Res	Type
1	S	571	HIS
1	S	576	GLN
1	S	603	HIS
1	S	671	ASN
1	S	711	ASN
1	S	738	GLN
1	S	756	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)

3 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	SIA	S	899	2	16,20,21	1.23	1 (6%)	18,28,31	2.37	9 (50%)
2	GAL	S	900	2	11,11,12	1.31	1 (9%)	14,15,17	3.17	9 (64%)
2	NGA	S	901	1,2	14,14,15	1.11	1 (7%)	15,19,21	3.29	6 (40%)

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	SIA	S	899	2	-	0/14/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	S	900	2	-	0/2/19/22	0/1/1/1
2	NGA	S	901	1,2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	901	NGA	C4-C3	2.03	1.57	1.52
2	S	900	GAL	C4-C3	2.51	1.59	1.52
2	S	899	SIA	C11-C10	2.85	1.56	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	901	NGA	C1-O5-C5	-8.50	101.46	112.25
2	S	900	GAL	C1-C2-C3	-7.90	100.19	109.54
2	S	900	GAL	O5-C1-C2	-4.50	103.56	110.86
2	S	899	SIA	C4-C5-N5	-2.19	105.65	110.41
2	S	899	SIA	O10-C10-N5	-2.01	117.76	121.86
2	S	900	GAL	C6-C5-C4	2.19	118.42	113.02
2	S	899	SIA	O8-C8-C9	2.22	114.40	109.22
2	S	901	NGA	O7-C7-C8	2.27	126.23	122.06
2	S	900	GAL	O3-C3-C2	2.29	114.13	110.00
2	S	899	SIA	O6-C2-C3	2.35	114.37	109.86
2	S	900	GAL	C2-C3-C4	2.35	115.03	111.04
2	S	900	GAL	O4-C4-C3	2.35	115.64	110.34
2	S	899	SIA	O7-C7-C8	2.44	114.89	108.75
2	S	900	GAL	O3-C3-C4	2.50	115.96	110.34
2	S	900	GAL	O4-C4-C5	2.54	115.97	109.24
2	S	899	SIA	C6-C5-N5	2.90	116.13	111.07
2	S	899	SIA	C5-N5-C10	3.33	131.65	123.10
2	S	901	NGA	C6-C5-C4	3.40	121.39	113.02
2	S	901	NGA	C2-N2-C7	3.97	128.14	123.04
2	S	901	NGA	O3-C3-C2	4.18	117.39	109.11
2	S	900	GAL	O2-C2-C1	4.31	117.86	109.21
2	S	899	SIA	O6-C6-C5	4.76	116.28	108.48
2	S	899	SIA	C3-C4-C5	4.83	116.86	111.47
2	S	901	NGA	C3-C2-N2	5.24	123.11	110.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	899	SIA	2	0

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	S	767/791 (96%)	0.19	23 (2%)	54	43	38, 90, 189, 215	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	343	LEU	4.3
1	S	300	LEU	3.9
1	S	342	GLN	3.8
1	S	275	HIS	3.6
1	S	336	SER	3.2
1	S	337	PRO	2.9
1	S	329	LYS	2.7
1	S	289	ASN	2.6
1	S	271	THR	2.5
1	S	280	TRP	2.5
1	S	340	THR	2.4
1	S	290	ARG	2.4
1	S	339	SER	2.3
1	S	273	SER	2.3
1	S	301	ASP	2.3
1	S	267	ASN	2.2
1	S	618	LEU	2.2
1	S	632	GLU	2.2
1	S	254	TYR	2.2
1	S	771	PRO	2.2
1	S	334	ASP	2.2
1	S	341	GLU	2.0
1	S	335	SER	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	NGA	S	901	14/15	0.93	0.20	-	104,104,106,106	0
2	GAL	S	900	11/12	0.83	0.16	-	103,106,112,116	0
2	SIA	S	899	20/21	0.84	0.24	-	112,112,114,114	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
3	CL	S	1001	1/1	0.92	0.22	-2.04	33,33,33,33	0
3	CL	S	1002	1/1	0.90	0.23	-	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.