Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:30 PM GMT

PDB ID	:	4F7C
Title	:	Crystal structure of bovine CD1d with bound C12-di-sulfatide
Authors	:	Wang, J.; Zajonc, D.M.
Deposited on	:	2012-05-15
Resolution	:	2.86 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

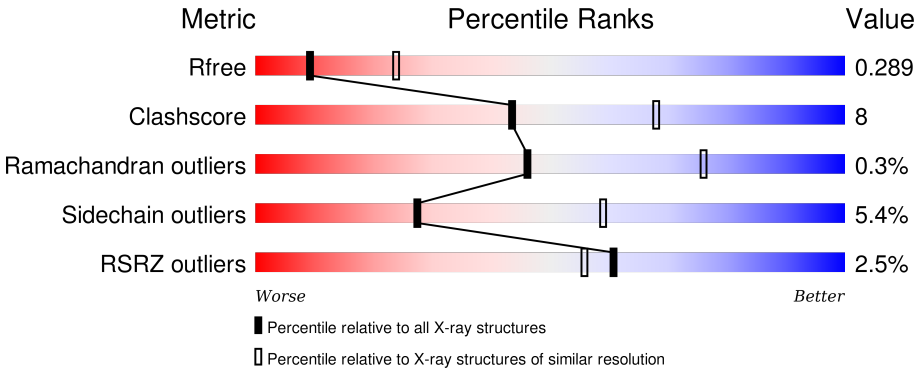
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.86 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	283	77% 14% • 5%
1	C	283	5% 74% 16% • 7%
2	B	98	80% 16% • •
2	D	98	81% 15% • •

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
5	0SG	C	308	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6216 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 CD1D antigen, d polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2176	1397	375	397	7			
1	C	263	Total	C	N	O	S	0	0	0
			2131	1370	368	386	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	HIS	-	EXPRESSION TAG	UNP A1L565
A	279	HIS	-	EXPRESSION TAG	UNP A1L565
A	280	HIS	-	EXPRESSION TAG	UNP A1L565
A	281	HIS	-	EXPRESSION TAG	UNP A1L565
A	282	HIS	-	EXPRESSION TAG	UNP A1L565
A	283	HIS	-	EXPRESSION TAG	UNP A1L565
C	278	HIS	-	EXPRESSION TAG	UNP A1L565
C	279	HIS	-	EXPRESSION TAG	UNP A1L565
C	280	HIS	-	EXPRESSION TAG	UNP A1L565
C	281	HIS	-	EXPRESSION TAG	UNP A1L565
C	282	HIS	-	EXPRESSION TAG	UNP A1L565
C	283	HIS	-	EXPRESSION TAG	UNP A1L565

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			811	520	141	148	2			
2	D	97	Total	C	N	O	S	0	0	0
			807	517	140	148	2			

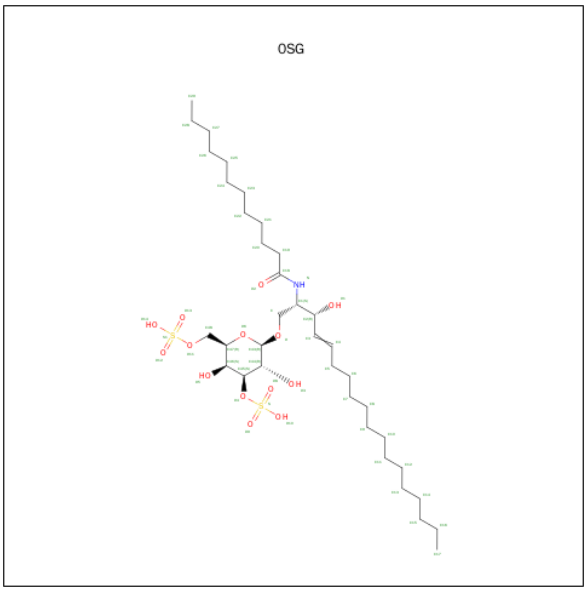
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is N-{(2S,3R,4E)-1-[(3,6-DI-O-SULFO-BETA-D-GALACTOPYRANOSYL)OXY]-3-HYDROXYOCTADEC-4-EN-2-YL}DODECANAMIDE (three-letter code: 0SG) (formula: $C_{36}H_{69}NO_{14}S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			53	36	1	14	2		
5	C	1	Total	C	N	O	S	0	0
			53	36	1	14	2		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is water.

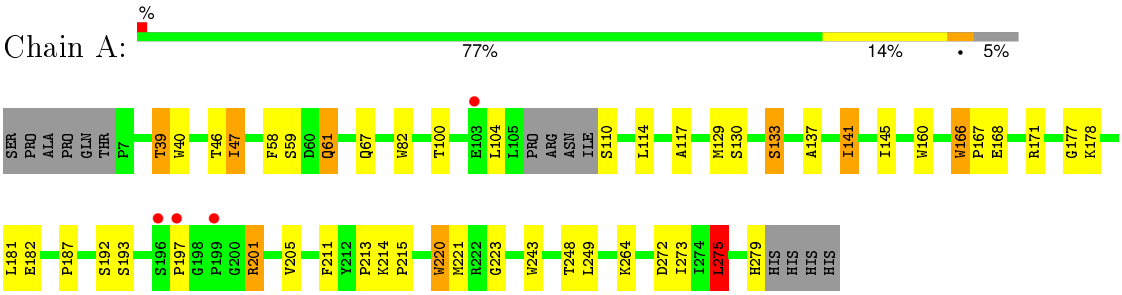
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	10	Total O 10 10	0	0
7	B	6	Total O 6 6	0	0
7	C	4	Total O 4 4	0	0
7	D	9	Total O 9 9	0	0

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.

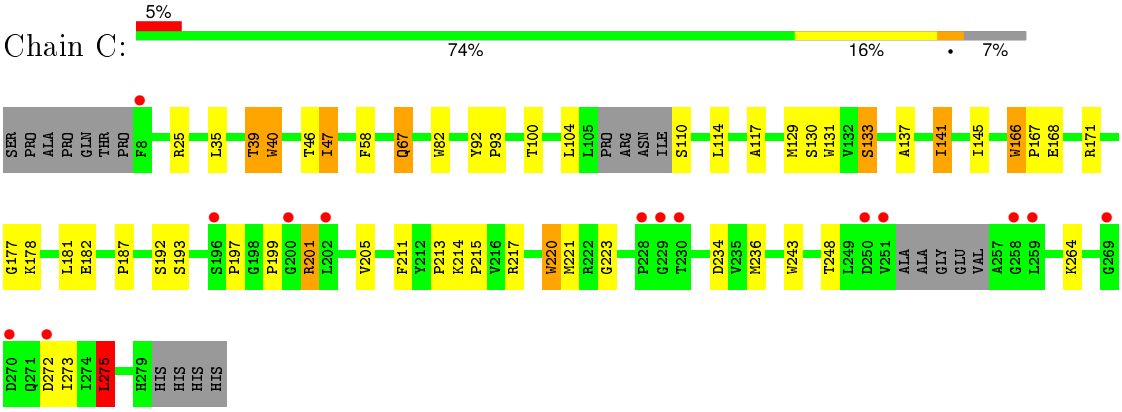
- Molecule 1: CD1D antigen, d polypeptide

Chain A:



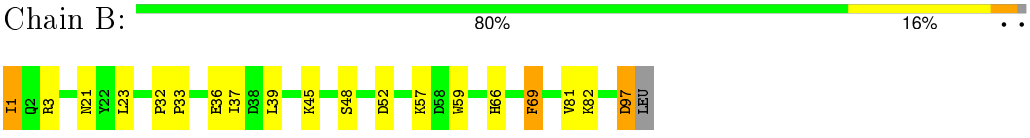
- Molecule 1: CD1D antigen, d polypeptide

Chain C:



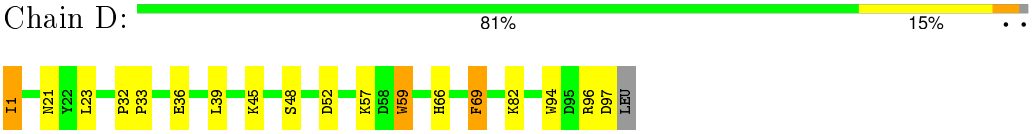
- Molecule 2: Beta-2-microglobulin

Chain B:



- Molecule 2: Beta-2-microglobulin

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α, β, γ	168.55Å 168.55Å 41.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.75 – 2.86 46.75 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.75-2.86) 98.4 (46.75-2.87)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	235.84 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.222 , 0.291 0.220 , 0.289	Depositor DCC
R_{free} test set	1515 reflections (5.80%)	DCC
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.6	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	1 of 27287 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6216	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 0SG

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	0.81	3/2242 (0.1%)	0.71	1/3052 (0.0%)
1	C	0.80	5/2195 (0.2%)	0.70	1/2987 (0.0%)
2	B	0.75	0/837	0.73	0/1135
2	D	0.74	2/833 (0.2%)	0.72	0/1131
All	All	0.79	10/6107 (0.2%)	0.71	2/8305 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	TRP	CD2-CE2	7.14	1.50	1.41
1	A	82	TRP	CD2-CE2	6.98	1.49	1.41
1	A	220	TRP	CD2-CE2	5.48	1.48	1.41
1	A	160	TRP	CD2-CE2	5.44	1.47	1.41
2	D	94	TRP	CD2-CE2	5.42	1.47	1.41
1	C	243	TRP	CD2-CE2	5.33	1.47	1.41
1	C	131	TRP	CD2-CE2	5.31	1.47	1.41
2	D	59	TRP	CD2-CE2	5.26	1.47	1.41
1	C	220	TRP	CD2-CE2	5.21	1.47	1.41
1	C	40	TRP	CD2-CE2	5.04	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	275	LEU	CA-CB-CG	5.67	128.34	115.30

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	2176	0	2098	36	0
1	C	2131	0	2051	37	0
2	B	811	0	786	16	0
2	D	807	0	775	17	0
3	A	28	0	25	0	0
4	A	39	0	34	0	0
4	C	39	0	34	0	0
5	A	53	0	69	0	0
5	C	53	0	69	0	0
6	C	50	0	43	1	0
7	A	10	0	0	2	0
7	B	6	0	0	0	0
7	C	4	0	0	0	0
7	D	9	0	0	0	0
All	All	6216	0	5984	98	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 8.

All (98) 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:C:39:THR:HG21	2:D:52:ASP:OD2	1.55	1.05
1:A:39:THR:HG21	2:B:52:ASP:OD2	1.65	0.96
1:C:133:SER:HB2	1:C:141:ILE:HD11	1.51	0.93
2:D:1:ILE:N	2:D:1:ILE:HD12	1.95	0.80
1:C:40:TRP:CE3	1:C:47:ILE:HG22	2.18	0.79
2:B:1:ILE:HD12	2:B:1:ILE:N	1.97	0.78
1:A:133:SER:HB2	1:A:141:ILE:HD11	1.66	0.78
1:A:40:TRP:CE3	1:A:47:ILE:HG22	2.21	0.75
1:C:168:GLU:HG3	1:C:171:ARG:HH22	1.53	0.74
2:D:1:ILE:H3	2:D:1:ILE:HD12	1.54	0.71
2:B:1:ILE:H3	2:B:1:ILE:HD12	1.57	0.69
2:D:39:LEU:HD12	2:D:48:SER:HB2	1.75	0.68
1:C:273:ILE:HG22	1:C:275:LEU:CD2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:CG2	2:B:52:ASP:OD2	2.42	0.66
1:A:205:VAL:HG22	1:A:248:THR:HG22	1.77	0.65
2:D:36:GLU:HB2	2:D:82:LYS:HB2	1.78	0.65
1:C:40:TRP:CZ3	1:C:47:ILE:HG22	2.31	0.64
1:A:40:TRP:CZ3	1:A:47:ILE:HG22	2.34	0.63
1:A:178:LYS:O	1:A:182:GLU:HG2	1.99	0.63
2:B:36:GLU:HB2	2:B:82:LYS:HB2	1.80	0.62
1:C:133:SER:HB2	1:C:141:ILE:CD1	2.29	0.60
1:A:168:GLU:HG3	1:A:171:ARG:HH22	1.66	0.60
2:D:32:PRO:HB2	2:D:33:PRO:CD	2.33	0.59
1:C:39:THR:CG2	2:D:52:ASP:OD2	2.41	0.59
1:A:214:LYS:N	1:A:215:PRO:CD	2.65	0.59
1:A:182:GLU:HA	7:A:408:HOH:O	2.01	0.58
1:A:100:THR:HG22	1:A:114:LEU:HG	1.85	0.57
1:C:205:VAL:HG22	1:C:248:THR:HG22	1.86	0.57
2:D:96:ARG:O	2:D:97:ASP:HB2	2.07	0.55
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.87	0.55
2:B:39:LEU:HD12	2:B:48:SER:HB2	1.88	0.55
1:C:214:LYS:N	1:C:215:PRO:CD	2.70	0.54
1:A:273:ILE:HG22	1:A:275:LEU:CD2	2.38	0.54
1:C:192:SER:OG	2:D:97:ASP:HB3	2.08	0.54
1:A:166:TRP:HB2	1:A:167:PRO:HD3	1.92	0.52
1:C:100:THR:HG22	1:C:114:LEU:HG	1.91	0.52
1:C:141:ILE:O	1:C:145:ILE:HG12	2.09	0.52
1:C:166:TRP:HB2	1:C:167:PRO:HD3	1.92	0.51
1:C:234:ASP:O	1:C:236:MET:HG3	2.10	0.51
1:C:187:PRO:HB3	1:C:211:PHE:HB3	1.91	0.50
1:A:192:SER:HB2	2:B:97:ASP:HB3	1.93	0.50
2:B:23:LEU:HD23	2:B:39:LEU:HD22	1.92	0.50
2:D:1:ILE:H1	2:D:1:ILE:HD12	1.73	0.49
2:B:32:PRO:HB2	2:B:33:PRO:CD	2.43	0.49
2:B:1:ILE:HD12	2:B:1:ILE:H1	1.74	0.49
1:C:117:ALA:HB2	2:D:59:TRP:CE2	2.48	0.49
1:A:46:THR:HB	1:A:67:GLN:HE21	1.77	0.49
1:C:178:LYS:O	1:C:182:GLU:HG2	2.12	0.48
1:C:177:GLY:O	1:C:181:LEU:HB2	2.14	0.48
1:C:46:THR:HB	1:C:67:GLN:HE21	1.78	0.48
1:C:214:LYS:N	1:C:215:PRO:HD3	2.29	0.47
2:B:21:ASN:HB3	2:B:69:PHE:CE1	2.50	0.47
2:D:1:ILE:H3	2:D:1:ILE:CD1	2.26	0.47
1:C:220:TRP:C	1:C:221:MET:HG2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:ILE:N	2:D:1:ILE:CD1	2.68	0.47
1:A:133:SER:HB2	1:A:141:ILE:CD1	2.40	0.47
1:C:213:PRO:HB2	1:C:215:PRO:HD2	1.97	0.47
1:A:214:LYS:H	1:A:215:PRO:HD3	1.81	0.46
1:A:137:ALA:HB1	1:A:141:ILE:HG12	1.96	0.46
1:A:213:PRO:HB2	1:A:215:PRO:HD2	1.97	0.46
1:C:35:LEU:HD12	1:C:181:LEU:HD12	1.97	0.46
1:C:220:TRP:O	1:C:221:MET:HG2	2.15	0.46
1:A:275:LEU:HD23	1:A:275:LEU:N	2.30	0.46
1:C:137:ALA:HB1	1:C:141:ILE:HG12	1.98	0.46
2:D:23:LEU:O	2:D:66:HIS:HA	2.16	0.46
1:A:177:GLY:O	1:A:181:LEU:HB2	2.16	0.45
2:D:32:PRO:CB	2:D:33:PRO:CD	2.95	0.45
1:A:214:LYS:N	1:A:215:PRO:HD3	2.31	0.45
2:D:32:PRO:HB2	2:D:33:PRO:HD2	1.99	0.44
2:B:1:ILE:CD1	2:B:1:ILE:N	2.70	0.44
1:A:117:ALA:HB2	2:B:59:TRP:CE2	2.52	0.44
2:B:32:PRO:HB2	2:B:33:PRO:HD2	2.00	0.43
1:C:197:PRO:HG2	1:C:201:ARG:HB3	2.00	0.43
1:A:46:THR:HB	1:A:67:GLN:NE2	2.34	0.43
1:C:46:THR:HB	1:C:67:GLN:NE2	2.34	0.43
1:C:264:LYS:HG2	1:C:272:ASP:OD2	2.19	0.43
1:A:214:LYS:HG3	1:A:243:TRP:CE2	2.53	0.42
1:C:275:LEU:N	1:C:275:LEU:HD23	2.35	0.42
2:B:37:ILE:HG12	2:B:81:VAL:HG22	2.01	0.42
1:A:141:ILE:O	1:A:145:ILE:HG12	2.19	0.42
1:A:213:PRO:HG3	7:A:408:HOH:O	2.17	0.42
1:C:40:TRP:CE3	1:C:47:ILE:CG2	2.96	0.42
1:A:201:ARG:HD2	1:A:201:ARG:HA	1.89	0.41
1:A:264:LYS:HG2	1:A:272:ASP:OD2	2.20	0.41
1:A:104:LEU:HA	1:A:110:SER:HA	2.02	0.41
1:A:59:SER:OG	1:A:61:GLN:HG3	2.21	0.41
2:D:21:ASN:HB3	2:D:69:PHE:CE1	2.56	0.41
1:A:40:TRP:CE3	1:A:47:ILE:CG2	2.98	0.41
1:C:104:LEU:HA	1:C:110:SER:HA	2.03	0.41
1:C:25:ARG:HB3	6:C:304:NAG:H82	2.02	0.41
1:C:217:ARG:HE	1:C:264:LYS:HD2	1.86	0.41
1:C:199:PRO:C	1:C:201:ARG:H	2.24	0.41
1:A:220:TRP:C	1:A:221:MET:HG2	2.41	0.41
1:C:92:TYR:HB3	1:C:93:PRO:HA	2.03	0.41
1:C:47:ILE:HD13	1:C:47:ILE:HG21	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PRO:HG2	1:A:201:ARG:HB3	2.03	0.40
2:B:23:LEU:O	2:B:66:HIS:HA	2.20	0.40
1:A:220:TRP:CD1	1:A:249:LEU:HB2	2.57	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	265/283 (94%)	253 (96%)	11 (4%)	1 (0%)	39 71
1	C	257/283 (91%)	247 (96%)	9 (4%)	1 (0%)	39 71
2	B	95/98 (97%)	91 (96%)	4 (4%)	0	100 100
2	D	95/98 (97%)	90 (95%)	5 (5%)	0	100 100
All	All	712/762 (93%)	681 (96%)	29 (4%)	2 (0%)	46 76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	223	GLY
1	A	223	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	236/250 (94%)	223 (94%)	13 (6%)	27	58
1	C	231/250 (92%)	219 (95%)	12 (5%)	29	60
2	B	92/94 (98%)	86 (94%)	6 (6%)	21	49
2	D	91/94 (97%)	87 (96%)	4 (4%)	35	68
All	All	650/688 (94%)	615 (95%)	35 (5%)	27	59

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	47	ILE
1	A	58	PHE
1	A	61	GLN
1	A	129	MET
1	A	130	SER
1	A	133	SER
1	A	141	ILE
1	A	166	TRP
1	A	193	SER
1	A	201	ARG
1	A	275	LEU
1	A	279	HIS
2	B	1	ILE
2	B	3	ARG
2	B	45	LYS
2	B	57	LYS
2	B	69	PHE
2	B	97	ASP
1	C	39	THR
1	C	47	ILE
1	C	58	PHE
1	C	67	GLN
1	C	129	MET
1	C	130	SER
1	C	133	SER
1	C	141	ILE
1	C	166	TRP
1	C	193	SER
1	C	201	ARG
1	C	275	LEU
2	D	1	ILE
2	D	45	LYS

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Mol	Chain	Res	Type
2	D	57	LYS
2	D	69	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
2	B	2	GLN
1	C	67	GLN
2	D	2	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

12 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	$\#\|Z\| > 2$
3	NAG	A	301	1,3	14,14,15	0.61	0	15,19,21	1.49	1 (6%)
3	NAG	A	302	3	14,14,15	0.54	0	15,19,21	1.51	3 (20%)
4	NAG	A	303	1,4	14,14,15	0.88	1 (7%)	15,19,21	1.69	3 (20%)
4	NAG	A	304	4	14,14,15	0.62	0	15,19,21	1.30	2 (13%)
4	BMA	A	305	4	11,11,12	0.57	0	14,15,17	1.61	2 (14%)
4	NAG	C	301	1,4	14,14,15	0.61	0	15,19,21	1.61	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	302	4	14,14,15	0.54	0	15,19,21	1.06	1 (6%)
4	BMA	C	303	4	11,11,12	0.55	0	14,15,17	1.68	2 (14%)
6	NAG	C	304	1,6	14,14,15	0.68	0	15,19,21	1.40	3 (20%)
6	NAG	C	305	6	14,14,15	0.64	0	15,19,21	1.41	2 (13%)
6	BMA	C	306	6	11,11,12	0.84	0	14,15,17	1.53	2 (14%)
6	BMA	C	307	6	11,11,12	0.66	0	14,15,17	1.83	2 (14%)

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	NAG	A	301	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	302	3	-	0/6/23/26	0/1/1/1
4	NAG	A	303	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	304	4	-	0/6/23/26	0/1/1/1
4	BMA	A	305	4	-	0/2/19/22	0/1/1/1
4	NAG	C	301	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	302	4	-	0/6/23/26	0/1/1/1
4	BMA	C	303	4	-	0/2/19/22	0/1/1/1
6	NAG	C	304	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	305	6	-	0/6/23/26	0/1/1/1
6	BMA	C	306	6	-	0/2/19/22	0/1/1/1
6	BMA	C	307	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	NAG	C2-N2	-2.30	1.42	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	303	NAG	C2-N2-C7	-4.72	116.97	123.04
3	A	302	NAG	C2-N2-C7	-3.71	118.27	123.04
3	A	301	NAG	C2-N2-C7	-3.51	118.53	123.04
6	C	304	NAG	C2-N2-C7	-3.35	118.73	123.04
4	C	301	NAG	O3-C3-C2	-2.92	103.32	109.11
4	A	303	NAG	C3-C4-C5	-2.61	105.64	110.20
6	C	304	NAG	C3-C4-C5	-2.52	105.80	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	303	NAG	C3-C2-N2	-2.30	105.06	110.56
6	C	304	NAG	C3-C2-N2	-2.20	105.30	110.56
4	A	304	NAG	C1-O5-C5	-2.18	109.48	112.25
4	C	303	BMA	O2-C2-C1	2.02	113.26	109.21
6	C	306	BMA	O3-C3-C2	2.18	113.93	110.00
3	A	302	NAG	C4-C3-C2	2.18	114.62	111.23
3	A	302	NAG	C1-O5-C5	2.29	115.16	112.25
4	C	302	NAG	C4-C3-C2	2.74	115.49	111.23
6	C	305	NAG	C3-C4-C5	2.77	115.03	110.20
4	A	304	NAG	C4-C3-C2	2.96	115.82	111.23
4	C	301	NAG	C4-C3-C2	3.09	116.03	111.23
4	C	301	NAG	C1-O5-C5	3.11	116.20	112.25
4	A	305	BMA	C3-C4-C5	3.20	115.78	110.20
6	C	307	BMA	C3-C4-C5	3.44	116.19	110.20
6	C	305	NAG	C4-C3-C2	3.78	117.10	111.23
4	A	305	BMA	C1-O5-C5	4.03	117.36	112.25
6	C	306	BMA	C3-C4-C5	4.27	117.64	110.20
4	C	303	BMA	C1-O5-C5	4.86	118.42	112.25
6	C	307	BMA	C1-O5-C5	5.08	118.69	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	304	NAG	1	0

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	0SG	A	306	-	52,53,53	1.24	7 (13%)	59,67,67	1.24	2 (3%)
5	0SG	C	308	-	52,53,53	1.33	6 (11%)	59,67,67	1.52	7 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	0SG	A	306	-	-	0/50/70/70	0/1/1/1
5	0SG	C	308	-	-	0/50/70/70	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	306	0SG	O4-C45	-2.12	1.41	1.46
5	C	308	0SG	O8-S	2.16	1.53	1.45
5	A	306	0SG	O13-S1	2.28	1.53	1.45
5	A	306	0SG	O8-S	2.28	1.53	1.45
5	A	306	0SG	O9-S	2.29	1.53	1.45
5	A	306	0SG	O12-S1	2.32	1.53	1.45
5	C	308	0SG	O9-S	2.57	1.54	1.45
5	C	308	0SG	O12-S1	2.59	1.54	1.45
5	C	308	0SG	O13-S1	2.75	1.55	1.45
5	A	306	0SG	C19-C18	2.87	1.56	1.51
5	C	308	0SG	C19-C18	3.51	1.58	1.51
5	C	308	0SG	C3-C4	4.51	1.53	1.31
5	A	306	0SG	C3-C4	4.54	1.53	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	306	0SG	C5-C4-C3	-5.75	107.90	125.14
5	C	308	0SG	C5-C4-C3	-5.39	108.96	125.14
5	C	308	0SG	C-O-C43	-5.13	103.04	113.82
5	A	306	0SG	C-O-C43	-4.36	104.67	113.82
5	C	308	0SG	O6-C47-C48	-3.56	99.34	106.61
5	C	308	0SG	C43-C44-C45	-2.83	104.90	110.00
5	C	308	0SG	C43-O6-C47	-2.78	108.35	113.75
5	C	308	0SG	C45-O4-S	2.14	122.85	118.77
5	C	308	0SG	O-C43-C44	4.20	113.34	108.04

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	269/283 (95%)	0.05	4 (1%) 76 73	23, 41, 80, 107	0
1	C	263/283 (92%)	0.17	14 (5%) 30 24	25, 46, 90, 117	0
2	B	97/98 (98%)	-0.34	0 100 100	20, 33, 60, 78	0
2	D	97/98 (98%)	-0.33	0 100 100	24, 36, 67, 84	0
All	All	726/762 (95%)	-0.01	18 (2%) 61 56	20, 41, 82, 117	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	GLY	3.6
1	C	270	ASP	3.5
1	A	199	PRO	3.3
1	C	202	LEU	3.2
1	C	228	PRO	2.9
1	A	197	PRO	2.7
1	A	196	SER	2.7
1	C	229	GLY	2.5
1	C	269	GLY	2.4
1	C	8	PHE	2.3
1	C	196	SER	2.2
1	A	103	GLU	2.2
1	C	251	VAL	2.1
1	C	272	ASP	2.1
1	C	250	ASP	2.1
1	C	259	LEU	2.1
1	C	258	GLY	2.0
1	C	230	THR	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	C	302	14/15	0.87	0.35	-	69,84,99,113	0
3	NAG	A	301	14/15	0.95	0.16	-	47,56,64,67	0
4	NAG	C	301	14/15	0.94	0.19	-	53,62,68,70	0
6	NAG	C	305	14/15	0.87	0.24	-	69,78,91,91	0
3	NAG	A	302	14/15	0.81	0.32	-	70,87,90,94	0
4	BMA	C	303	11/12	0.57	0.30	-	77,106,113,113	0
6	NAG	C	304	14/15	0.95	0.13	-	36,42,49,61	0
4	BMA	A	305	11/12	0.71	0.26	-	82,96,105,106	0
4	NAG	A	304	14/15	0.84	0.20	-	64,79,87,92	0
6	BMA	C	307	11/12	0.69	0.25	-	95,110,113,114	0
4	NAG	A	303	14/15	0.96	0.15	-	37,39,46,57	0
6	BMA	C	306	11/12	0.75	0.26	-	94,101,106,110	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	0SG	C	308	53/53	0.88	0.30	3.55	40,66,112,125	0
5	0SG	A	306	53/53	0.92	0.25	1.91	43,64,98,102	0

6.5 Other polymers (i)

There are no such residues in this entry.