Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:56 PM GMT

PDB ID	:	1Z5L
Title	:	Structure of a highly potent short-chain galactosyl ceramide agonist bound to CD1D
Authors	:	Zajonc, D.M.; Cantu, C.; Mattner, J.; Zhou, D.; Savage, P.B.; Bendelac, A.; Wilson, I.A.; Teyton, L.
Deposited on	:	2005-03-18
Resolution	:	2.20 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:

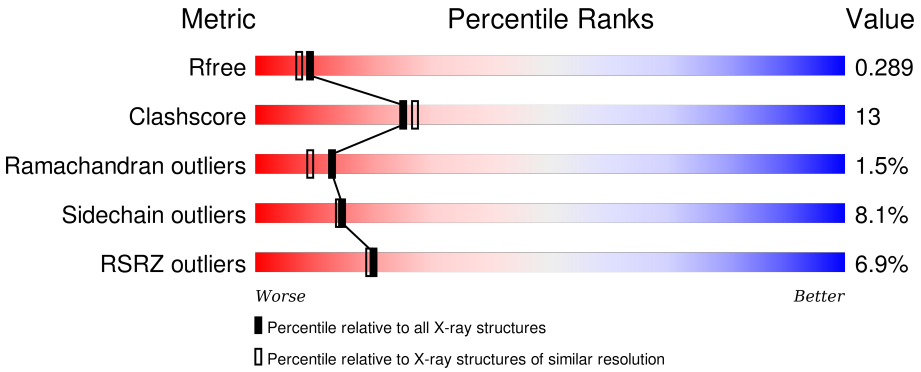
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	285	8% 62% 26% • • 7%
1	C	285	6% 62% 25% 5% • 7%
2	B	99	4% 73% 20% 6% •
2	D	99	4% 60% 30% 8% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	R16	A	701	-	-	-	X
6	R16	C	702	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6290 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 T-cell surface glycoprotein CD1d antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	42	0	0
			2140	1368	366	393	13			
1	C	266	Total	C	N	O	S	66	0	0
			2151	1373	370	395	13			

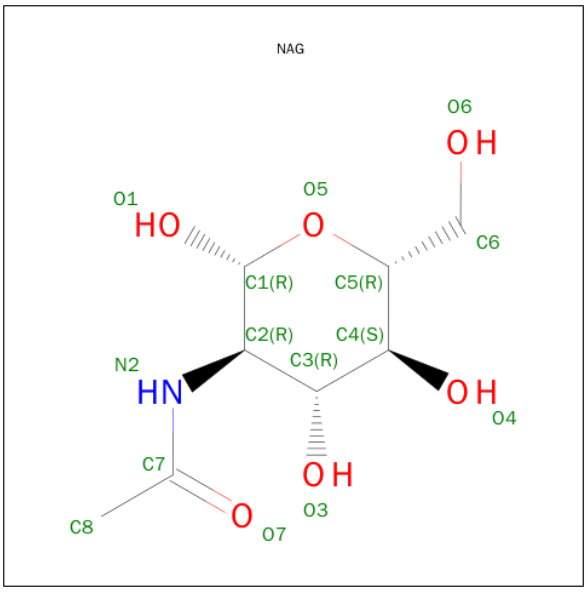
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	HIS	-	EXPRESSION TAG	GB 50333
A	281	HIS	-	EXPRESSION TAG	GB 50333
A	282	HIS	-	EXPRESSION TAG	GB 50333
A	283	HIS	-	EXPRESSION TAG	GB 50333
A	284	HIS	-	EXPRESSION TAG	GB 50333
A	285	HIS	-	EXPRESSION TAG	GB 50333
C	280	HIS	-	EXPRESSION TAG	GB 50333
C	281	HIS	-	EXPRESSION TAG	GB 50333
C	282	HIS	-	EXPRESSION TAG	GB 50333
C	283	HIS	-	EXPRESSION TAG	GB 50333
C	284	HIS	-	EXPRESSION TAG	GB 50333
C	285	HIS	-	EXPRESSION TAG	GB 50333

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	37	0	0
			810	517	137	149	7			
2	D	98	Total	C	N	O	S	37	0	0
			810	517	137	149	7			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

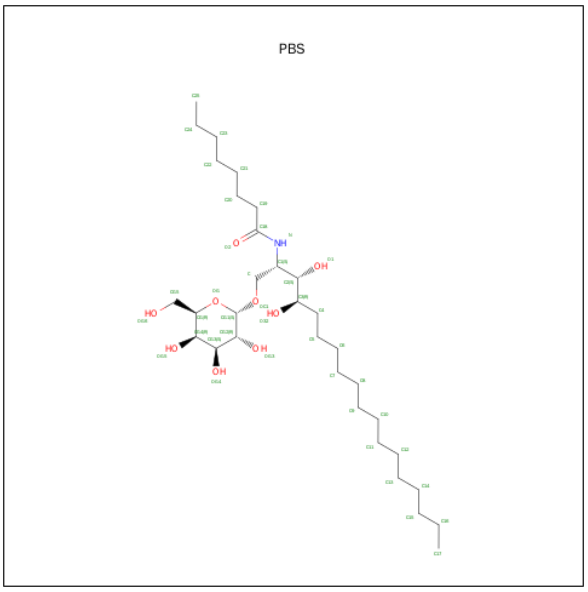


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

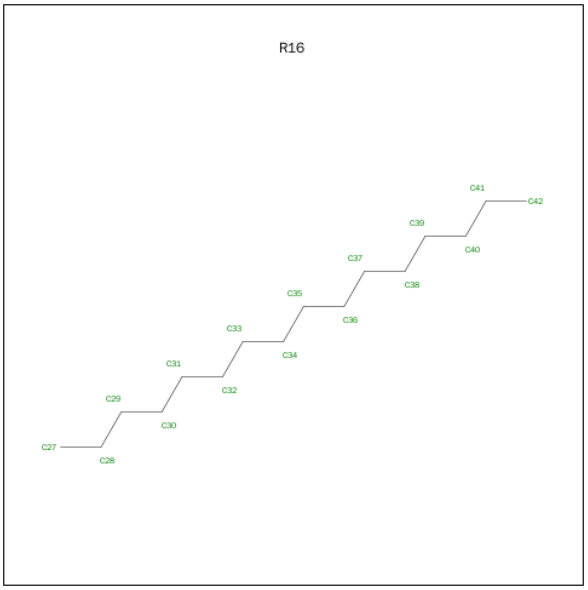
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total C N O 28 16 2 10	0	0
4	C	2	Total C N O 28 16 2 10	0	0

- Molecule 5 is (2S,3S,4R)-N-OCTANOYL-1-[(ALPHA-D-GALACTOPYRANOSYL)OXY]-2 -AMINO-OCTADECANE-3,4-DIOL (three-letter code: PBS) (formula: $C_{32}H_{63}NO_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 42 32 1 9	0	0
5	C	1	Total C N O 42 32 1 9	0	0

- Molecule 6 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 16 16	0	0
6	C	1	Total C 16 16	0	0

- Molecule 7 is water.

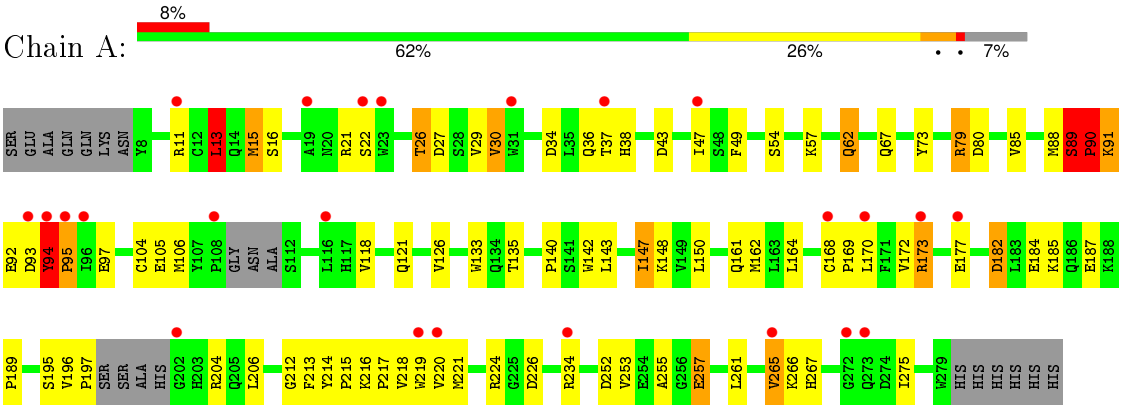
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	50	Total O 50 50	0	0
7	B	24	Total O 24 24	0	0
7	C	66	Total O 66 66	0	0
7	D	25	Total O 25 25	0	0

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.

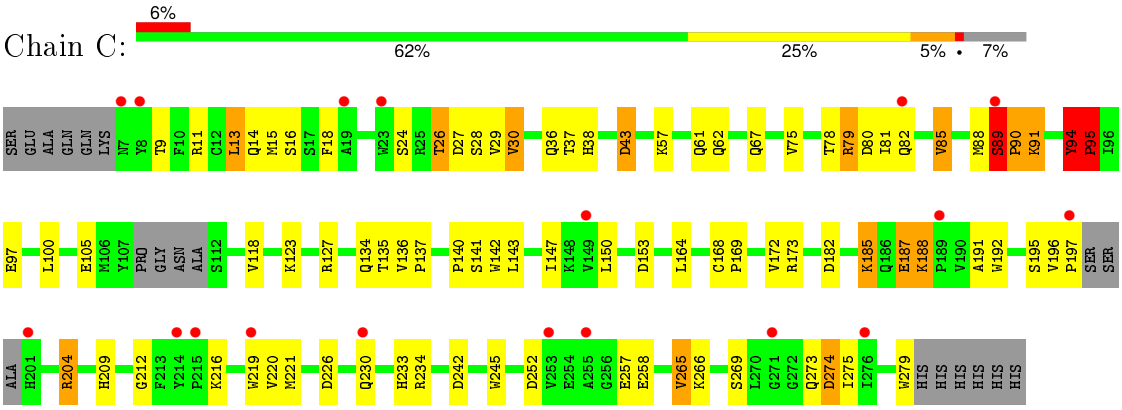
- Molecule 1: T-cell surface glycoprotein CD1d antigen

Chain A:



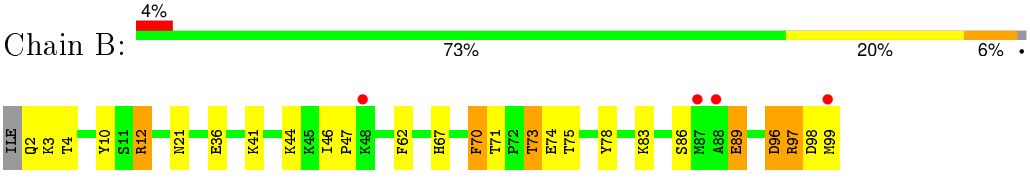
- Molecule 1: T-cell surface glycoprotein CD1d antigen

Chain C:



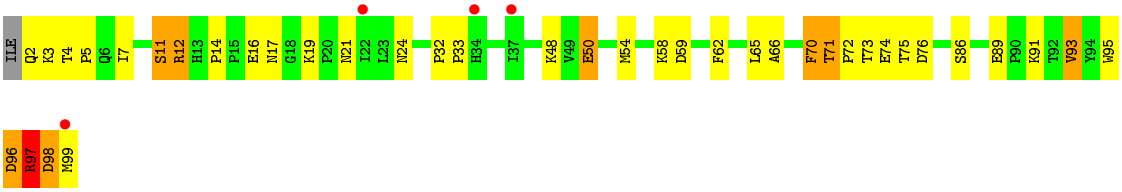
- Molecule 2: Beta-2-microglobulin

Chain B:



- Molecule 2: Beta-2-microglobulin

Chain D:


ILE
Q2
K3
T4
P5
Q6
I7
S11
R12
H13
P14
P15
E16
N17
G18
K19
P20
N21
I22
L23
N24
P32
P33
H34
I37
K48
V49
E50
M54
K58
D59
F62
L65
A66
F70
T71
P72
T73
E74
T75
D76
S86
E89
P90
K91
T92
V93
Y94
W95
D96
R97
D98
M99

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.45Å 77.05Å 111.01Å 90.00° 107.63° 90.00°	Depositor
Resolution (Å)	39.68 – 2.20 39.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (39.68-2.20) 93.7 (39.68-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.242 , 0.294 0.241 , 0.289	Depositor DCC
R_{free} test set	1414 reflections (3.21%)	DCC
Wilson B-factor (Å^2)	49.2	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.5	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.37$	Xtriage
Outliers	1 of 45428 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6290	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.60 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.4033e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: R16, NAG, PBS

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	0.97	5/2202 (0.2%)	1.07	15/2991 (0.5%)
1	C	1.02	7/2213 (0.3%)	1.03	12/3005 (0.4%)
2	B	1.06	3/836 (0.4%)	1.04	2/1133 (0.2%)
2	D	0.88	4/836 (0.5%)	1.03	7/1133 (0.6%)
All	All	0.99	19/6087 (0.3%)	1.05	36/8262 (0.4%)

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	A	0	1
1	C	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	91	LYS	CA-CB	-23.40	1.02	1.53
1	C	273	GLN	CA-CB	-19.75	1.10	1.53
1	A	184	GLU	CA-CB	-17.88	1.14	1.53
2	B	3	LYS	CA-CB	-16.09	1.18	1.53
1	A	62	GLN	CA-CB	-14.99	1.21	1.53
1	A	255	ALA	CA-CB	-11.78	1.27	1.52
1	C	257	GLU	CA-CB	-10.58	1.30	1.53
2	D	48	LYS	CA-CB	-10.38	1.31	1.53
1	C	173	ARG	CA-CB	-10.15	1.31	1.53
1	A	105	GLU	CA-CB	-9.81	1.32	1.53
2	B	89	GLU	CA-CB	8.53	1.72	1.53
2	B	83	LYS	CA-CB	-8.50	1.35	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	ARG	CA-CB	-7.43	1.37	1.53
2	D	58	LYS	CA-CB	-7.41	1.37	1.53
2	D	16	GLU	CA-CB	7.25	1.69	1.53
1	A	257	GLU	CA-CB	-6.71	1.39	1.53
1	C	61	GLN	CA-CB	6.27	1.67	1.53
1	C	188	LYS	CA-CB	-6.08	1.40	1.53
2	D	19	LYS	CA-CB	5.73	1.66	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	184	GLU	CB-CA-C	11.76	133.93	110.40
1	C	62	GLN	N-CA-CB	11.72	131.69	110.60
1	C	79	ARG	N-CA-CB	11.71	131.67	110.60
1	A	257	GLU	N-CA-CB	10.91	130.24	110.60
2	D	3	LYS	N-CA-CB	-10.15	92.33	110.60
1	C	257	GLU	CB-CA-C	9.28	128.96	110.40
1	A	62	GLN	CB-CA-C	8.04	126.49	110.40
2	D	48	LYS	N-CA-CB	7.17	123.51	110.60
1	A	252	ASP	CB-CG-OD2	7.12	124.71	118.30
2	B	3	LYS	CB-CA-C	6.76	123.92	110.40
1	A	184	GLU	CA-CB-CG	6.57	127.85	113.40
1	C	43	ASP	CB-CG-OD2	6.42	124.08	118.30
1	C	153	ASP	CB-CG-OD2	6.37	124.03	118.30
2	B	96	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	105	GLU	N-CA-CB	6.24	121.83	110.60
1	A	62	GLN	N-CA-CB	6.19	121.75	110.60
2	D	96	ASP	CB-CG-OD2	6.03	123.73	118.30
1	C	150	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	255	ALA	N-CA-CB	5.91	118.38	110.10
2	D	59	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	150	LEU	CA-CB-CG	5.87	128.79	115.30
1	C	95	PRO	N-CD-CG	-5.83	94.45	103.20
2	D	89	GLU	N-CA-CB	-5.80	100.17	110.60
1	A	27	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	62	GLN	CA-CB-CG	5.73	126.01	113.40
1	A	34	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	21	ARG	CA-CB-CG	-5.41	101.50	113.40
1	C	80	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	226	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	13	LEU	CB-CG-CD1	5.35	120.09	111.00
2	D	98	ASP	CB-CG-OD2	5.19	122.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	173	ARG	CB-CA-C	5.17	120.75	110.40
1	C	273	GLN	CB-CA-C	5.16	120.71	110.40
2	D	76	ASP	CB-CG-OD2	5.15	122.93	118.30
1	C	27	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	226	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	TYR	Peptide
1	C	94	TYR	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	2140	0	2050	58	1
1	C	2151	0	2057	56	0
2	B	810	0	783	15	1
2	D	810	0	783	31	0
3	A	28	0	26	0	0
3	C	14	0	13	0	0
4	A	28	0	25	1	0
4	C	28	0	25	0	0
5	A	42	0	63	2	0
5	C	42	0	63	0	0
6	A	16	0	34	0	0
6	C	16	0	34	2	0
7	A	50	0	0	2	0
7	B	24	0	0	1	0
7	C	66	0	0	3	0
7	D	25	0	0	0	0
All	All	6290	0	5956	148	1

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 13.

All (148) 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:30:VAL:HG13	1:C:38:HIS:HB2	1.15	1.09
1:A:89:SER:HB3	1:A:90:PRO:HD2	1.39	1.00
1:A:182:ASP:O	1:A:185:LYS:HG2	1.64	0.96
2:D:73:THR:HG22	2:D:75:THR:H	1.30	0.94
2:B:73:THR:HG22	2:B:75:THR:H	1.29	0.94
1:C:30:VAL:CG1	1:C:38:HIS:HB2	1.99	0.93
2:B:96:ASP:O	2:B:98:ASP:N	2.05	0.89
1:A:16:SER:OG	1:A:26:THR:HB	1.74	0.88
1:A:213:PHE:CE2	1:A:218:VAL:HG21	2.09	0.88
1:A:89:SER:HB3	1:A:90:PRO:CD	2.08	0.82
1:C:89:SER:HB3	1:C:90:PRO:HD2	1.68	0.76
1:A:265:VAL:HG13	1:A:275:ILE:HB	1.69	0.74
1:A:15:MET:HG2	2:B:62:PHE:HE2	1.54	0.71
1:A:213:PHE:CD2	1:A:218:VAL:HG21	2.24	0.71
1:C:266:LYS:HG2	1:C:274:ASP:OD2	1.89	0.71
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.72	0.70
1:A:218:VAL:HG22	1:A:267:HIS:HD2	1.54	0.70
1:C:29:VAL:HG23	1:C:36:GLN:NE2	2.07	0.69
1:A:216:LYS:O	1:A:218:VAL:HG23	1.95	0.66
1:C:89:SER:O	1:C:90:PRO:C	2.32	0.66
1:C:233:HIS:HB3	7:C:717:HOH:O	1.96	0.65
2:D:96:ASP:O	2:D:98:ASP:N	2.22	0.64
1:C:97:GLU:HG3	7:C:746:HOH:O	1.96	0.64
2:B:2:GLN:HG2	2:B:86:SER:HB3	1.81	0.63
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.80	0.62
1:A:94:TYR:O	1:A:95:PRO:O	2.18	0.61
1:A:195:SER:OG	1:A:204:ARG:NH2	2.34	0.61
1:A:30:VAL:HG13	1:A:38:HIS:HB2	1.81	0.60
1:C:89:SER:CB	1:C:90:PRO:HD2	2.32	0.60
1:C:168:CYS:HB3	1:C:169:PRO:HD3	1.84	0.60
1:C:258:GLU:HB3	1:C:279:TRP:CD1	2.36	0.60
1:A:218:VAL:HG22	1:A:267:HIS:CD2	2.37	0.59
2:D:17:ASN:HA	2:D:72:PRO:O	2.02	0.59
2:B:10:TYR:HB3	2:B:99:MET:HG2	1.83	0.59
1:C:30:VAL:HG13	1:C:38:HIS:CB	2.10	0.58
1:C:212:GLY:HA3	2:D:12:ARG:NH2	2.20	0.57
1:A:140:PRO:HD2	1:A:143:LEU:HD12	1.87	0.56
1:A:161:GLN:HB3	4:A:511:NAG:H82	1.87	0.56
2:B:96:ASP:C	2:B:98:ASP:H	2.02	0.56
1:C:187:GLU:HA	1:C:187:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:MET:HA	1:C:142:TRP:CE3	2.41	0.56
2:B:67:HIS:HE1	7:B:112:HOH:O	1.87	0.56
1:A:106:MET:HG3	1:A:172:VAL:HG11	1.88	0.55
1:C:242:ASP:OD2	2:D:12:ARG:NH1	2.39	0.55
1:C:94:TYR:O	1:C:95:PRO:O	2.25	0.55
1:A:89:SER:O	1:A:90:PRO:C	2.46	0.55
2:D:73:THR:HG22	2:D:75:THR:N	2.10	0.54
1:A:49:PHE:HB3	1:A:54:SER:HB2	1.89	0.54
1:A:213:PHE:CE2	1:A:218:VAL:CG2	2.88	0.54
1:A:30:VAL:HG22	1:A:37:THR:OG1	2.08	0.53
1:C:100:LEU:HG	1:C:118:VAL:HG22	1.90	0.53
2:B:74:GLU:CD	2:B:74:GLU:H	2.12	0.53
1:C:123:LYS:HD2	7:C:768:HOH:O	2.08	0.53
1:A:57:LYS:NZ	1:C:230:GLN:OE1	2.25	0.53
2:D:11:SER:HB2	2:D:99:MET:OXT	2.08	0.53
1:C:78:THR:O	1:C:82:GLN:HG3	2.10	0.52
1:A:89:SER:O	1:A:91:LYS:N	2.42	0.52
2:B:36:GLU:HA	2:B:36:GLU:OE1	2.11	0.51
1:A:212:GLY:HA3	2:B:12:ARG:NH2	2.25	0.51
1:C:212:GLY:CA	2:D:12:ARG:NH2	2.74	0.51
1:C:182:ASP:O	1:C:185:LYS:HD2	2.11	0.51
1:A:118:VAL:HB	1:A:126:VAL:HB	1.91	0.51
1:C:29:VAL:CG2	1:C:36:GLN:NE2	2.74	0.50
1:A:135:THR:HG23	1:A:147:ILE:HG12	1.94	0.50
1:A:15:MET:HG2	2:B:62:PHE:CE2	2.42	0.50
1:C:94:TYR:HB3	1:C:95:PRO:CD	2.42	0.50
1:C:192:TRP:CE3	2:D:14:PRO:HG3	2.47	0.49
1:C:14:GLN:HB2	6:C:702:R16:H282	1.94	0.49
1:C:219:TRP:HB3	1:C:266:LYS:HB2	1.95	0.49
1:C:195:SER:OG	1:C:204:ARG:NH2	2.46	0.49
2:B:41:LYS:HG3	2:B:78:TYR:CE2	2.49	0.48
1:C:16:SER:OG	1:C:26:THR:HB	2.14	0.48
1:C:219:TRP:HA	1:C:234:ARG:HH22	1.79	0.48
1:A:206:LEU:HD22	1:A:253:VAL:HG11	1.95	0.48
2:D:73:THR:CG2	2:D:75:THR:OG1	2.62	0.48
1:A:29:VAL:CG2	1:A:36:GLN:NE2	2.77	0.47
1:C:89:SER:CB	1:C:90:PRO:CD	2.92	0.47
2:D:7:ILE:HB	2:D:93:VAL:HG11	1.96	0.47
1:A:224:ARG:NH2	1:A:257:GLU:O	2.42	0.47
1:A:47:ILE:HD12	1:A:67:GLN:HG3	1.96	0.47
1:C:9:THR:O	1:C:11:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ALA:HA	1:C:209:HIS:O	2.15	0.47
2:D:50:GLU:O	2:D:66:ALA:HA	2.15	0.47
1:C:136:VAL:HG13	1:C:137:PRO:HD2	1.97	0.46
1:A:89:SER:CB	1:A:90:PRO:CD	2.89	0.46
1:A:88:MET:HA	1:A:142:TRP:CE3	2.50	0.46
1:C:29:VAL:HG23	1:C:36:GLN:HE21	1.80	0.46
1:A:29:VAL:HG23	1:A:36:GLN:NE2	2.30	0.46
2:D:73:THR:CG2	2:D:74:GLU:N	2.79	0.45
1:A:91:LYS:O	1:A:93:ASP:N	2.49	0.45
1:C:15:MET:HE1	2:D:54:MET:CG	2.47	0.45
1:A:121:GLN:HA	1:A:121:GLN:OE1	2.16	0.45
1:A:30:VAL:CG1	1:A:38:HIS:HB2	2.45	0.45
1:C:168:CYS:O	1:C:172:VAL:HG23	2.16	0.45
1:A:79:ARG:NE	1:A:80:ASP:OD1	2.44	0.45
1:C:196:VAL:HA	1:C:197:PRO:HD2	1.69	0.45
2:D:74:GLU:H	2:D:74:GLU:CD	2.21	0.44
2:D:32:PRO:HB2	2:D:33:PRO:HD2	1.99	0.44
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.52	0.44
2:D:73:THR:HG22	2:D:74:GLU:N	2.32	0.44
1:C:13:LEU:O	1:C:28:SER:HA	2.16	0.44
2:D:95:TRP:CZ2	2:D:97:ARG:HA	2.52	0.44
1:C:15:MET:HG2	2:D:62:PHE:HE2	1.83	0.44
1:C:216:LYS:HD3	1:C:245:TRP:CE2	2.51	0.44
1:C:221:MET:HE2	1:C:221:MET:HB3	1.87	0.44
1:A:218:VAL:HG12	1:A:219:TRP:N	2.33	0.44
1:A:220:VAL:O	1:A:221:MET:HG2	2.18	0.44
1:C:265:VAL:HG13	1:C:275:ILE:HB	2.00	0.44
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.99	0.43
1:C:127:ARG:HD3	1:C:134:GLN:OE1	2.17	0.43
1:C:220:VAL:HG22	1:C:265:VAL:HB	1.99	0.43
1:A:85:VAL:HG22	1:A:88:MET:HE3	2.00	0.43
1:C:135:THR:HG23	1:C:147:ILE:HG12	2.01	0.43
2:D:73:THR:HG21	2:D:75:THR:OG1	2.18	0.43
2:D:7:ILE:HD12	2:D:91:LYS:HD2	2.00	0.43
2:B:73:THR:CG2	2:B:74:GLU:N	2.81	0.43
1:C:30:VAL:HG22	1:C:37:THR:OG1	2.19	0.43
1:A:94:TYR:HB3	1:A:95:PRO:CD	2.49	0.43
2:D:71:THR:HA	2:D:72:PRO:HD2	1.72	0.43
1:A:73:TYR:HE1	5:A:601:PBS:H62	1.84	0.43
2:D:5:PRO:O	2:D:91:LYS:NZ	2.45	0.42
2:D:2:GLN:HG2	2:D:86:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:PHE:CD2	1:C:24:SER:OG	2.68	0.42
1:C:188:LYS:HA	1:C:269:SER:OG	2.18	0.42
1:C:15:MET:HE1	2:D:54:MET:HG2	2.01	0.42
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.54	0.42
1:A:220:VAL:H	1:A:234:ARG:HH21	1.67	0.42
1:A:214:TYR:CG	1:A:215:PRO:HA	2.55	0.42
1:A:11:ARG:HB2	1:A:13:LEU:HD13	2.00	0.42
1:A:266:LYS:NZ	7:A:744:HOH:O	2.52	0.42
1:A:218:VAL:HG12	1:A:219:TRP:H	1.85	0.42
1:C:28:SER:OG	6:C:702:R16:H291	2.20	0.42
1:C:9:THR:HA	1:C:105:GLU:HA	2.02	0.42
2:B:46:ILE:HA	2:B:47:PRO:HD3	1.91	0.42
2:D:32:PRO:CB	2:D:33:PRO:HD2	2.50	0.41
1:C:81:ILE:O	1:C:85:VAL:HB	2.20	0.41
1:A:224:ARG:NH1	1:A:261:LEU:HD21	2.35	0.41
2:D:95:TRP:CE2	2:D:97:ARG:HA	2.55	0.41
1:A:173:ARG:O	1:A:177:GLU:HG3	2.21	0.41
2:D:4:THR:O	2:D:4:THR:HG23	2.20	0.41
1:C:15:MET:HG2	2:D:62:PHE:CE2	2.56	0.41
1:A:215:PRO:HB2	1:A:217:PRO:HD2	2.03	0.41
1:A:168:CYS:O	1:A:172:VAL:HG23	2.22	0.40
1:A:133:TRP:CH2	5:A:601:PBS:H81	2.57	0.40
1:A:22:SER:HA	7:A:745:HOH:O	2.20	0.40
1:A:196:VAL:HA	1:A:197:PRO:HD2	1.86	0.40
1:A:16:SER:OG	1:A:26:THR:CB	2.58	0.40
1:C:140:PRO:HD2	1:C:143:LEU:HD12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:MET:CG	2:B:97:ARG:NH2[1_655]	1.99	0.21

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	259/285 (91%)	249 (96%)	5 (2%)	5 (2%)	10 6
1	C	260/285 (91%)	250 (96%)	6 (2%)	4 (2%)	13 9
2	B	96/99 (97%)	90 (94%)	5 (5%)	1 (1%)	19 16
2	D	96/99 (97%)	90 (94%)	5 (5%)	1 (1%)	19 16
All	All	711/768 (93%)	679 (96%)	21 (3%)	11 (2%)	13 9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	92	GLU
1	A	94	TYR
1	A	95	PRO
2	B	97	ARG
1	C	89	SER
1	C	90	PRO
1	C	94	TYR
1	C	95	PRO
2	D	97	ARG
1	A	89	SER

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	233/249 (94%)	213 (91%)	20 (9%)	13 12
1	C	234/249 (94%)	215 (92%)	19 (8%)	15 14
2	B	92/93 (99%)	85 (92%)	7 (8%)	16 16
2	D	92/93 (99%)	85 (92%)	7 (8%)	16 16
All	All	651/684 (95%)	598 (92%)	53 (8%)	15 14

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	15	MET
1	A	26	THR
1	A	30	VAL
1	A	43	ASP
1	A	62	GLN
1	A	79	ARG
1	A	89	SER
1	A	90	PRO
1	A	91	LYS
1	A	97	GLU
1	A	104	CYS
1	A	147	ILE
1	A	148	LYS
1	A	164	LEU
1	A	170	LEU
1	A	173	ARG
1	A	182	ASP
1	A	187	GLU
1	A	265	VAL
2	B	4	THR
2	B	12	ARG
2	B	44	LYS
2	B	70	PHE
2	B	71	THR
2	B	73	THR
2	B	89	GLU
1	C	13	LEU
1	C	26	THR
1	C	30	VAL
1	C	43	ASP
1	C	57	LYS
1	C	67	GLN
1	C	75	VAL
1	C	79	ARG
1	C	85	VAL
1	C	89	SER
1	C	91	LYS
1	C	141	SER
1	C	164	LEU
1	C	185	LYS
1	C	187	GLU

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Mol	Chain	Res	Type
1	C	204	ARG
1	C	252	ASP
1	C	265	VAL
1	C	274	ASP
2	D	11	SER
2	D	12	ARG
2	D	50	GLU
2	D	70	PHE
2	D	71	THR
2	D	93	VAL
2	D	97	ARG

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
1	C	7	ASN
1	C	36	GLN
1	C	117	HIS

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

4 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	$\#\|Z\|>2$
4	NAG	A	511	1,4	14,14,15	0.76	0	15,19,21	1.38	2 (13%)
4	NAG	A	512	4	14,14,15	0.53	0	15,19,21	1.78	3 (20%)
4	NAG	C	511	1,4	14,14,15	0.59	0	15,19,21	1.31	2 (13%)
4	NAG	C	512	4	14,14,15	0.61	0	15,19,21	1.27	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	511	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	512	4	-	0/6/23/26	0/1/1/1
4	NAG	C	511	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	512	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	512	NAG	C2-N2-C7	-2.91	119.30	123.04
4	C	511	NAG	C1-O5-C5	-2.34	109.28	112.25
4	A	511	NAG	C3-C4-C5	-2.23	106.32	110.20
4	C	511	NAG	C3-C4-C5	-2.07	106.58	110.20
4	C	512	NAG	O3-C3-C4	-2.03	105.76	110.34
4	A	511	NAG	C6-C5-C4	2.13	118.26	113.02
4	C	512	NAG	C1-O5-C5	2.63	115.59	112.25
4	A	512	NAG	O4-C4-C5	2.77	116.58	109.24
4	A	512	NAG	C1-O5-C5	5.06	118.67	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
4	A	511	NAG	1	0

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
3	NAG	A	500	1	14,14,15	0.74	0	15,19,21	1.49	1 (6%)
3	NAG	A	501	1	14,14,15	0.77	1 (7%)	15,19,21	1.38	2 (13%)
5	PBS	A	601	-	41,42,42	1.00	2 (4%)	47,51,51	1.39	5 (10%)
6	R16	A	701	-	15,15,15	0.75	0	14,14,14	0.44	0
3	NAG	C	501	1	14,14,15	0.52	0	15,19,21	1.67	3 (20%)
5	PBS	C	602	-	41,42,42	0.65	1 (2%)	47,51,51	0.84	2 (4%)
6	R16	C	702	-	15,15,15	0.64	0	14,14,14	0.31	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	NAG	A	500	1	-	0/6/23/26	0/1/1/1
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
5	PBS	A	601	-	-	0/40/60/60	0/1/1/1
6	R16	A	701	-	-	0/13/13/13	0/0/0/0
3	NAG	C	501	1	-	0/6/23/26	0/1/1/1
5	PBS	C	602	-	-	0/40/60/60	0/1/1/1
6	R16	C	702	-	-	0/13/13/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAG	O5-C1	-2.08	1.40	1.43
5	C	602	PBS	OC1-CG1	2.19	1.44	1.40
5	A	601	PBS	C1-N	2.36	1.50	1.46
5	A	601	PBS	OC1-CG1	4.37	1.48	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	NAG	C2-N2-C7	-2.74	119.52	123.04
5	C	602	PBS	C5-C4-C3	-2.41	109.88	114.20
5	A	601	PBS	O2-C18-C19	-2.04	118.46	121.98
3	C	501	NAG	O4-C4-C5	2.03	114.62	109.24
5	C	602	PBS	C-OC1-CG1	2.08	118.19	113.82
5	A	601	PBS	C2-C1-N	2.20	114.67	110.31
3	A	501	NAG	C4-C3-C2	2.49	115.10	111.23
5	A	601	PBS	OG-CG-CG4	2.50	114.37	109.68
3	A	501	NAG	C1-O5-C5	2.68	115.65	112.25
5	A	601	PBS	C-OC1-CG1	3.60	121.38	113.82
5	A	601	PBS	OC1-CG1-CG2	4.11	113.23	108.04
3	C	501	NAG	C1-O5-C5	4.51	117.97	112.25
3	A	500	NAG	C1-O5-C5	4.73	118.25	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	PBS	2	0
6	C	702	R16	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	265/285 (92%)	0.93	24 (9%)	11	11	61, 73, 82, 91	9 (3%)
1	C	266/285 (93%)	0.72	18 (6%)	20	20	65, 73, 82, 88	12 (4%)
2	B	98/99 (98%)	0.62	4 (4%)	41	39	67, 73, 81, 87	7 (7%)
2	D	98/99 (98%)	0.62	4 (4%)	41	39	65, 73, 80, 89	7 (7%)
All	All	727/768 (94%)	0.77	50 (6%)	20	19	61, 73, 82, 91	35 (4%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	GLY	5.2
1	C	7	ASN	4.1
1	C	201	HIS	3.9
1	A	93	ASP	3.8
1	A	23	TRP	3.6
1	A	272	GLY	3.5
1	C	271	GLY	3.5
1	A	95	PRO	3.4
2	B	99	MET	3.3
1	A	108	PRO	3.1
2	B	88	ALA	3.1
1	C	8	TYR	3.1
1	A	168	CYS	3.1
1	A	19	ALA	3.0
1	C	230	GLN	2.9
1	A	22	SER	2.8
1	A	96	ILE	2.7
1	C	276	ILE	2.7
1	A	219	TRP	2.7
1	C	149	VAL	2.6
1	A	94	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	19	ALA	2.6
1	A	47	ILE	2.5
1	C	215	PRO	2.5
1	C	189	PRO	2.4
1	A	170	LEU	2.3
1	A	173	ARG	2.3
2	D	99	MET	2.3
1	C	219	TRP	2.3
1	C	214	TYR	2.3
2	D	22	ILE	2.2
1	A	116	LEU	2.2
1	A	37	THR	2.2
2	B	48	LYS	2.2
2	D	34	HIS	2.2
1	C	23	TRP	2.2
1	A	177	GLU	2.2
1	A	265	VAL	2.2
1	A	234	ARG	2.1
1	A	273	GLN	2.1
1	C	89	SER	2.1
2	B	87	MET	2.1
1	C	82	GLN	2.1
1	C	197	PRO	2.1
1	A	220	VAL	2.1
1	A	31	TRP	2.1
1	C	255	ALA	2.1
2	D	37	ILE	2.0
1	C	253	VAL	2.0
1	A	11	ARG	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	511	14/15	0.92	0.21	0.49	64,67,71,72	0
4	NAG	A	511	14/15	0.95	0.22	0.44	63,68,70,71	0
4	NAG	A	512	14/15	0.83	0.24	-	67,71,76,78	0
4	NAG	C	512	14/15	0.90	0.21	-	70,72,75,75	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
6	R16	C	702	16/16	0.75	0.32	5.53	82,84,86,87	0
6	R16	A	701	16/16	0.72	0.35	4.92	80,83,87,87	0
5	PBS	C	602	42/42	0.92	0.20	1.56	72,78,84,87	0
5	PBS	A	601	42/42	0.88	0.19	0.25	74,79,88,93	0
3	NAG	A	501	14/15	0.90	0.17	-	71,74,76,77	0
3	NAG	C	501	14/15	0.86	0.15	-	75,77,80,83	0
3	NAG	A	500	14/15	0.56	0.31	-	74,76,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.