



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:19 AM GMT

PDB ID : 3SDD
Title : Crystal structure of autoreactive-Valpha14-Vbeta6NKT TCR in complex with CD1d-beta-lactosylceramide
Authors : Clarke, A.J.; Rossjohn, J.
Deposited on : 2011-06-09
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

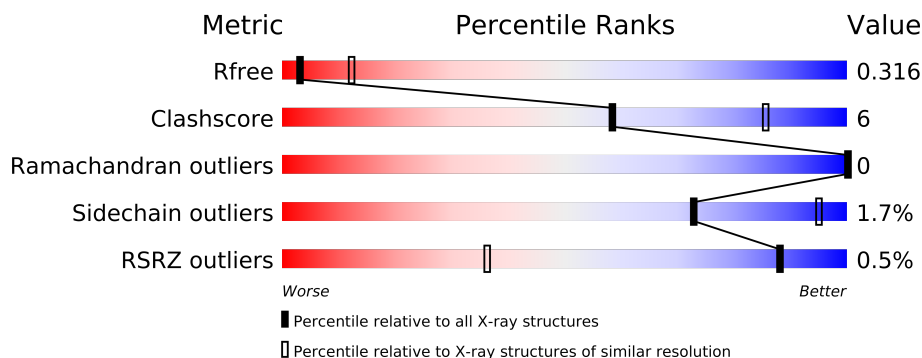
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	302	
2	B	99	
3	C	207	
4	D	245	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	3GD	A	307	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6647 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	2333	1486	406	427	14	6	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	EXPRESSION TAG	UNP P11609
A	281	SER	-	EXPRESSION TAG	UNP P11609
A	282	LEU	-	EXPRESSION TAG	UNP P11609
A	283	HIS	-	EXPRESSION TAG	UNP P11609
A	284	HIS	-	EXPRESSION TAG	UNP P11609
A	285	ILE	-	EXPRESSION TAG	UNP P11609
A	286	LEU	-	EXPRESSION TAG	UNP P11609
A	287	ASP	-	EXPRESSION TAG	UNP P11609
A	288	ALA	-	EXPRESSION TAG	UNP P11609
A	289	GLN	-	EXPRESSION TAG	UNP P11609
A	290	LYS	-	EXPRESSION TAG	UNP P11609
A	291	MET	-	EXPRESSION TAG	UNP P11609
A	292	VAL	-	EXPRESSION TAG	UNP P11609
A	293	TRP	-	EXPRESSION TAG	UNP P11609
A	294	ASN	-	EXPRESSION TAG	UNP P11609
A	295	HIS	-	EXPRESSION TAG	UNP P11609
A	296	ARG	-	EXPRESSION TAG	UNP P11609
A	297	HIS	-	EXPRESSION TAG	UNP P11609
A	298	HIS	-	EXPRESSION TAG	UNP P11609
A	299	HIS	-	EXPRESSION TAG	UNP P11609
A	300	HIS	-	EXPRESSION TAG	UNP P11609
A	301	HIS	-	EXPRESSION TAG	UNP P11609
A	302	HIS	-	EXPRESSION TAG	UNP P11609

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	1	0	0
			814	520	138	149	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	SEE REMARK 999	UNP P01887

- Molecule 3 is a protein called NKT TCR Valpha14 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	189	Total	C	N	O	S	3	0	0
			1462	905	252	298	7			

- Molecule 4 is a protein called NKT TCR autoreactive-Vbeta6 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	238	Total	C	N	O	S	6	0	0
			1886	1191	324	364	7			

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

There are 24 discrepancies between the modelled and reference sequences:

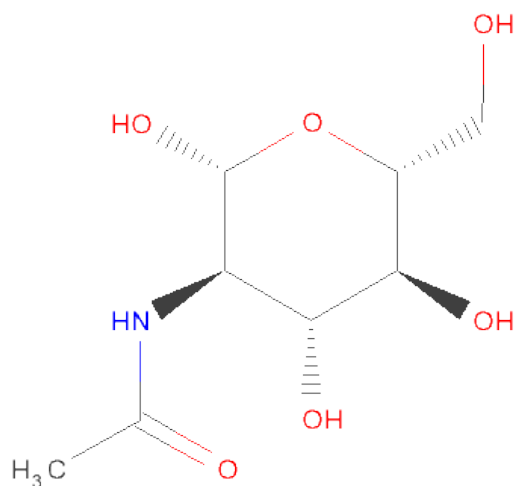
Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	EXPRESSION TAG	UNP P11609
A	281	SER	-	EXPRESSION TAG	UNP P11609
A	282	LEU	-	EXPRESSION TAG	UNP P11609
A	283	HIS	-	EXPRESSION TAG	UNP P11609
A	284	HIS	-	EXPRESSION TAG	UNP P11609
A	285	ILE	-	EXPRESSION TAG	UNP P11609
A	286	LEU	-	EXPRESSION TAG	UNP P11609
A	287	ASP	-	EXPRESSION TAG	UNP P11609
A	288	ALA	-	EXPRESSION TAG	UNP P11609
A	289	GLN	-	EXPRESSION TAG	UNP P11609
A	290	LYS	-	EXPRESSION TAG	UNP P11609
A	291	MET	-	EXPRESSION TAG	UNP P11609

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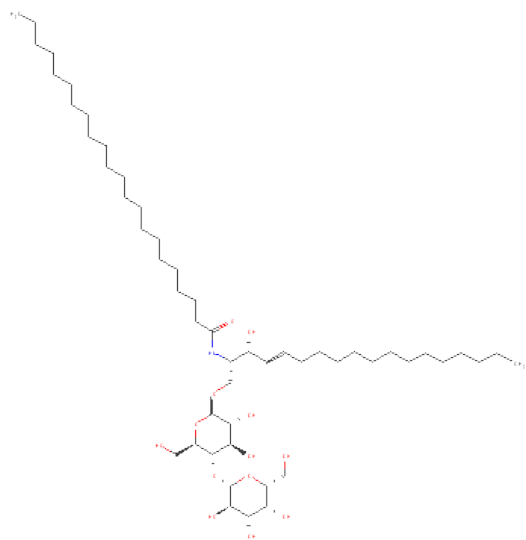
Chain	Residue	Modelled	Actual	Comment	Reference
A	292	VAL	-	EXPRESSION TAG	UNP P11609
A	293	TRP	-	EXPRESSION TAG	UNP P11609
A	294	ASN	-	EXPRESSION TAG	UNP P11609
A	295	HIS	-	EXPRESSION TAG	UNP P11609
A	296	ARG	-	EXPRESSION TAG	UNP P11609
A	297	HIS	-	EXPRESSION TAG	UNP P11609
A	298	HIS	-	EXPRESSION TAG	UNP P11609
A	299	HIS	-	EXPRESSION TAG	UNP P11609
A	300	HIS	-	EXPRESSION TAG	UNP P11609
A	301	HIS	-	EXPRESSION TAG	UNP P11609
A	302	HIS	-	EXPRESSION TAG	UNP P11609

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is N-[(2S,3R,4E)-1-{[4-O-(BETA-D-GALACTOPYRANOSYL)-BETA-D-GALACTOPYRANOSYL]OXY}-3-HYDROXYOCTADEC-4-EN-2-YL]DOCOSANAMIDE (three-letter code: 3GD) (formula: $C_{52}H_{99}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			66	52	1	13		

- Molecule 8 is water.

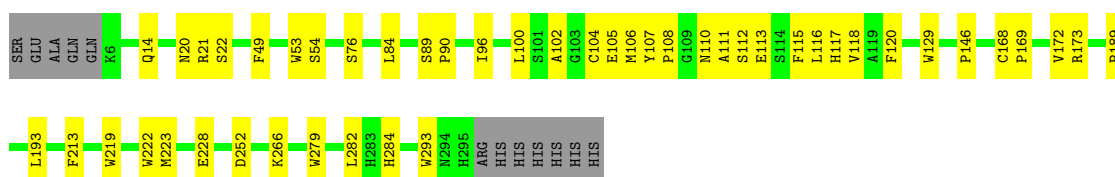
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	14	Total	O	0	0
			14	14		
8	B	2	Total	O	0	0
			2	2		
8	C	3	Total	O	0	0
			3	3		
8	D	11	Total	O	0	0
			11	11		

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: Antigen-presenting glycoprotein CD1d1

Chain A: 



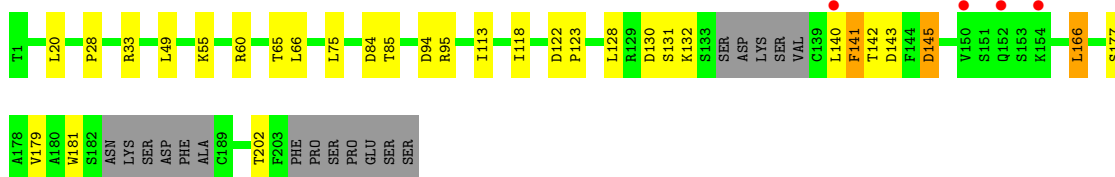
- Molecule 2: Beta-2-microglobulin

Chain B: 



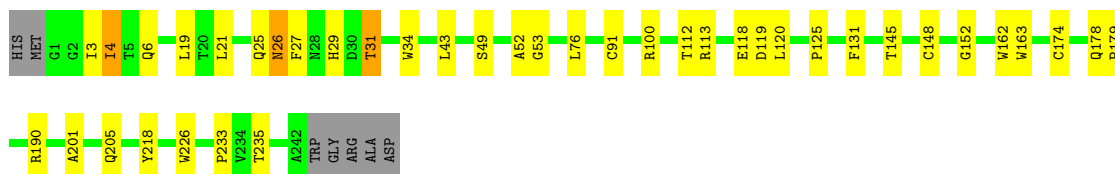
- Molecule 3: NKT TCR Valpha14 chain

Chain C: 



- Molecule 4: NKT TCR autoreactive-Vbeta6 chain

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.47Å 94.47Å 291.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.85 – 3.00 89.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (89.85-3.00) 99.7 (89.85-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.258 , 0.318 0.258 , 0.316	Depositor DCC
R_{free} test set	1371 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 27353 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6647	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 3GD

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	0.62	2/2403 (0.1%)	0.55	2/3266 (0.1%)
2	B	0.49	0/840	0.49	0/1140
3	C	0.41	1/1485 (0.1%)	0.48	0/2015
4	D	0.48	2/1931 (0.1%)	0.52	0/2617
All	All	0.52	5/6659 (0.1%)	0.52	2/9038 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	181	TRP	CD2-CE2	5.03	1.47	1.41
1	A	293	TRP	CD2-CE2	5.02	1.47	1.41
4	D	34	TRP	CD2-CE2	5.02	1.47	1.41
4	D	163	TRP	CD2-CE2	5.01	1.47	1.41
1	A	53	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	SER	N-CA-CB	-5.55	102.18	110.50
1	A	22	SER	N-CA-C	5.18	124.98	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2333	0	2233	26	0
2	B	814	0	788	2	0
3	C	1462	0	1413	20	0
4	D	1886	0	1820	37	0
5	A	28	0	25	0	0
6	A	28	0	26	0	0
7	A	66	0	99	0	0
8	A	14	0	0	0	0
8	B	2	0	0	0	0
8	C	3	0	0	0	0
8	D	11	0	0	1	0
All	All	6647	0	6404	80	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (80) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:52:ALA:CB	4:D:53:GLY:HA3	1.70	1.21
4:D:52:ALA:HB1	4:D:53:GLY:HA3	1.13	1.10
4:D:52:ALA:CB	4:D:53:GLY:CA	2.50	0.89
4:D:3:ILE:O	4:D:26:ASN:ND2	2.04	0.89
4:D:43:LEU:HD12	4:D:43:LEU:N	1.95	0.80
4:D:52:ALA:HB1	4:D:53:GLY:CA	2.07	0.79
4:D:43:LEU:HD12	4:D:43:LEU:H	1.49	0.77
4:D:26:ASN:ND2	4:D:26:ASN:H	1.86	0.74
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.69	0.74
1:A:107:TYR:CD2	1:A:111:ALA:HB3	2.24	0.71
1:A:110:ASN:HB2	1:A:173:ARG:NH1	2.05	0.71
1:A:107:TYR:HD2	1:A:111:ALA:HB3	1.55	0.70
4:D:26:ASN:HD22	4:D:26:ASN:H	1.38	0.69
4:D:25:GLN:NE2	4:D:29:HIS:HB2	2.08	0.68
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.77	0.67
3:C:166:LEU:HB3	4:D:174:CYS:HB2	1.77	0.67
1:A:102:ALA:HB2	1:A:116:LEU:HD13	1.78	0.65
1:A:89:SER:OG	1:A:90:PRO:HD3	1.98	0.64
4:D:3:ILE:H	4:D:26:ASN:ND2	1.94	0.63
4:D:52:ALA:HB3	4:D:53:GLY:HA3	1.74	0.60
3:C:123:PRO:HB2	3:C:202:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:TYR:HB2	1:A:111:ALA:HB3	1.82	0.60
3:C:128:LEU:HB3	4:D:131:PHE:HB3	1.83	0.60
3:C:60:ARG:NH2	3:C:84:ASP:OD2	2.33	0.59
4:D:4:ILE:HD12	4:D:25:GLN:HB2	1.84	0.59
4:D:25:GLN:NE2	4:D:27:PHE:O	2.35	0.59
1:A:49:PHE:HD2	1:A:54:SER:HB2	1.67	0.58
3:C:85:THR:HG23	3:C:113:ILE:HA	1.85	0.58
1:A:76:SER:HA	3:C:95:ARG:HH21	1.69	0.58
4:D:201:ALA:O	4:D:205:GLN:HG2	2.05	0.56
4:D:26:ASN:ND2	4:D:26:ASN:N	2.54	0.56
4:D:148:CYS:HB2	4:D:162:TRP:CZ2	2.42	0.55
1:A:279:TRP:O	1:A:284:HIS:ND1	2.39	0.55
4:D:52:ALA:HB3	4:D:53:GLY:CA	2.34	0.54
3:C:55:LYS:HG2	3:C:65:THR:HG22	1.90	0.54
3:C:130:ASP:N	3:C:131:SER:HA	2.23	0.53
4:D:43:LEU:H	4:D:43:LEU:CD1	2.18	0.53
4:D:6:GLN:HE22	4:D:91:CYS:H	1.57	0.53
3:C:20:LEU:HD12	3:C:75:LEU:HD23	1.91	0.53
4:D:43:LEU:N	4:D:43:LEU:CD1	2.69	0.52
3:C:49:LEU:HD13	3:C:66:LEU:HB2	1.92	0.52
1:A:106:MET:HE3	1:A:172:VAL:HG21	1.92	0.51
1:A:115:PHE:HB2	1:A:117:HIS:CD2	2.45	0.51
2:B:36:GLU:HB3	2:B:83:LYS:HB2	1.92	0.51
1:A:14:GLN:HB3	1:A:100:LEU:HB2	1.93	0.51
4:D:152:GLY:HA2	4:D:190:ARG:HD3	1.93	0.50
4:D:6:GLN:NE2	4:D:91:CYS:H	2.11	0.49
4:D:113:ARG:HG3	8:D:258:HOH:O	2.13	0.48
4:D:21:LEU:HD22	4:D:112:THR:HG21	1.95	0.48
3:C:128:LEU:HD11	3:C:140:LEU:HD12	1.96	0.48
1:A:49:PHE:CD2	1:A:54:SER:HB2	2.47	0.47
3:C:28:PRO:HG2	3:C:94:ASP:O	2.15	0.47
4:D:118:GLU:HA	4:D:119:ASP:HA	1.56	0.47
4:D:218:TYR:HA	4:D:235:THR:HG23	1.97	0.47
1:A:129:TRP:HA	1:A:129:TRP:CE3	2.49	0.47
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.97	0.46
1:A:193:LEU:HD22	1:A:222:TRP:CH2	2.50	0.46
3:C:33:ARG:NH1	4:D:100:ARG:O	2.45	0.45
3:C:118:ILE:HD11	3:C:145:ASP:HA	1.99	0.45
3:C:131:SER:HB2	3:C:132:LYS:HA	1.98	0.45
1:A:219:TRP:HB3	1:A:266:LYS:HB2	1.99	0.44
1:A:84:LEU:HD22	1:A:146:PRO:HB3	1.99	0.44
4:D:125:PRO:HD3	4:D:233:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:MET:HG2	1:A:228:GLU:HA	2.00	0.43
3:C:166:LEU:H	3:C:166:LEU:HD13	1.83	0.43
1:A:100:LEU:HG	1:A:118:VAL:HG22	2.01	0.43
4:D:178:GLN:HA	4:D:179:PRO:HD3	1.91	0.43
3:C:140:LEU:HD11	4:D:145:THR:HB	2.00	0.42
1:A:20:ASN:O	1:A:21:ARG:C	2.57	0.42
3:C:141:PHE:O	3:C:177:SER:HA	2.19	0.42
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.01	0.42
3:C:122:ASP:O	3:C:143:ASP:HB2	2.20	0.42
3:C:142:THR:HG22	3:C:143:ASP:H	1.86	0.41
4:D:31:THR:HA	4:D:49:SER:O	2.21	0.41
1:A:104:CYS:HA	1:A:113:GLU:O	2.20	0.41
4:D:25:GLN:HE22	4:D:29:HIS:HB2	1.83	0.41
1:A:105:GLU:O	1:A:112:SER:HA	2.20	0.41
4:D:3:ILE:N	4:D:26:ASN:ND2	2.67	0.40
1:A:96:ILE:HG23	1:A:120:PHE:HE1	1.86	0.40
4:D:21:LEU:HD12	4:D:76:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	288/302 (95%)	279 (97%)	9 (3%)	0	100	100
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	C	183/207 (88%)	173 (94%)	10 (6%)	0	100	100
4	D	236/245 (96%)	224 (95%)	12 (5%)	0	100	100
All	All	804/853 (94%)	771 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	253/264 (96%)	251 (99%)	2 (1%)	89	98
2	B	92/93 (99%)	92 (100%)	0	100	100
3	C	169/186 (91%)	165 (98%)	4 (2%)	61	92
4	D	206/211 (98%)	200 (97%)	6 (3%)	55	90
All	All	720/754 (96%)	708 (98%)	12 (2%)	73	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	A	282	LEU
3	C	141	PHE
3	C	145	ASP
3	C	166	LEU
3	C	179	VAL
4	D	4	ILE
4	D	19	LEU
4	D	26	ASN
4	D	31	THR
4	D	120	LEU
4	D	226	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
1	A	248	GLN
2	B	42	ASN
3	C	72	HIS
3	C	127	GLN
4	D	6	GLN
4	D	25	GLN
4	D	26	ASN
4	D	84	ASN

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Mol	Chain	Res	Type
4	D	187	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	305	1,5	12,14,15	0.64	0	15,19,21	1.32	4 (26%)
5	NAG	A	306	5	12,14,15	0.67	0	15,19,21	1.02	1 (6%)

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	NAG	A	305	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	306	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	305	NAG	C4-C3-C2	2.32	116.99	111.32
5	A	305	NAG	C3-C4-C5	2.27	114.27	110.20
5	A	306	NAG	O5-C5-C6	2.21	109.31	106.98
5	A	305	NAG	O4-C4-C3	-2.21	105.39	110.35
5	A	305	NAG	C3-C2-N2	-2.00	108.71	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

3 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
6	NAG	A	303	1	12,14,15	0.45	0	15,19,21	1.53	3 (20%)
6	NAG	A	304	1	12,14,15	0.64	0	15,19,21	0.95	1 (6%)
7	3GD	A	307	-	67,67,67	1.05	4 (5%)	81,81,81	1.49	6 (7%)

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
6	NAG	A	303	1	-	0/6/23/26	0/1/1/1
6	NAG	A	304	1	-	0/6/23/26	0/1/1/1
7	3GD	A	307	-	-	0/57/97/97	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	307	3GD	O-C	4.60	1.53	1.43
7	A	307	3GD	CBW-CBV	4.55	1.53	1.31
7	A	307	3GD	OBC-CBB	2.75	1.45	1.40
7	A	307	3GD	C-CBW	2.32	1.54	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	307	3GD	C-CBW-CBV	-7.27	114.40	125.12
7	A	307	3GD	CA-C-CBW	7.02	121.37	111.84
6	A	303	NAG	O5-C5-C4	3.94	115.65	110.65
6	A	303	NAG	O5-C5-C6	3.28	110.42	106.98
7	A	307	3GD	OBC-CBB-CAW	3.11	112.14	108.18
7	A	307	3GD	CBU-CBV-CBW	-2.40	116.20	125.64
6	A	304	NAG	O5-C5-C6	2.21	109.30	106.98
7	A	307	3GD	CBB-OBG-CAZ	-2.15	109.54	113.73
6	A	303	NAG	C3-C4-C5	2.14	114.02	110.20
7	A	307	3GD	OBF-CAL-OAU	-2.13	105.38	110.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	290/302 (96%)	-0.04	0	100 100	53, 66, 81, 97	4 (1%)
2	B	99/99 (100%)	0.03	0	100 100	54, 67, 80, 84	1 (1%)
3	C	189/207 (91%)	0.13	4 (2%)	60 12	57, 76, 136, 144	2 (1%)
4	D	238/245 (97%)	0.04	0	100 100	57, 94, 119, 126	3 (1%)
All	All	816/853 (95%)	0.03	4 (0%)	88 36	53, 72, 121, 144	10 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	140	LEU	2.7
3	C	152	GLN	2.6
3	C	154	LYS	2.4
3	C	150	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	305	14/15	0.20	2.44	74,76,77,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	306	14/15	0.18	0.39	81,82,84,84	0

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	3GD	A	307	66/66	0.46	3.57	60,68,90,92	20
6	NAG	A	304	14/15	0.17	-1.11	74,75,76,76	0
6	NAG	A	303	14/15	0.16	-2.16	82,84,84,84	0

6.5 Other polymers

There are no such residues in this entry.