



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:35 PM GMT

PDB ID : 4EN3
Title : Crystal structure of a human Valpha24(-) NKT TCR in complex with CD1d/
alpha-galactosylceramide
Authors : Lopez-Sagaseta, J; Adams, E.J.
Deposited on : 2012-04-12
Resolution : 2.57 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>

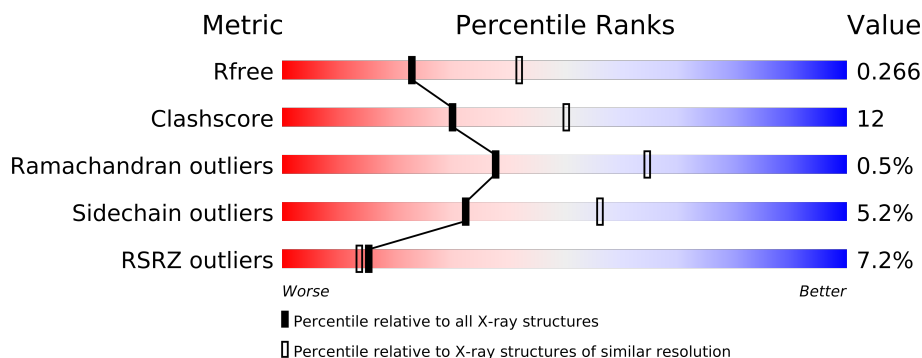
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.57 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	2347 (2.60-2.52)
Clashscore	79885	2876 (2.60-2.52)
Ramachandran outliers	78287	2826 (2.60-2.52)
Sidechain outliers	78261	2826 (2.60-2.52)
RSRZ outliers	66119	2347 (2.60-2.52)

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	C	284	
2	A	220	
3	B	259	
4	D	100	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	B	302	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6389 atoms, of which 8 are hydrogens 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 CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	257	Total	C	N	O	S	0	0	0
			2056	1323	351	375	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	EXPRESSION TAG	UNP P15813
C	1	ASP	-	EXPRESSION TAG	UNP P15813
C	2	PRO	-	EXPRESSION TAG	UNP P15813
C	278	HIS	-	EXPRESSION TAG	UNP P15813
C	279	HIS	-	EXPRESSION TAG	UNP P15813
C	280	HIS	-	EXPRESSION TAG	UNP P15813
C	281	HIS	-	EXPRESSION TAG	UNP P15813
C	282	HIS	-	EXPRESSION TAG	UNP P15813
C	283	HIS	-	EXPRESSION TAG	UNP P15813

- Molecule 2 is a protein called HUMAN NKT TCR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	186	Total	C	N	O	S	0	0	0
			1369	858	231	273	7			

- Molecule 3 is a protein called HUMAN NKT TCR BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	240	Total	C	N	O	S	0	0	0
			1892	1193	326	365	8			

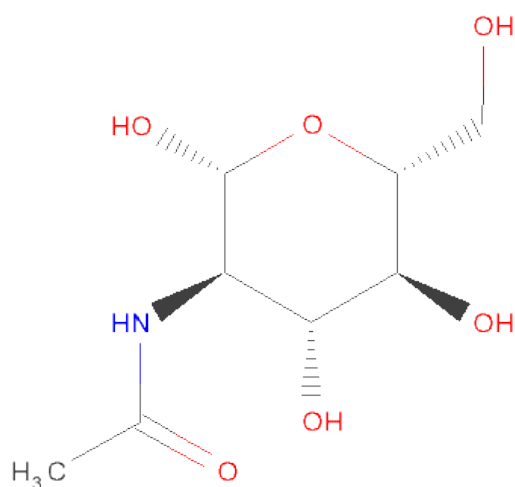
- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	99	Total	C	N	O	S	0	0	0
			811	517	135	157	2			

There is a discrepancy between the modelled and reference sequences:

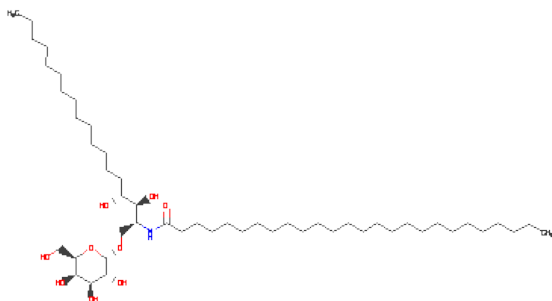
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PRO	-	EXPRESSION TAG	UNP P61769

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



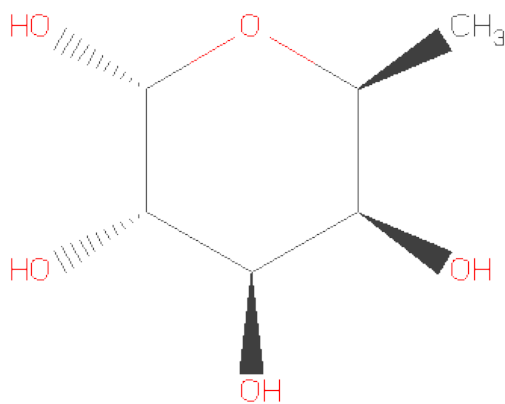
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O		0	0
			14	8	1	5			
5	C	1	Total	C	N	O		0	0
			14	8	1	5			
5	C	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	B	1	Total	C	N	O		0	0
			14	8	1	5			

- Molecule 6 is SUGAR (N-{(1S,2R,3S)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}HEXACOSANAMIDE) (three-letter code: AGH) (formula: $C_{50}H_{99}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			60	50	1	9		

- Molecule 7 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

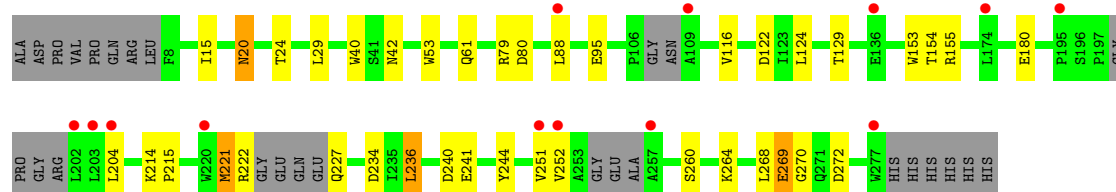
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	33	Total	H	O	0	0
			35	2	33		
9	A	20	Total	H	O	0	0
			22	2	20		
9	B	26	Total	H	O	0	0
			30	4	26		
9	D	22	Total	O		0	0
			22	22			

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.

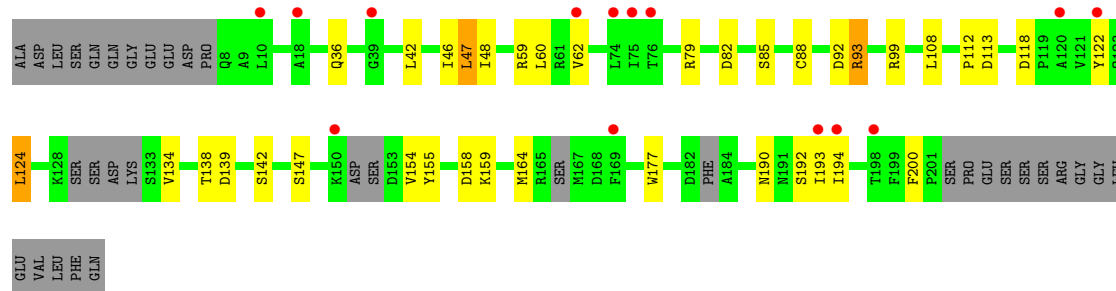
- Molecule 1: Antigen-presenting glycoprotein CD1d

Chain C: 



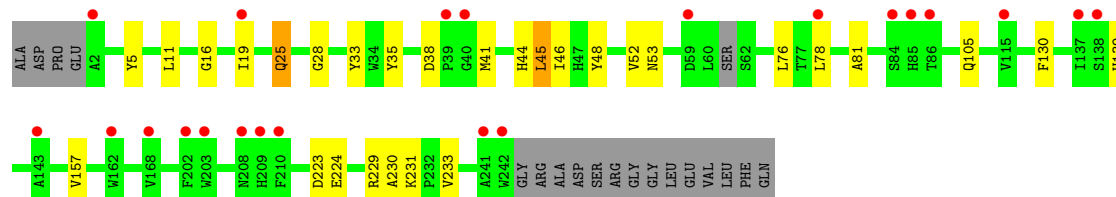
- Molecule 2: HUMAN NKT TCR ALPHA CHAIN

Chain A: 



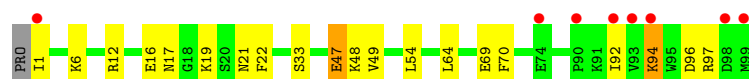
- Molecule 3: HUMAN NKT TCR BETA CHAIN

Chain B: 



- Molecule 4: Beta-2-microglobulin

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.11Å 72.57Å 113.75Å 90.00° 103.31° 90.00°	Depositor
Resolution (Å)	44.01 – 2.57 44.01 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.01-2.57) 93.1 (44.01-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.208 , 0.266 0.208 , 0.266	Depositor DCC
R_{free} test set	1378 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.9	EDS
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 28902 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6389	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: GOL, AGH, FUC, NAG

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	C	0.21	0/2116	0.37	0/2882
2	A	0.21	0/1392	0.37	0/1896
3	B	0.21	0/1944	0.39	0/2651
4	D	0.21	0/834	0.37	0/1134
All	All	0.21	0/6286	0.38	0/8563

There are no bond length outliers.

There are no bond angle outliers.

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	C	2056	0	15	25	0
2	A	1369	0	12	23	0
3	B	1892	0	31	17	0
4	D	811	0	48	10	0
5	A	14	0	13	6	0
5	B	14	0	13	2	0
5	C	42	0	39	8	0
6	C	60	0	99	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	10	0	10	4	0
8	B	12	0	16	4	0
9	A	20	2	0	2	0
9	B	26	4	0	1	0
9	C	33	2	0	0	0
9	D	22	0	0	1	0
All	All	6381	8	296	79	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 12.

All (79) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:301:NAG:H4	5:C:302:NAG:C1	2.03	0.88
2:A:200:PHE:CE2	5:A:302:NAG:H5	2.18	0.78
1:C:264:LYS:NZ	1:C:272:ASP:OD2	2.17	0.78
1:C:240:ASP:OD2	4:D:12:ARG:NH1	2.21	0.73
5:C:301:NAG:O4	5:C:302:NAG:H4	1.89	0.73
2:A:99:ARG:NH2	9:A:1116:HOH:O	2.21	0.72
1:C:42:ASN:ND2	5:C:301:NAG:C1	2.53	0.71
1:C:153:TRP:CZ3	6:C:304:AGH:HAB1	2.29	0.68
5:C:301:NAG:C4	5:C:302:NAG:C1	2.73	0.67
8:B:301:GOL:O3	8:B:301:GOL:O1	2.12	0.66
4:D:47:GLU:O	4:D:49:VAL:N	2.30	0.65
1:C:79:ARG:NH2	2:A:92:ASP:OD2	2.30	0.65
3:B:25:GLN:OE1	3:B:28:GLY:N	2.32	0.63
1:C:80:ASP:OD1	2:A:93:ARG:NH1	2.32	0.62
3:B:230:ALA:O	9:B:414:HOH:O	2.17	0.60
2:A:142:SER:O	2:A:159:LYS:NZ	2.35	0.60
3:B:223:ASP:O	3:B:231:LYS:NZ	2.36	0.59
1:C:61:GLN:OE1	1:C:61:GLN:N	2.37	0.58
1:C:20:ASN:ND2	5:C:303:NAG:C1	2.68	0.56
5:C:301:NAG:O7	5:C:301:NAG:C1	2.52	0.55
4:D:21:ASN:OD1	4:D:22:PHE:N	2.40	0.55
1:C:268:LEU:O	1:C:270:GLY:N	2.40	0.55
1:C:154:THR:CG2	6:C:304:AGH:HAB2	2.38	0.54
2:A:158:ASP:OD1	2:A:159:LYS:N	2.41	0.54
5:B:302:NAG:O3	5:B:302:NAG:H83	2.08	0.53
1:C:15:ILE:CD1	4:D:54:LEU:CD1	2.88	0.52
7:A:301:FUC:O5	5:A:302:NAG:N2	2.43	0.51
3:B:35:TYR:OH	3:B:105:GLN:OE1	2.28	0.51
1:C:95:GLU:OE2	4:D:33:SER:OG	2.29	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:16:GLY:N	3:B:81:ALA:O	2.44	0.50
2:A:46:ILE:CG2	2:A:62:VAL:CG2	2.89	0.50
2:A:47:LEU:CD1	2:A:48:ILE:N	2.73	0.50
7:A:301:FUC:C1	5:A:302:NAG:C3	2.91	0.49
3:B:52:VAL:O	3:B:53:ASN:CB	2.60	0.48
2:A:122:TYR:OH	3:B:139:HIS:ND1	2.47	0.48
3:B:38:ASP:O	3:B:41:MET:N	2.46	0.48
2:A:59:ARG:NH1	2:A:82:ASP:OD2	2.47	0.48
4:D:1:ILE:O	4:D:1:ILE:CG1	2.62	0.47
2:A:147:SER:N	2:A:192:SER:OG	2.46	0.47
1:C:129:THR:O	1:C:155:ARG:CG	2.62	0.47
4:D:16:GLU:CG	4:D:19:LYS:HE3	2.45	0.47
4:D:17:ASN:OD1	4:D:97:ARG:NH2	2.47	0.47
3:B:53:ASN:ND2	5:B:302:NAG:C1	2.78	0.47
1:C:116:VAL:CG1	1:C:124:LEU:CG	2.93	0.47
7:A:301:FUC:C1	5:A:302:NAG:H3	2.45	0.46
1:C:40:TRP:CE3	6:C:304:AGH:HAM1	2.50	0.46
3:B:41:MET:CA	3:B:41:MET:CE	2.94	0.46
2:A:79:ARG:O	2:A:82:ASP:N	2.49	0.46
3:B:48:TYR:CE2	8:B:301:GOL:H2	2.51	0.46
1:C:24:THR:O	5:C:301:NAG:O7	2.35	0.45
2:A:193:ILE:N	2:A:193:ILE:CD1	2.80	0.45
7:A:301:FUC:C1	5:A:302:NAG:O3	2.65	0.45
1:C:221:MET:N	1:C:260:SER:O	2.50	0.45
4:D:94:LYS:NZ	9:D:101:HOH:O	2.50	0.44
3:B:44:HIS:CA	8:B:303:GOL:H11	2.47	0.44
6:C:304:AGH:N2	6:C:304:AGH:H51	2.28	0.44
1:C:236:LEU:O	1:C:244:TYR:N	2.51	0.44
2:A:138:THR:OG1	2:A:139:ASP:N	2.51	0.44
1:C:234:ASP:OD2	4:D:6:LYS:NZ	2.51	0.44
2:A:47:LEU:CD1	2:A:47:LEU:C	2.86	0.44
2:A:113:ASP:N	9:A:1104:HOH:O	2.50	0.43
1:C:251:VAL:CG1	1:C:252:VAL:N	2.81	0.43
2:A:190:ASN:ND2	5:A:302:NAG:C7	2.82	0.43
3:B:231:LYS:O	3:B:233:VAL:N	2.51	0.43
1:C:53:TRP:NE1	1:C:180:GLU:OE1	2.52	0.43
2:A:112:PRO:O	2:A:142:SER:OG	2.37	0.42
1:C:116:VAL:CG1	1:C:124:LEU:CD1	2.97	0.42
1:C:214:LYS:N	1:C:215:PRO:CD	2.83	0.42
2:A:36:GLN:N	2:A:85:SER:O	2.53	0.42
3:B:45:LEU:N	8:B:303:GOL:H11	2.35	0.42
5:C:303:NAG:C7	5:C:303:NAG:HO3	2.33	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:118:ASP:N	2:A:139:ASP:O	2.52	0.41
1:C:204:LEU:N	1:C:204:LEU:CD1	2.83	0.41
1:C:240:ASP:O	1:C:241:GLU:CB	2.68	0.41
2:A:134:VAL:CG2	3:B:130:PHE:CE2	3.03	0.41
2:A:155:TYR:CD2	2:A:177:TRP:NE1	2.88	0.41
3:B:19:ILE:CD1	3:B:19:ILE:N	2.83	0.41
2:A:124:LEU:N	2:A:124:LEU:CD2	2.84	0.40
3:B:19:ILE:O	3:B:78:LEU:N	2.55	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	C	247/284 (87%)	240 (97%)	6 (2%)	1 (0%)	43	69
2	A	176/220 (80%)	165 (94%)	10 (6%)	1 (1%)	33	60
3	B	236/259 (91%)	220 (93%)	16 (7%)	0	100	100
4	D	97/100 (97%)	91 (94%)	4 (4%)	2 (2%)	11	18
All	All	756/863 (88%)	716 (95%)	36 (5%)	4 (0%)	38	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	48	LYS
1	C	269	GLU
2	A	164	MET
4	D	47	GLU

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	C	224/249 (90%)	215 (96%)	9 (4%)	42	70
2	A	137/195 (70%)	128 (93%)	9 (7%)	24	42
3	B	203/227 (89%)	193 (95%)	10 (5%)	35	59
4	D	90/95 (95%)	84 (93%)	6 (7%)	23	41
All	All	654/766 (85%)	620 (95%)	34 (5%)	32	56

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	ASN
1	C	29	LEU
1	C	88	LEU
1	C	122	ASP
1	C	221	MET
1	C	222	ARG
1	C	227	GLN
1	C	236	LEU
1	C	269	GLU
2	A	42	LEU
2	A	47	LEU
2	A	60	LEU
2	A	88	CYS
2	A	93	ARG
2	A	108	LEU
2	A	124	LEU
2	A	154	VAL
2	A	194	ILE
3	B	5	TYR
3	B	11	LEU
3	B	25	GLN
3	B	33	TYR
3	B	45	LEU
3	B	46	ILE
3	B	76	LEU
3	B	157	VAL
3	B	224	GLU
3	B	229	ARG
4	D	64	LEU
4	D	69	GLU

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Mol	Chain	Res	Type
4	D	70	PHE
4	D	92	ILE
4	D	94	LYS
4	D	96	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
7	FUC	A	301	-	9,10,11	0.85	0	10,14,16	1.25	1 (10%)
5	NAG	A	302	-	12,14,15	0.68	0	15,19,21	1.46	1 (6%)
8	GOL	B	301	-	5,5,5	0.32	0	5,5,5	0.31	0
5	NAG	B	302	-	12,14,15	0.69	1 (8%)	15,19,21	0.71	1 (6%)
8	GOL	B	303	-	5,5,5	0.33	0	5,5,5	0.30	0
5	NAG	C	301	-	12,14,15	0.58	0	15,19,21	1.15	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	302	-	12,14,15	0.54	0	15,19,21	0.94	1 (6%)
5	NAG	C	303	-	12,14,15	0.67	0	15,19,21	0.73	0
6	AGH	C	304	-	60,60,60	0.33	0	69,69,69	0.89	3 (4%)

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
7	FUC	A	301	-	-	0/0/17/20	0/1/1/1
5	NAG	A	302	-	-	0/6/23/26	0/1/1/1
8	GOL	B	301	-	-	0/4/4/4	0/0/0/0
5	NAG	B	302	-	-	0/6/23/26	0/1/1/1
8	GOL	B	303	-	-	0/4/4/4	0/0/0/0
5	NAG	C	301	-	-	0/6/23/26	0/1/1/1
5	NAG	C	302	-	-	0/6/23/26	0/1/1/1
5	NAG	C	303	-	-	1/6/23/26	0/1/1/1
6	AGH	C	304	-	-	0/58/78/78	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	302	NAG	O5-C5	-2.07	1.41	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	302	NAG	C3-C4-C5	3.25	116.01	110.20
6	C	304	AGH	C1-C2-N2	-3.12	105.36	109.74
6	C	304	AGH	C3-C2-N2	-2.95	104.92	110.91
7	A	301	FUC	O5-C5-C4	2.84	114.51	110.22
5	C	301	NAG	O5-C5-C4	2.83	114.24	110.65
5	C	302	NAG	O5-C5-C4	2.25	113.51	110.65
6	C	304	AGH	C4-C3-C2	-2.20	110.30	113.61
5	B	302	NAG	O5-C5-C6	2.00	109.08	106.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	303	NAG	C3-C2-N2-C7

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	C	257/284 (90%)	0.51	13 (5%) 27 26	35, 55, 89, 97	0
2	A	186/220 (84%)	0.57	14 (7%) 14 12	40, 67, 108, 124	0
3	B	240/259 (92%)	0.66	22 (9%) 9 8	35, 61, 106, 118	0
4	D	99/100 (99%)	0.56	8 (8%) 12 10	33, 59, 92, 113	0
All	All	782/863 (90%)	0.58	57 (7%) 15 13	33, 59, 102, 124	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	1	ILE	7.6
3	B	242	TRP	4.5
3	B	39	PRO	4.3
1	C	252	VAL	4.2
1	C	202	LEU	4.1
3	B	210	PHE	4.0
1	C	195	PRO	3.9
3	B	203	TRP	3.8
3	B	84	SER	3.5
1	C	251	VAL	3.3
1	C	257	ALA	3.1
1	C	136	GLU	3.1
4	D	74	GLU	3.1
2	A	120	ALA	3.0
4	D	99	MET	3.0
4	D	98	ASP	3.0
4	D	94	LYS	2.8
3	B	85	HIS	2.8
3	B	138	SER	2.8
3	B	202	PHE	2.7
4	D	93	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	B	2	ALA	2.6
3	B	208	ASN	2.6
3	B	209	HIS	2.5
2	A	193	ILE	2.5
3	B	19	ILE	2.5
3	B	59	ASP	2.5
1	C	109	ALA	2.5
3	B	137	ILE	2.5
1	C	204	LEU	2.5
2	A	169	PHE	2.4
3	B	78	LEU	2.4
2	A	62	VAL	2.4
3	B	40	GLY	2.4
3	B	168	VAL	2.3
2	A	150	LYS	2.3
1	C	88	LEU	2.3
3	B	86	THR	2.3
1	C	174	LEU	2.2
1	C	203	LEU	2.2
3	B	143	ALA	2.2
2	A	198	THR	2.2
2	A	39	GLY	2.2
1	C	277	TRP	2.2
4	D	90	PRO	2.2
2	A	75	ILE	2.1
4	D	92	ILE	2.1
3	B	115	VAL	2.1
2	A	76	THR	2.1
2	A	18	ALA	2.1
2	A	194	ILE	2.1
2	A	10	LEU	2.1
1	C	220	TRP	2.1
3	B	162	TRP	2.1
3	B	241	ALA	2.1
2	A	122	TYR	2.1
2	A	74	LEU	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 ⓘ

There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
5	NAG	B	302	14/15	0.22	3.00	104,105,108,109	0
8	GOL	B	301	6/6	0.24	1.95	55,60,62,62	0
6	AGH	C	304	60/60	0.23	1.74	32,48,61,63	0
8	GOL	B	303	6/6	0.24	0.68	41,57,59,61	0
5	NAG	A	302	14/15	0.26	0.53	98,105,112,114	0
5	NAG	C	303	14/15	0.21	0.42	75,92,95,96	0
5	NAG	C	301	14/15	0.19	-0.07	54,70,82,83	0
7	FUC	A	301	10/11	0.21	-0.31	112,116,121,124	0
5	NAG	C	302	14/15	0.15	-	102,107,111,112	0

6.5 Other polymers ⓘ

There are no such residues in this entry.