



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:35 am GMT

PDB ID : 3SDC  
Title : Crystal structure of autoreactive-Valpha14-Vbeta6 NKT TCR in complex with CD1d-globotrihexosylceramide  
Authors : Clarke, A.J.; Rossjohn, J.  
Deposited on : 2011-06-09  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

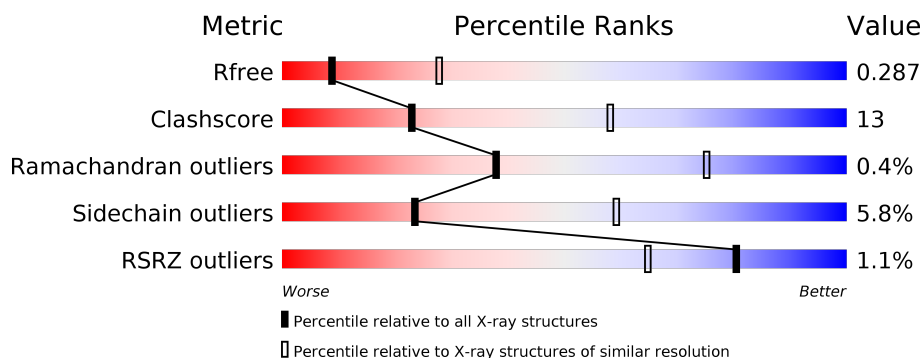
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	302	<div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
2	B	99	<div> <div>86%</div> <div>12%</div> <div>•</div> </div>
3	C	207	<div> <div>%</div> <div>66%</div> <div>22%</div> <div>• • 8%</div> </div>
4	D	245	<div> <div>3%</div> <div>71%</div> <div>22%</div> <div>• •</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6690 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	6	0	0
			2324	1480	404	426	14			

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	191	Total	C	N	O	S	3	0	0
			1478	915	254	302	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	5	0	0
			1900	1202	326	365	7			

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

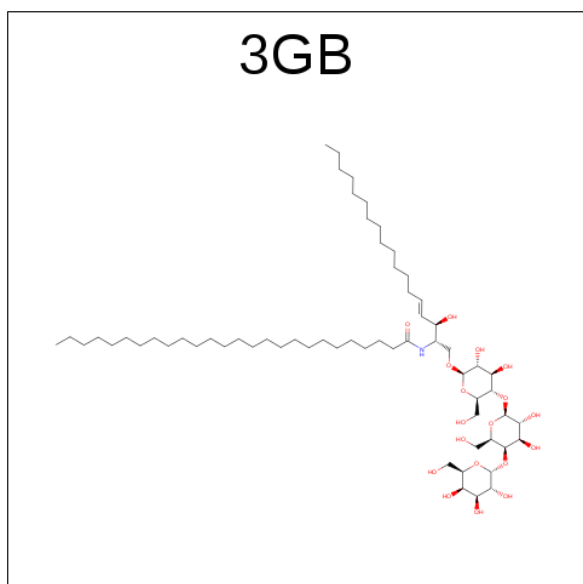
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

- 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-{[ALPHA-D-GALACTOPYRANOSYL-(1->4)-BETA-D-GALACTOPYRANOSYL-(1->4)-BETA-D-GLUCOPYRANOSYL]OXY}-3-HYDROXYOCTADEC-4-EN-2-YL]HEXACOSANAMIDE (three-letter code: 3GB) (formula:  $C_{62}H_{117}NO_{18}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			81	62	1	18		

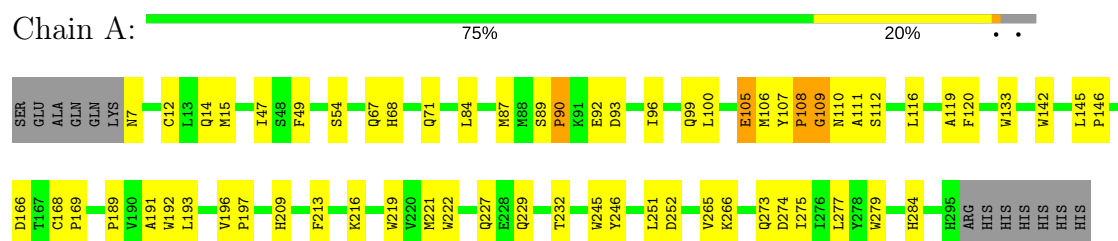
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	16	Total	O	0	0
			16	16		
8	B	8	Total	O	0	0
			8	8		
8	C	10	Total	O	0	0
			10	10		
8	D	3	Total	O	0	0
			3	3		

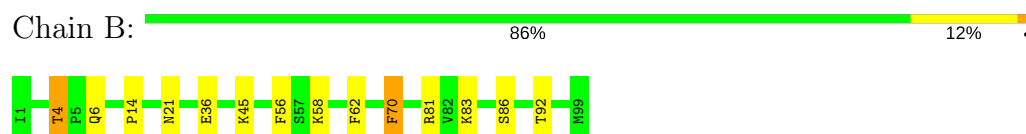
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

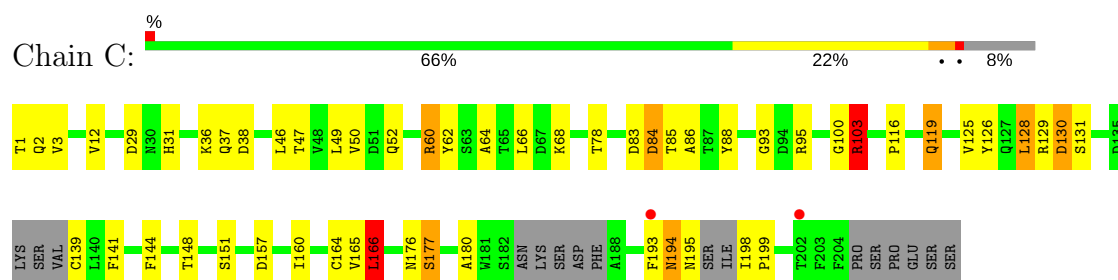
- Molecule 1: Antigen-presenting glycoprotein CD1d1



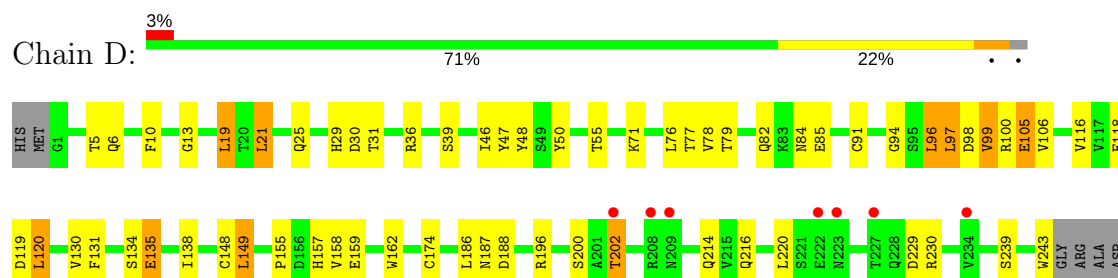
- Molecule 2: Beta-2-microglobulin



- Molecule 3: NKT TCR Valpha14 chain



- Molecule 4: NKT TCR autoreactive-Vbeta6 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.35Å 94.35Å 287.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.72 – 3.10 66.72 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (66.72-3.10) 97.5 (66.72-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.22	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.240 , 0.292 0.237 , 0.287	Depositor DCC
$R_{free}$ test set	1225 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 3GB, 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	A	0.46	0/2394	0.59	1/3255 (0.0%)
2	B	0.40	0/840	0.57	0/1140
3	C	0.40	0/1501	0.59	1/2035 (0.0%)
4	D	0.48	0/1947	0.60	0/2640
All	All	0.45	0/6682	0.59	2/9070 (0.0%)

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
3	C	0	1
4	D	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	GLY	N-CA-C	-6.64	96.49	113.10
3	C	166	LEU	CA-CB-CG	5.40	127.73	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PRO	Peptide

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Mol	Chain	Res	Type	Group
3	C	103	ARG	Mainchain
4	D	118	GLU	Peptide

## 5.2 Too-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 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	2324	0	2220	46	2
2	B	814	0	788	8	0
3	C	1478	0	1419	80	0
4	D	1900	0	1830	51	0
5	A	28	0	25	0	0
6	A	28	0	26	0	0
7	A	81	0	116	6	0
8	A	16	0	0	0	0
8	B	8	0	0	0	0
8	C	10	0	0	1	0
8	D	3	0	0	1	0
All	All	6690	0	6424	168	2

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 (168) 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)
3:C:129:ARG:N	3:C:130:ASP:HB2	1.35	1.38
4:D:96:LEU:C	4:D:97:LEU:HD23	1.51	1.29
3:C:129:ARG:CA	3:C:130:ASP:HB2	1.72	1.18
4:D:97:LEU:HD23	4:D:97:LEU:N	1.47	1.12
3:C:103:ARG:HD2	8:C:217:HOH:O	1.58	1.02
3:C:38:ASP:HA	3:C:86:ALA:HB2	1.48	0.94
3:C:129:ARG:N	3:C:130:ASP:CB	2.30	0.92
3:C:129:ARG:H	3:C:130:ASP:HB2	1.19	0.92
3:C:126:TYR:HB3	4:D:134:SER:HB3	1.53	0.90
3:C:38:ASP:HA	3:C:86:ALA:CB	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:ARG:CA	3:C:130:ASP:CB	2.52	0.87
3:C:37:GLN:O	3:C:86:ALA:HB1	1.76	0.85
3:C:103:ARG:HG2	3:C:103:ARG:HH11	1.38	0.85
3:C:60:ARG:NH2	3:C:84:ASP:OD1	2.11	0.84
3:C:95:ARG:HB2	3:C:100:GLY:HA3	1.62	0.81
4:D:120:LEU:HD11	4:D:220:LEU:HD21	1.62	0.81
3:C:60:ARG:HG2	3:C:78:THR:O	1.83	0.79
3:C:103:ARG:NH1	3:C:103:ARG:HG2	1.96	0.77
3:C:129:ARG:HA	3:C:130:ASP:HB2	1.61	0.77
3:C:177:SER:HB3	4:D:196:ARG:HD3	1.65	0.77
4:D:96:LEU:O	4:D:97:LEU:HD23	1.87	0.74
3:C:37:GLN:C	3:C:86:ALA:HB1	2.07	0.74
4:D:29:HIS:NE2	4:D:105:GLU:HG2	2.03	0.74
1:A:15:MET:HG2	2:B:62:PHE:HE2	1.54	0.72
1:A:14:GLN:HB3	1:A:100:LEU:HB2	1.72	0.72
3:C:129:ARG:HA	3:C:130:ASP:CB	2.19	0.71
3:C:128:LEU:CD1	3:C:139:CYS:HA	2.21	0.71
3:C:128:LEU:HD13	3:C:128:LEU:H	1.55	0.70
3:C:126:TYR:HB3	4:D:134:SER:CB	2.21	0.70
4:D:187:ASN:O	4:D:188:ASP:CG	2.31	0.69
3:C:128:LEU:HD11	3:C:139:CYS:HA	1.74	0.69
4:D:214:GLN:HA	4:D:239:SER:HB3	1.76	0.68
4:D:100:ARG:O	4:D:106:VAL:N	2.26	0.67
3:C:52:GLN:HA	3:C:68:LYS:HG3	1.77	0.66
4:D:19:LEU:HB2	4:D:78:VAL:HB	1.78	0.66
1:A:92:GLU:HG3	1:A:142:TRP:CZ2	2.32	0.65
1:A:109:GLY:HA3	1:A:110:ASN:C	2.17	0.65
3:C:129:ARG:H	3:C:130:ASP:CB	2.01	0.65
4:D:148:CYS:HB2	4:D:162:TRP:CH2	2.32	0.64
4:D:148:CYS:HB2	4:D:162:TRP:CZ2	2.31	0.64
2:B:21:ASN:HB3	2:B:70:PHE:CE2	2.33	0.64
3:C:31:HIS:HE1	4:D:99:VAL:HG21	1.63	0.63
1:A:145:LEU:HB3	1:A:146:PRO:HD3	1.79	0.63
4:D:188:ASP:OD1	4:D:188:ASP:C	2.37	0.63
1:A:89:SER:OG	1:A:90:PRO:HD3	1.99	0.62
3:C:128:LEU:HA	3:C:129:ARG:HB2	1.82	0.62
4:D:96:LEU:C	4:D:97:LEU:CD2	2.47	0.62
1:A:168:CYS:HB2	7:A:307:3GB:HDA	1.82	0.61
4:D:85:GLU:HB3	4:D:116:VAL:HG21	1.82	0.61
1:A:219:TRP:HB3	1:A:266:LYS:HB2	1.82	0.61
3:C:119:GLN:HE21	3:C:119:GLN:HA	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:CYS:O	3:C:177:SER:N	2.33	0.61
3:C:126:TYR:O	3:C:139:CYS:HB2	2.02	0.60
1:A:49:PHE:CD2	1:A:54:SER:HB2	2.37	0.59
3:C:139:CYS:N	3:C:180:ALA:O	2.36	0.59
3:C:38:ASP:HA	3:C:86:ALA:HB1	1.85	0.59
4:D:98:ASP:O	4:D:99:VAL:C	2.38	0.59
3:C:177:SER:CB	4:D:196:ARG:HD3	2.34	0.58
1:A:109:GLY:CA	1:A:110:ASN:C	2.72	0.58
1:A:12:CYS:HB3	7:A:307:3GB:HCOA	1.85	0.57
4:D:21:LEU:HD11	4:D:76:LEU:HD23	1.85	0.57
3:C:29:ASP:OD2	3:C:68:LYS:HD3	2.05	0.57
3:C:128:LEU:HA	3:C:129:ARG:CB	2.35	0.56
3:C:131:SER:O	4:D:130:VAL:O	2.22	0.56
1:A:191:ALA:HA	1:A:209:HIS:O	2.05	0.56
3:C:103:ARG:CG	3:C:103:ARG:HH11	2.12	0.56
3:C:160:ILE:HG21	3:C:193:PHE:HB3	1.88	0.55
4:D:77:THR:HG23	8:D:248:HOH:O	2.07	0.55
1:A:246:TYR:CD2	1:A:246:TYR:C	2.80	0.55
3:C:193:PHE:O	3:C:198:ILE:HD11	2.07	0.55
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.87	0.55
1:A:15:MET:HG2	2:B:62:PHE:CE2	2.40	0.55
7:A:307:3GB:OAV	3:C:68:LYS:NZ	2.40	0.54
3:C:36:LYS:HE2	3:C:86:ALA:HB3	1.90	0.54
4:D:187:ASN:O	4:D:188:ASP:CB	2.55	0.54
1:A:116:LEU:HD11	7:A:307:3GB:HCK	1.90	0.53
3:C:166:LEU:HB3	4:D:174:CYS:HB2	1.90	0.53
4:D:13:GLY:O	4:D:116:VAL:HA	2.09	0.53
1:A:265:VAL:HB	1:A:275:ILE:HB	1.90	0.53
4:D:85:GLU:HB3	4:D:116:VAL:CG2	2.38	0.53
1:A:105:GLU:HG2	1:A:107:TYR:CZ	2.44	0.53
4:D:94:GLY:HA2	4:D:105:GLU:O	2.10	0.52
3:C:38:ASP:CA	3:C:86:ALA:CB	2.83	0.52
1:A:266:LYS:HE2	1:A:274:ASP:OD2	2.09	0.52
4:D:6:GLN:NE2	4:D:91:CYS:H	2.08	0.52
3:C:29:ASP:OD1	3:C:29:ASP:N	2.41	0.52
4:D:21:LEU:CD1	4:D:76:LEU:HB3	2.39	0.51
1:A:279:TRP:O	1:A:284:HIS:ND1	2.43	0.51
3:C:160:ILE:HD13	3:C:193:PHE:HB3	1.93	0.51
1:A:106:MET:O	1:A:107:TYR:CD1	2.64	0.51
1:A:193:LEU:HG	1:A:277:LEU:HD23	1.92	0.51
3:C:49:LEU:HD13	3:C:66:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD12	1:A:67:GLN:HG3	1.93	0.50
3:C:95:ARG:HB2	3:C:100:GLY:CA	2.37	0.50
3:C:166:LEU:HD12	3:C:177:SER:OG	2.11	0.50
3:C:46:LEU:HD22	3:C:62:TYR:CE1	2.46	0.50
1:A:133:TRP:CZ2	7:A:307:3GB:HBS	2.46	0.50
3:C:141:PHE:HB2	3:C:193:PHE:HZ	1.77	0.50
4:D:159:GLU:HB2	4:D:216:GLN:HB3	1.94	0.50
3:C:47:THR:HG21	3:C:64:ALA:HB3	1.94	0.49
3:C:194:ASN:O	3:C:195:ASN:HB2	2.12	0.49
1:A:107:TYR:O	1:A:109:GLY:O	2.30	0.49
3:C:177:SER:CB	4:D:196:ARG:CD	2.90	0.49
3:C:141:PHE:HB2	3:C:193:PHE:CZ	2.48	0.49
7:A:307:3GB:N	7:A:307:3GB:HBB	2.28	0.49
1:A:107:TYR:HB2	1:A:111:ALA:HB3	1.93	0.49
2:B:81:ARG:HD3	2:B:92:THR:OG1	2.13	0.49
3:C:128:LEU:O	3:C:128:LEU:HD22	2.13	0.48
1:A:84:LEU:HD22	1:A:146:PRO:HB3	1.95	0.48
3:C:1:THR:HG23	3:C:3:VAL:H	1.78	0.48
1:A:219:TRP:CZ2	1:A:221:MET:HG3	2.49	0.48
3:C:128:LEU:HB2	3:C:130:ASP:N	2.28	0.48
3:C:83:ASP:C	3:C:85:THR:H	2.17	0.48
4:D:82:GLN:HB2	4:D:85:GLU:HB2	1.95	0.48
1:A:196:VAL:HB	1:A:197:PRO:HD2	1.96	0.48
1:A:192:TRP:CE3	2:B:14:PRO:HG3	2.48	0.48
3:C:194:ASN:OD1	3:C:194:ASN:N	2.47	0.47
3:C:95:ARG:CB	3:C:100:GLY:HA3	2.38	0.47
1:A:105:GLU:HG2	1:A:107:TYR:CE1	2.50	0.47
4:D:36:ARG:HB2	4:D:46:ILE:HD11	1.97	0.47
2:B:36:GLU:HB3	2:B:83:LYS:HB2	1.96	0.47
3:C:128:LEU:HA	3:C:129:ARG:C	2.35	0.47
3:C:194:ASN:HA	3:C:198:ILE:HD12	1.97	0.46
4:D:10:PHE:HB3	4:D:157:HIS:ND1	2.30	0.46
1:A:49:PHE:CG	1:A:54:SER:HB2	2.50	0.46
3:C:38:ASP:CA	3:C:86:ALA:HB1	2.46	0.46
4:D:131:PHE:HE1	4:D:149:LEU:HB2	1.81	0.46
1:A:68:HIS:HA	1:A:71:GLN:OE1	2.16	0.46
4:D:96:LEU:O	4:D:97:LEU:CD2	2.60	0.45
1:A:92:GLU:CG	1:A:142:TRP:CZ2	2.99	0.45
4:D:135:GLU:HA	4:D:138:ILE:HD13	1.96	0.45
3:C:166:LEU:CD1	3:C:177:SER:OG	2.64	0.45
4:D:21:LEU:HD12	4:D:76:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:O	1:A:169:PRO:HD2	2.18	0.44
3:C:38:ASP:N	3:C:86:ALA:HB1	2.31	0.44
3:C:86:ALA:O	3:C:88:TYR:CE1	2.70	0.44
1:A:99:GLN:HG2	2:B:56:PHE:CE2	2.53	0.44
3:C:1:THR:OG1	3:C:2:GLN:N	2.48	0.44
1:A:96:ILE:HD12	1:A:120:PHE:CZ	2.53	0.43
1:A:216:LYS:HE3	1:A:245:TRP:CZ2	2.53	0.43
3:C:60:ARG:NH2	3:C:84:ASP:CG	2.70	0.43
3:C:128:LEU:CA	3:C:129:ARG:C	2.87	0.43
3:C:128:LEU:CA	3:C:129:ARG:HB2	2.48	0.43
3:C:116:PRO:HB3	3:C:165:VAL:HG11	2.00	0.43
1:A:87:MET:HG3	4:D:50:TYR:CD2	2.54	0.43
3:C:130:ASP:HA	4:D:131:PHE:HD2	1.82	0.43
3:C:194:ASN:HA	3:C:198:ILE:CD1	2.49	0.42
1:A:222:TRP:HD1	1:A:232:THR:HG23	1.84	0.42
3:C:93:GLY:HA2	3:C:103:ARG:O	2.19	0.42
3:C:144:PHE:CZ	3:C:176:ASN:HB3	2.54	0.42
1:A:105:GLU:HG2	1:A:107:TYR:OH	2.20	0.42
3:C:166:LEU:H	3:C:166:LEU:HD13	1.85	0.41
4:D:30:ASP:OD2	4:D:71:LYS:HE3	2.20	0.41
1:A:99:GLN:HB2	1:A:119:ALA:HB3	2.01	0.41
4:D:46:ILE:HG22	4:D:47:TYR:HD2	1.86	0.41
1:A:227:GLN:HE21	1:A:229:GLN:HE22	1.67	0.41
3:C:31:HIS:CE1	4:D:99:VAL:HG21	2.49	0.41
3:C:130:ASP:H	4:D:131:PHE:HD2	1.69	0.41
1:A:189:PRO:HB3	1:A:213:PHE:HB3	2.02	0.41
4:D:155:PRO:O	4:D:157:HIS:N	2.48	0.41
1:A:168:CYS:HB3	1:A:169:PRO:HD3	2.03	0.41
3:C:31:HIS:HE1	4:D:99:VAL:CG2	2.31	0.41
4:D:200:SER:HB3	4:D:202:THR:HG23	2.04	0.40
4:D:48:TYR:HE1	4:D:50:TYR:CE1	2.39	0.40
1:A:251:LEU:HD12	1:A:252:ASP:H	1.85	0.40
2:B:4:THR:HA	2:B:86:SER:HG	1.86	0.40
3:C:50:VAL:HG21	4:D:100:ARG:NH2	2.37	0.40
4:D:229:ASP:HB3	4:D:230:ARG:HE	1.87	0.40

All (2) 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:93:ASP:OD2	1:A:273:GLN:OE1[6_424]	1.25	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:OD2	1:A:273:GLN:CD[6_424]	1.96	0.24

## 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	287/302 (95%)	272 (95%)	14 (5%)	1 (0%)	44	79
2	B	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
3	C	183/207 (88%)	171 (93%)	11 (6%)	1 (0%)	32	71
4	D	237/245 (97%)	219 (92%)	17 (7%)	1 (0%)	38	75
All	All	804/853 (94%)	753 (94%)	48 (6%)	3 (0%)	38	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	105	GLU
1	A	90	PRO
3	C	84	ASP

### 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	252/264 (96%)	249 (99%)	3 (1%)	75	91
2	B	92/93 (99%)	87 (95%)	5 (5%)	26	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	170/186 (91%)	156 (92%)	14 (8%)	13	45
4	D	207/211 (98%)	187 (90%)	20 (10%)	9	35
All	All	721/754 (96%)	679 (94%)	42 (6%)	23	59

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	105	GLU
1	A	112	SER
2	B	4	THR
2	B	6	GLN
2	B	45	LYS
2	B	58	LYS
2	B	70	PHE
3	C	12	VAL
3	C	60	ARG
3	C	103	ARG
3	C	119	GLN
3	C	125	VAL
3	C	128	LEU
3	C	130	ASP
3	C	148	THR
3	C	151	SER
3	C	157	ASP
3	C	166	LEU
3	C	177	SER
3	C	194	ASN
3	C	199	PRO
4	D	5	THR
4	D	19	LEU
4	D	21	LEU
4	D	25	GLN
4	D	31	THR
4	D	39	SER
4	D	55	THR
4	D	79	THR
4	D	84	ASN
4	D	96	LEU
4	D	97	LEU
4	D	99	VAL

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Mol	Chain	Res	Type
4	D	119	ASP
4	D	120	LEU
4	D	135	GLU
4	D	149	LEU
4	D	158	VAL
4	D	186	LEU
4	D	202	THR
4	D	243	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	134	GLN
1	A	154	GLN
1	A	186	GLN
1	A	209	HIS
1	A	229	GLN
1	A	248	GLN
2	B	38	GLN
2	B	84	HIS
3	C	119	GLN
4	D	6	GLN
4	D	122	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

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	14,14,15	0.57	0	15,19,21	1.51	2 (13%)
5	NAG	A	306	5	14,14,15	0.69	0	15,19,21	1.83	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
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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	306	NAG	C1-O5-C5	-5.32	104.84	112.17
5	A	305	NAG	O4-C4-C3	-3.77	102.16	110.36
5	A	306	NAG	C4-C3-C2	3.00	115.42	111.02
5	A	305	NAG	C4-C3-C2	3.27	115.81	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	14,14,15	0.50	0	15,19,21	1.98	1 (6%)
6	NAG	A	304	1	14,14,15	0.48	0	15,19,21	1.61	1 (6%)
7	3GB	A	307	-	82,83,83	1.16	5 (6%)	99,103,103	1.07	9 (9%)

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	3GB	A	307	-	-	0/67/127/127	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	307	3GB	O-C	-6.37	1.30	1.43
7	A	307	3GB	CBU-CBV	-2.19	1.38	1.50
7	A	307	3GB	CCK-CCJ	-2.15	1.39	1.51
7	A	307	3GB	CCM-CCL	-2.02	1.40	1.51
7	A	307	3GB	O1-CAO	2.11	1.49	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	307	3GB	CB-OBC-CBB	-3.67	106.23	113.76
7	A	307	3GB	C1-O1-CAO	-3.48	109.52	118.00
7	A	307	3GB	CAL-OBF-CAY	-3.47	109.53	118.00
7	A	307	3GB	C-CBW-CBV	-2.54	121.80	125.22
7	A	307	3GB	CBB-OBG-CAZ	-2.26	109.47	113.72
7	A	307	3GB	C1-O5-C5	-2.25	109.47	113.72
7	A	307	3GB	CAL-OAU-CAP	-2.23	109.52	113.72
7	A	307	3GB	CCM-CCL-CCK	2.15	125.55	114.45
7	A	307	3GB	O-C-CA	2.84	115.56	107.90
6	A	304	NAG	C1-O5-C5	5.36	119.56	112.17
6	A	303	NAG	C1-O5-C5	6.55	121.19	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	307	3GB	6	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	289/302 (95%)	-0.07	0	100 100	38, 51, 65, 73	5 (1%)
2	B	99/99 (100%)	-0.10	0	100 100	41, 54, 65, 69	1 (1%)
3	C	191/207 (92%)	0.13	2 (1%)	82 67	38, 64, 112, 122	5 (2%)
4	D	239/245 (97%)	0.21	7 (2%)	52 28	40, 73, 96, 98	5 (2%)
All	All	818/853 (95%)	0.05	9 (1%)	80 65	38, 56, 101, 122	16 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	223	ASN	6.5
4	D	202	THR	3.9
4	D	208	ARG	3.6
4	D	227	THR	3.4
3	C	202	THR	2.8
4	D	234	VAL	2.5
4	D	222	GLU	2.4
3	C	193	PHE	2.3
4	D	209	ASN	2.2

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	306	14/15	0.84	0.23	-	67,68,70,70	0
5	NAG	A	305	14/15	0.96	0.25	-	55,56,60,64	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	3GB	A	307	81/81	0.94	0.34	1.69	37,45,60,61	0
6	NAG	A	304	14/15	0.89	0.19	-0.79	60,62,63,63	0
6	NAG	A	303	14/15	0.84	0.22	-	62,64,65,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.