



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:10 PM GMT

PDB ID : 3SDC
Title : Crystal structure of autoreactive-Valpha14-Vbeta6NKT 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 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>

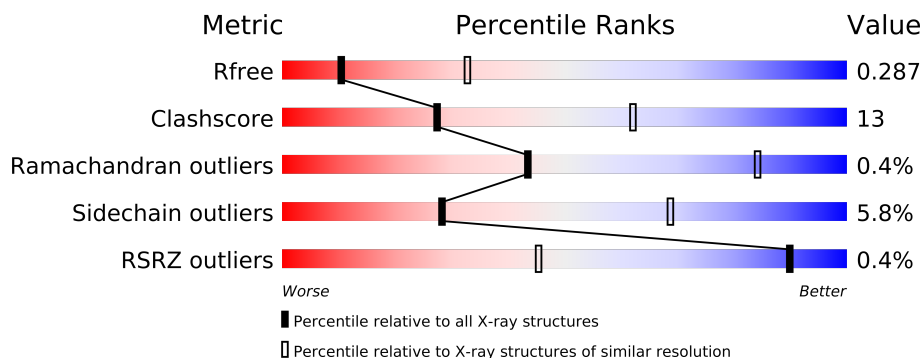
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6690 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	289	2324	1480	404	426	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	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		

There are 24 discrepancies between the modelled and reference sequences:

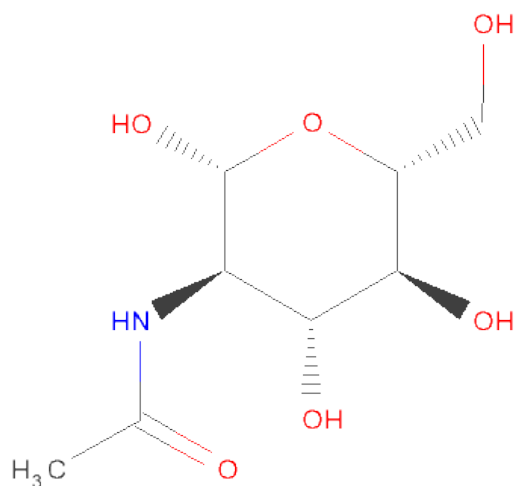
Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	EXPRESSION TAG	UNP P11609
A	281	SER	-	EXPRESSION TAG	UNP P11609
A	282	LEU	-	EXPRESSION TAG	UNP P11609
A	283	HIS	-	EXPRESSION TAG	UNP P11609
A	284	HIS	-	EXPRESSION TAG	UNP P11609
A	285	ILE	-	EXPRESSION 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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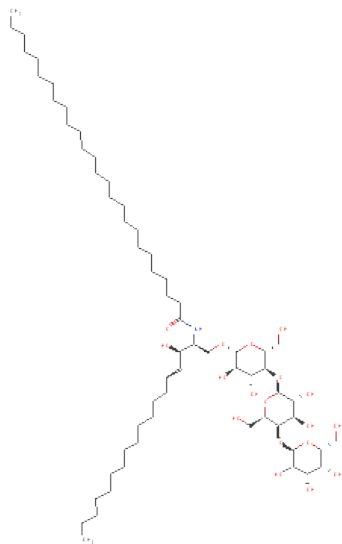
Chain	Residue	Modelled	Actual	Comment	Reference
A	292	VAL	-	EXPRESSION TAG	UNP P11609
A	293	TRP	-	EXPRESSION TAG	UNP P11609
A	294	ASN	-	EXPRESSION TAG	UNP P11609
A	295	HIS	-	EXPRESSION TAG	UNP P11609
A	296	ARG	-	EXPRESSION TAG	UNP P11609
A	297	HIS	-	EXPRESSION TAG	UNP P11609
A	298	HIS	-	EXPRESSION TAG	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-{[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.

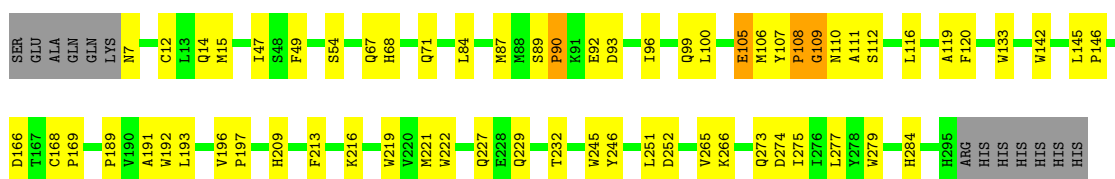
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	16	Total	O	0	0
			16	16		
8	B	8	Total	O	0	0
			8	8		
8	C	10	Total	O	0	0
			10	10		
8	D	3	Total	O	0	0
			3	3		

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 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:



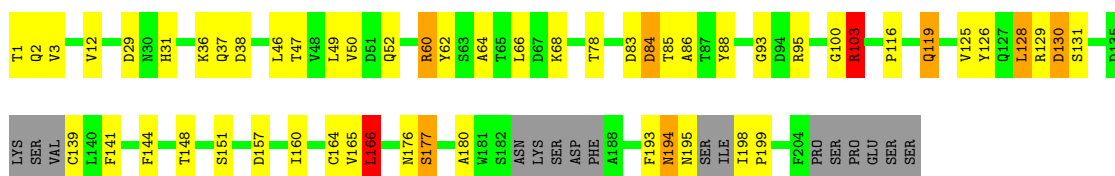
- Molecule 2: Beta-2-microglobulin

Chain B:



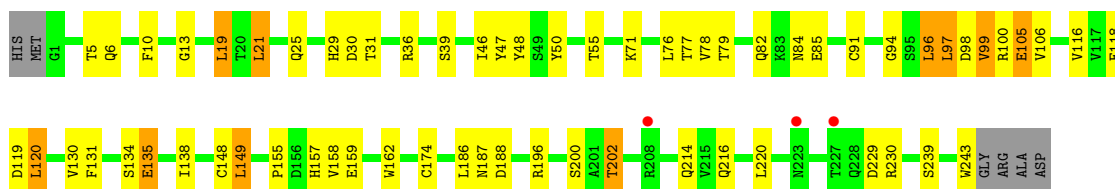
- Molecule 3: NKT TCR Valpha14 chain

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	94.35Å 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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	66.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 18.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 23951 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6690	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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 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	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

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 13.

All (168) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
3:C:129:ARG:H	3:C:130:ASP:CB	2.01	0.65
1:A:109:GLY:HA3	1:A:110:ASN:C	2.17	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
4:D:188:ASP:OD1	4:D:188:ASP:C	2.37	0.63
1:A:145:LEU:HB3	1:A:146:PRO:HD3	1.79	0.63
3:C:128:LEU:HA	3:C:129:ARG:HB2	1.82	0.62
1:A:89:SER:OG	1:A:90:PRO:HD3	1.99	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:HA	3:C:119:GLN:HE21	1.65	0.61
3:C:164:CYS:O	3:C:177:SER:N	2.33	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:15:MET:HG2	2:B:62:PHE:CE2	2.40	0.55
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.87	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
3:C:166:LEU:HB3	4:D:174:CYS:HB2	1.90	0.53
1:A:116:LEU:HD11	7:A:307:3GB:HCK	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:N	3:C:29:ASP:OD1	2.41	0.52
4:D:21:LEU:CD1	4:D:76:LEU:HB3	2.39	0.51
3:C:160:ILE:HD13	3:C:193:PHE:HB3	1.93	0.51
1:A:279:TRP:O	1:A:284:HIS:ND1	2.43	0.51
1:A:106:MET:O	1:A:107:TYR:CD1	2.64	0.51
3:C:49:LEU:HD13	3:C:66:LEU:HB2	1.92	0.51
1:A:193:LEU:HG	1:A:277:LEU:HD23	1.92	0.51
3:C:95:ARG:HB2	3:C:100:GLY:CA	2.37	0.50
1:A:47:ILE:HD12	1:A:67:GLN:HG3	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:C:177:SER:CB	4:D:196:ARG:CD	2.90	0.49
1:A:107:TYR:O	1:A:109:GLY:O	2.30	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
4:D:82:GLN:HB2	4:D:85:GLU:HB2	1.95	0.48
3:C:83:ASP:C	3:C:85:THR:H	2.17	0.48
1:A:192:TRP:CE3	2:B:14:PRO:HG3	2.48	0.48
1:A:196:VAL:HB	1:A:197:PRO:HD2	1.96	0.48
3:C:194:ASN:N	3:C:194:ASN:OD1	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
3:C:128:LEU:HA	3:C:129:ARG:C	2.35	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: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
3:C:38:ASP:CA	3:C:86:ALA:HB1	2.46	0.46
1:A:49:PHE:CG	1:A:54:SER:HB2	2.50	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
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:166:ASP:O	1:A:169:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:C:130:ASP:HA	4:D:131:PHE:HD2	1.82	0.43
1:A:87:MET:HG3	4:D:50:TYR:CD2	2.54	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:HD13	3:C:166:LEU:H	1.85	0.41
4:D:30:ASP:OD2	4:D:71:LYS:HE3	2.20	0.41
4:D:46:ILE:HG22	4:D:47:TYR:HD2	1.86	0.41
1:A:99:GLN:HB2	1:A:119:ALA:HB3	2.01	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
4:D:155:PRO:O	4:D:157:HIS:N	2.48	0.41
1:A:189:PRO:HB3	1:A:213:PHE:HB3	2.02	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:48:TYR:HE1	4:D:50:TYR:CE1	2.39	0.40
4:D:200:SER:HB3	4:D:202:THR:HG23	2.04	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	Distance(Å)	Clash(Å)
1:A:93:ASP:OD2	1:A:273:GLN:OE1[6_424]	1.25	0.95
1:A:93:ASP:OD2	1:A:273:GLN:CD[6_424]	1.96	0.24

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	287/302 (95%)	272 (95%)	14 (5%)	1 (0%)	50	87
2	B	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
3	C	183/207 (88%)	171 (93%)	11 (6%)	1 (0%)	38	81
4	D	237/245 (97%)	219 (92%)	17 (7%)	1 (0%)	43	84
All	All	804/853 (94%)	753 (94%)	48 (6%)	3 (0%)	43	84

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 ⓘ

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%)	82	96
2	B	92/93 (99%)	87 (95%)	5 (5%)	31	72
3	C	170/186 (91%)	156 (92%)	14 (8%)	17	53
4	D	207/211 (98%)	187 (90%)	20 (10%)	12	41
All	All	721/754 (96%)	679 (94%)	42 (6%)	28	69

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
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 ⓘ

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	0.63	0	15,19,21	1.59	3 (20%)
5	NAG	A	306	5	12,14,15	0.70	0	15,19,21	1.59	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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	306	NAG	O5-C5-C6	3.74	110.91	106.98
5	A	305	NAG	O4-C4-C3	-3.65	102.16	110.35
5	A	305	NAG	O5-C5-C6	3.13	110.27	106.98
5	A	306	NAG	C3-C2-N2	-2.96	107.25	111.76
5	A	305	NAG	C3-C2-N2	-2.36	108.17	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	0.51	0	15,19,21	0.78	0
6	NAG	A	304	1	12,14,15	0.55	0	15,19,21	0.88	0
7	3GB	A	307	-	83,83,83	1.11	3 (3%)	103,103,103	1.26	13 (12%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	307	3GB	O-C	-5.89	1.30	1.43
7	A	307	3GB	CBU-CBV	-2.65	1.38	1.50
7	A	307	3GB	O1-CAO	2.04	1.49	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	307	3GB	CB-CA-C	-5.71	97.96	113.12
7	A	307	3GB	CB-OBC-CBB	-3.80	106.23	113.81
7	A	307	3GB	C-CA-N	-3.64	103.28	110.25
7	A	307	3GB	C1-O1-CAO	-3.32	109.52	117.99
7	A	307	3GB	CAL-OBF-CAY	-3.31	109.53	117.99
7	A	307	3GB	OBC-CB-CA	3.24	115.86	107.93
7	A	307	3GB	C-CBW-CBV	-2.25	121.80	125.12
7	A	307	3GB	CBB-OBG-CAZ	-2.19	109.47	113.73
7	A	307	3GB	C1-O5-C5	-2.19	109.47	113.73
7	A	307	3GB	CAL-OAU-CAP	-2.16	109.52	113.73
7	A	307	3GB	O-C-CA	2.15	115.56	108.80
7	A	307	3GB	CA-C-CBW	2.07	114.65	111.84
7	A	307	3GB	CCM-CCL-CCK	2.02	125.55	114.61

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	289/302 (95%)	-0.11	0	100 100	38, 51, 65, 73	5 (1%)
2	B	99/99 (100%)	-0.11	0	100 100	41, 54, 65, 69	1 (1%)
3	C	191/207 (92%)	0.01	0	100 100	38, 64, 112, 122	5 (2%)
4	D	239/245 (97%)	0.03	3 (1%)	74 19	40, 73, 96, 98	5 (2%)
All	All	818/853 (95%)	-0.04	3 (0%)	90 45	38, 56, 101, 122	16 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	223	ASN	2.6
4	D	208	ARG	2.2
4	D	227	THR	2.1

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	0.22	0.92	55,56,60,64	0
5	NAG	A	306	14/15	0.20	-0.80	67,68,70,70	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	3GB	A	307	81/81	0.36	1.94	37,45,60,61	0
6	NAG	A	303	14/15	0.20	0.03	62,64,65,66	0
6	NAG	A	304	14/15	0.19	-0.75	60,62,63,63	0

6.5 Other polymers

There are no such residues in this entry.