



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:43 PM GMT

PDB ID : 3RUG
Title : Crystal structure of Valpha10-Vbeta8.1 NKT TCR in complex with CD1d-al
phaglucoylceramide (C20:2)
Authors : Patel, O.; Rossjohn, J.
Deposited on : 2011-05-05
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

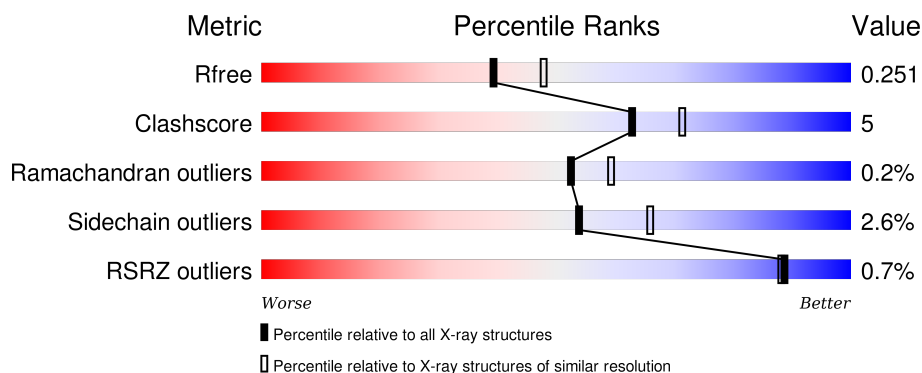
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





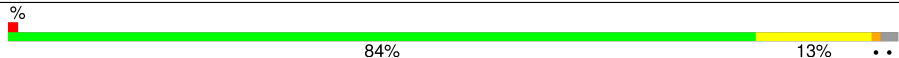
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>5%</div> </div> </div>
1	C	302	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
2	B	99	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>2%</div> </div> </div>
2	D	99	<div> <div></div> <div> <div></div> <div>85%</div> <div>12%</div> <div>3%</div> </div> </div>
3	E	204	<div> <div></div> <div> <div></div> <div>88%</div> <div>9%</div> <div>3%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	204	
4	F	241	
4	H	241	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DB6	A	303	-	-	-	X
5	DB6	C	303	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13311 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	286	Total	C	N	O	S	0	0	0
			2267	1450	390	413	14			
1	C	285	Total	C	N	O	S	0	0	0
			2250	1441	387	408	14			

There are 48 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
C	201	HIS	ASP	SEE REMARK 999	UNP P11609

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			785	501	133	144	7			
2	D	98	Total	C	N	O	S	0	0	0
			794	508	133	146	7			

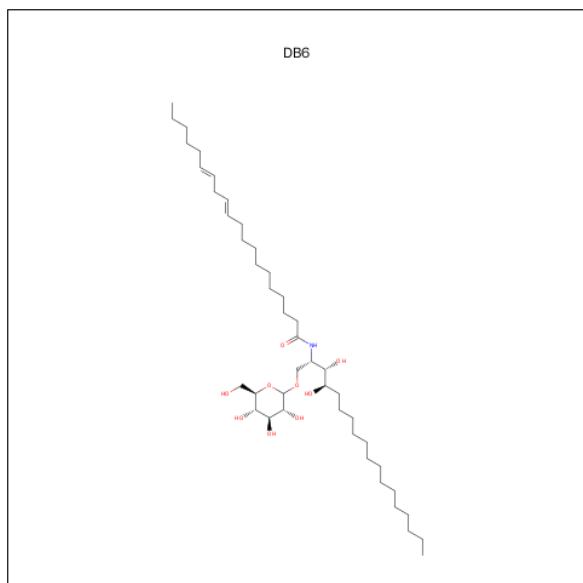
- Molecule 3 is a protein called Valpha10(mouse variable domain, human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	198	Total	C	N	O	S	0	0	0
			1474	917	240	309	8			
3	G	198	Total	C	N	O	S	0	0	0
			1466	910	236	312	8			

- Molecule 4 is a protein called Vbeta8.1(mouse variable domain, human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	236	Total	C	N	O	S	0	0	0
			1850	1174	319	351	6			
4	H	236	Total	C	N	O	S	0	0	0
			1850	1174	322	348	6			

- Molecule 5 is (11E,14E)-N-[(2S,3S,4R)-1-(ALPHA-D-GLUCOPYRANOSYLOXY)-3,4-DIHYDROXYOCTADECAN-2-YL]ICOSA-11,14-DIENAMIDE (three-letter code: DB6) (formula: $C_{44}H_{83}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			54	44	1	9		
5	C	1	Total	C	N	O	0	0
			54	44	1	9		

- 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		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	60	Total	O	0	0
			60	60		
8	B	19	Total	O	0	0
			19	19		
8	C	49	Total	O	0	0
			49	49		

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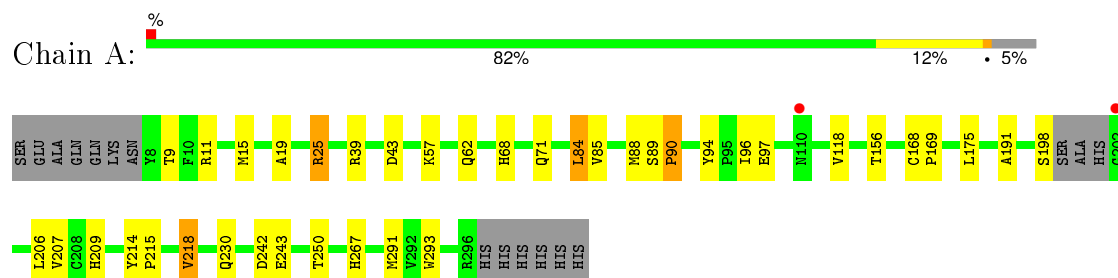
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	25	Total 25	O 25	0	0
8	E	33	Total 33	O 33	0	0
8	F	60	Total 60	O 60	0	0
8	G	47	Total 47	O 47	0	0
8	H	62	Total 62	O 62	0	0

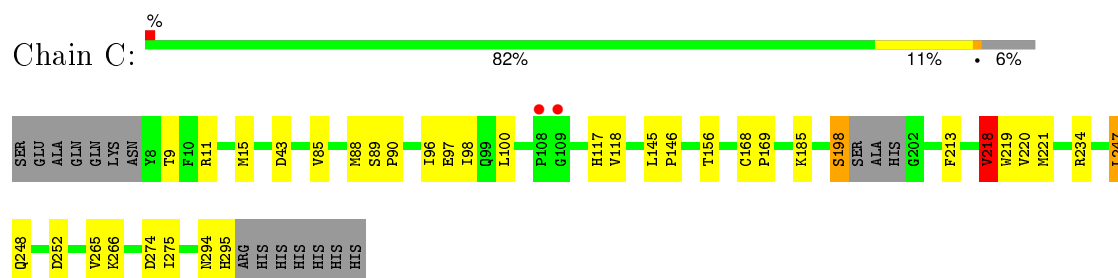
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

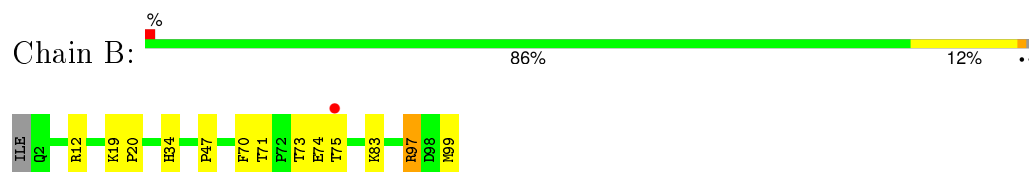
- Molecule 1: Antigen-presenting glycoprotein CD1d1



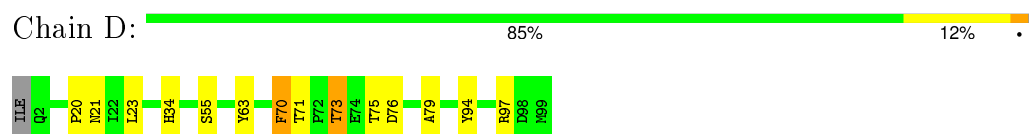
- Molecule 1: Antigen-presenting glycoprotein CD1d1



- Molecule 2: Beta-2 microglobulin

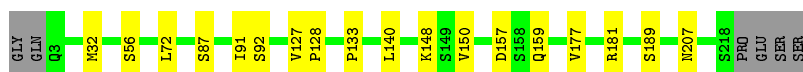


- Molecule 2: Beta-2 microglobulin

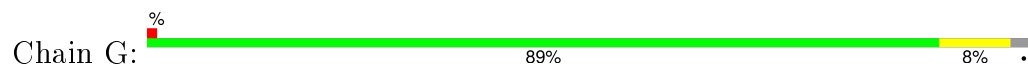


- Molecule 3: Valpha10(mouse variable domain, human constant domain)

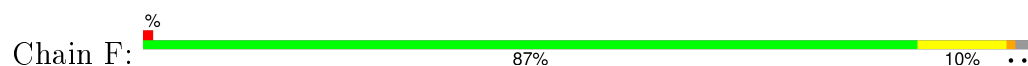




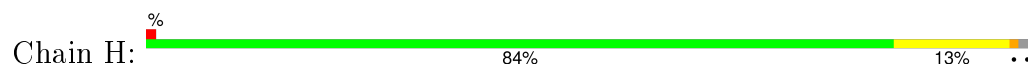
- Molecule 3: Valpha10(mouse variable domain, human constant domain)



- Molecule 4: Vbeta8.1(mouse variable domain, human constant domain)



- Molecule 4: Vbeta8.1(mouse variable domain, human constant domain)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.14Å 118.83Å 108.12Å 90.00° 110.24° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 48.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.20) 99.6 (48.22-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.210 , 0.254 0.208 , 0.251	Depositor DCC
R_{free} test set	4866 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.9	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 97190 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13311	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.02 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.2311e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, DB6

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	0.58	0/2335	0.70	1/3179 (0.0%)
1	C	0.63	0/2318	0.72	1/3157 (0.0%)
2	B	0.59	0/811	0.69	0/1107
2	D	0.70	0/820	0.70	0/1117
3	E	0.61	0/1504	0.66	0/2048
3	G	0.60	0/1496	0.69	0/2041
4	F	0.67	1/1902 (0.1%)	0.73	0/2594
4	H	0.66	0/1902	0.71	1/2593 (0.0%)
All	All	0.63	1/13088 (0.0%)	0.70	3/17836 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	169	GLU	CG-CD	5.04	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	VAL	CB-CA-C	-6.67	98.72	111.40
4	H	159	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	175	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2267	0	2140	28	0
1	C	2250	0	2126	27	0
2	B	785	0	731	6	0
2	D	794	0	745	10	0
3	E	1474	0	1360	11	0
3	G	1466	0	1333	10	0
4	F	1850	0	1735	17	0
4	H	1850	0	1743	34	0
5	A	54	0	83	3	0
5	C	54	0	83	3	0
6	A	28	0	26	0	0
6	C	28	0	26	0	0
7	A	28	0	25	1	0
7	C	28	0	25	0	0
8	A	60	0	0	2	0
8	B	19	0	0	0	0
8	C	49	0	0	1	0
8	D	25	0	0	2	0
8	E	33	0	0	1	0
8	F	60	0	0	2	0
8	G	47	0	0	0	0
8	H	62	0	0	8	0
All	All	13311	0	12181	134	0

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 5.

All (134) 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)
4:H:47:GLY:HA3	4:H:48:HIS:CD2	1.96	1.01
4:H:45:ASP:O	4:H:47:GLY:HA2	1.66	0.95
4:H:46:THR:HA	4:H:48:HIS:NE2	1.82	0.93
4:H:150:HIS:NE2	8:H:340:HOH:O	1.94	0.91
1:A:62:GLN:OE1	8:A:352:HOH:O	1.97	0.83
2:B:73:THR:HG22	2:B:75:THR:H	1.48	0.76
4:H:45:ASP:O	4:H:47:GLY:CA	2.33	0.76
4:H:44:GLN:HB2	4:H:50:LEU:HD22	1.66	0.76
4:H:150:HIS:CE1	8:H:340:HOH:O	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:47:GLY:HA3	4:H:48:HIS:CG	2.24	0.73
1:C:266:LYS:HE3	1:C:274:ASP:OD2	1.90	0.72
1:A:207:VAL:HG22	1:A:250:THR:HG22	1.71	0.72
4:H:46:THR:HA	4:H:48:HIS:CE1	2.25	0.72
1:C:294:ASN:OD1	1:C:295:HIS:N	2.23	0.72
4:H:62:THR:HG22	8:H:295:HOH:O	1.91	0.70
3:E:140:LEU:HB2	3:E:150:VAL:HG23	1.75	0.67
1:C:97:GLU:OE2	2:D:34:HIS:HE1	1.79	0.66
4:H:29:HIS:HD2	4:H:106:SER:OG	1.81	0.64
1:A:97:GLU:OE2	2:B:34:HIS:HE1	1.81	0.62
2:D:73:THR:HG22	2:D:76:ASP:H	1.64	0.62
2:D:73:THR:HG22	2:D:75:THR:H	1.65	0.61
1:A:89:SER:OG	1:A:90:PRO:HD3	2.00	0.60
4:H:46:THR:HA	4:H:48:HIS:CD2	2.36	0.60
4:H:47:GLY:CA	4:H:48:HIS:CD2	2.80	0.59
4:F:46:THR:HA	4:F:48:HIS:CD2	2.38	0.58
3:E:148:LYS:HE2	4:F:161:THR:HG21	1.85	0.58
1:C:145:LEU:HB3	1:C:146:PRO:HD3	1.84	0.58
4:H:46:THR:CA	4:H:48:HIS:NE2	2.64	0.57
3:E:189:SER:OG	4:F:206:ARG:HD3	2.04	0.57
3:E:32:MET:SD	3:E:87:SER:HB2	2.46	0.55
4:H:129:ASP:OD1	4:H:131:LYS:HB2	2.07	0.55
1:C:117:HIS:HE1	8:C:346:HOH:O	1.89	0.55
3:G:173:THR:HG21	4:H:204:SER:OG	2.07	0.55
3:E:72:LEU:CD1	3:E:91:ILE:HG12	2.37	0.55
3:E:128:PRO:HD3	3:E:177:VAL:HG21	1.90	0.54
3:G:32:MET:SD	3:G:87:SER:HB2	2.48	0.54
4:H:43:ARG:HB3	4:H:53:ILE:HD11	1.90	0.53
1:A:218:VAL:HG13	1:A:267:HIS:HD2	1.73	0.53
3:G:72:LEU:CD1	3:G:91:ILE:HG12	2.39	0.53
5:A:303:DB6:CAN	5:A:303:DB6:HAJA	2.40	0.52
4:H:220:HIS:HD2	8:H:264:HOH:O	1.93	0.52
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.91	0.52
1:A:19:ALA:O	1:A:94:TYR:HB3	2.10	0.52
1:A:39:ARG:HD2	8:A:333:HOH:O	2.10	0.52
1:A:9:THR:HG21	1:A:11:ARG:NH2	2.25	0.52
2:D:20:PRO:HA	2:D:71:THR:HG22	1.92	0.51
4:H:44:GLN:HB2	4:H:50:LEU:CD2	2.39	0.51
1:C:100:LEU:HG	1:C:118:VAL:HG22	1.91	0.51
1:A:118:VAL:HG11	5:A:303:DB6:H13A	1.93	0.51
3:G:72:LEU:HD12	3:G:91:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:THR:HG21	1:C:11:ARG:NH2	2.27	0.50
3:G:134:ASP:OD1	8:H:340:HOH:O	2.19	0.50
2:D:73:THR:HG23	8:D:101:HOH:O	2.11	0.50
1:A:68:HIS:HA	1:A:71:GLN:HE21	1.77	0.49
4:F:170:LEU:HD23	4:F:170:LEU:C	2.32	0.49
1:C:219:TRP:HA	1:C:234:ARG:HH21	1.76	0.49
4:H:129:ASP:O	8:H:33:HOH:O	2.19	0.49
3:G:139:GLN:O	4:H:144:SER:HB2	2.13	0.49
4:F:135:PRO:HD3	4:F:243:PRO:HB3	1.94	0.48
4:F:31:TYR:CE2	4:F:109:GLY:O	2.66	0.48
3:E:181:ARG:HH11	3:E:181:ARG:HG3	1.77	0.48
1:C:85:VAL:HB	1:C:88:MET:HE3	1.96	0.48
1:C:294:ASN:O	1:C:295:HIS:HB2	2.13	0.48
2:D:97:ARG:HB2	8:D:108:HOH:O	2.13	0.47
1:C:168:CYS:HB3	1:C:169:PRO:CD	2.44	0.47
4:F:162:GLY:O	4:F:200:ARG:HD2	2.15	0.47
1:C:220:VAL:H	1:C:234:ARG:HH21	1.63	0.47
1:C:219:TRP:HA	1:C:234:ARG:NH2	2.29	0.47
4:F:47:GLY:HA2	4:F:48:HIS:CD2	2.49	0.47
4:H:3:ALA:HB1	4:H:27:ASN:HD21	1.78	0.47
1:A:156:THR:HG23	5:A:303:DB6:HABA	1.97	0.47
1:A:168:CYS:HB3	1:A:169:PRO:CD	2.45	0.47
1:A:85:VAL:HB	1:A:88:MET:CE	2.45	0.47
3:E:133:PRO:HG2	4:H:218:ARG:HE	1.79	0.47
8:E:240:HOH:O	4:H:177:LYS:HE3	2.15	0.47
4:F:132:ASN:HB3	8:F:260:HOH:O	2.14	0.47
4:F:44:GLN:HB2	4:F:50:LEU:HD22	1.96	0.46
4:F:132:ASN:HB2	8:F:279:HOH:O	2.15	0.46
1:C:89:SER:HA	1:C:90:PRO:HA	1.82	0.46
1:A:68:HIS:HA	1:A:71:GLN:NE2	2.30	0.46
1:C:88:MET:HE1	1:C:96:ILE:HD11	1.97	0.46
1:C:168:CYS:HB3	1:C:169:PRO:HD3	1.97	0.46
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.51	0.46
4:H:186:ASP:OD1	4:H:206:ARG:NH1	2.45	0.46
4:F:104:CYS:SG	4:F:105:ALA:N	2.89	0.46
3:E:157:ASP:HB3	3:E:159:GLN:OE1	2.15	0.45
1:A:97:GLU:OE2	2:B:34:HIS:CE1	2.67	0.45
1:A:206:LEU:O	1:A:250:THR:HA	2.16	0.45
1:A:293:TRP:CD1	2:B:97:ARG:HD2	2.50	0.45
1:C:219:TRP:CZ2	1:C:221:MET:HG3	2.52	0.45
1:C:118:VAL:HG11	5:C:303:DB6:H13A	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:105:ALA:HB1	3:G:116:LEU:HG	1.99	0.45
3:G:134:ASP:CG	8:H:340:HOH:O	2.55	0.44
1:C:198:SER:OG	1:C:252:ASP:OD1	2.33	0.44
1:A:94:TYR:CD2	1:A:96:ILE:HD12	2.52	0.44
4:H:10:SER:HG	4:H:228:TYR:HD2	1.65	0.44
1:A:84:LEU:HD23	1:A:84:LEU:C	2.38	0.44
1:C:247:LEU:HG	1:C:248:GLN:N	2.33	0.44
1:C:265:VAL:HB	1:C:275:ILE:HB	1.99	0.44
3:E:159:GLN:HG3	4:H:220:HIS:HB3	2.00	0.43
1:C:88:MET:HE1	1:C:96:ILE:CD1	2.48	0.43
1:C:213:PHE:CE2	1:C:218:VAL:HG22	2.54	0.43
2:D:79:ALA:HB2	2:D:94:TYR:CD2	2.53	0.43
2:B:73:THR:CG2	2:B:74:GLU:N	2.80	0.43
4:H:220:HIS:CD2	8:H:264:HOH:O	2.70	0.43
4:H:29:HIS:CD2	4:H:106:SER:OG	2.67	0.43
1:A:57:LYS:HD3	1:A:57:LYS:HA	1.86	0.43
1:A:89:SER:OG	1:A:90:PRO:CD	2.66	0.43
1:C:85:VAL:HB	1:C:88:MET:CE	2.48	0.43
1:A:218:VAL:HG13	1:A:267:HIS:CD2	2.53	0.43
1:C:98:ILE:HD11	5:C:303:DB6:H18B	1.99	0.43
1:A:242:ASP:O	1:A:243:GLU:HB2	2.19	0.42
4:F:188:GLN:HA	4:F:189:PRO:HD3	1.94	0.42
4:F:196:LEU:HB2	4:F:199:SER:HB2	2.00	0.42
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.94	0.42
4:F:31:TYR:HA	4:F:56:SER:O	2.19	0.42
3:G:127:VAL:HG13	3:G:158:SER:CB	2.50	0.42
1:C:156:THR:HG23	5:C:303:DB6:HABA	2.02	0.41
4:H:220:HIS:HE1	4:H:251:GLU:OE1	2.03	0.41
4:H:31:TYR:HB2	4:H:107:ARG:HG2	2.03	0.41
4:F:29:HIS:HD2	4:F:106:SER:OG	2.03	0.41
2:D:55:SER:HB3	2:D:63:TYR:CZ	2.55	0.41
1:A:25:ARG:HG3	7:A:305:NAG:H82	2.01	0.41
4:H:31:TYR:HA	4:H:56:SER:O	2.21	0.41
4:H:123:ARG:NH1	4:H:166:ASP:OD1	2.52	0.41
1:A:191:ALA:HA	1:A:209:HIS:O	2.20	0.41
1:A:85:VAL:HG11	1:A:96:ILE:HD13	2.03	0.40
4:F:43:ARG:HB3	4:F:53:ILE:HD11	2.03	0.40
1:C:219:TRP:HB3	1:C:266:LYS:HB2	2.02	0.40
4:H:220:HIS:HB2	4:H:253:TRP:CZ3	2.55	0.40
3:E:181:ARG:NH1	3:E:181:ARG:HG3	2.37	0.40
1:A:214:TYR:CD2	1:A:215:PRO:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:178:LEU:C	3:G:178:LEU:HD12	2.42	0.40
2:D:23:LEU:HA	2:D:23:LEU:HD12	1.91	0.40

There are no symmetry-related clashes.

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	282/302 (93%)	275 (98%)	6 (2%)	1 (0%)	39	42
1	C	281/302 (93%)	277 (99%)	4 (1%)	0	100	100
2	B	96/99 (97%)	92 (96%)	2 (2%)	2 (2%)	9	5
2	D	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
3	E	196/204 (96%)	192 (98%)	4 (2%)	0	100	100
3	G	196/204 (96%)	192 (98%)	4 (2%)	0	100	100
4	F	232/241 (96%)	222 (96%)	10 (4%)	0	100	100
4	H	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
All	All	1611/1692 (95%)	1566 (97%)	42 (3%)	3 (0%)	52	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97	ARG
2	B	47	PRO
1	A	90	PRO

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	240/264 (91%)	232 (97%)	8 (3%)	45	56
1	C	238/264 (90%)	232 (98%)	6 (2%)	55	67
2	B	86/93 (92%)	81 (94%)	5 (6%)	25	28
2	D	87/93 (94%)	85 (98%)	2 (2%)	58	71
3	E	166/182 (91%)	162 (98%)	4 (2%)	57	69
3	G	165/182 (91%)	160 (97%)	5 (3%)	48	60
4	F	195/207 (94%)	193 (99%)	2 (1%)	82	91
4	H	195/207 (94%)	191 (98%)	4 (2%)	61	74
All	All	1372/1492 (92%)	1336 (97%)	36 (3%)	54	66

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	25	ARG
1	A	43	ASP
1	A	84	LEU
1	A	198	SER
1	A	218	VAL
1	A	230	GLN
1	A	291	MET
2	B	12	ARG
2	B	70	PHE
2	B	71	THR
2	B	83	LYS
2	B	99	MET
1	C	15	MET
1	C	43	ASP
1	C	185	LYS
1	C	198	SER
1	C	218	VAL
1	C	247	LEU

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Mol	Chain	Res	Type
2	D	70	PHE
2	D	73	THR
3	E	56	SER
3	E	92	SER
3	E	127	VAL
3	E	207	ASN
4	F	48	HIS
4	F	206	ARG
3	G	150	VAL
3	G	175	LYS
3	G	181	ARG
3	G	198	ASP
3	G	218	SER
4	H	43	ARG
4	H	144	SER
4	H	188	GLN
4	H	206	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	117	HIS
1	A	273	GLN
2	B	31	HIS
2	B	34	HIS
1	C	71	GLN
1	C	117	HIS
1	C	248	GLN
2	D	31	HIS
2	D	34	HIS
4	F	29	HIS
4	F	48	HIS
4	F	116	GLN
4	F	220	HIS
4	H	27	ASN
4	H	29	HIS
4	H	167	HIS
4	H	220	HIS
4	H	246	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	305	1,7	14,14,15	0.51	0	15,19,21	1.27	1 (6%)
7	NAG	A	306	7	14,14,15	0.57	0	15,19,21	1.90	1 (6%)
7	NAG	C	305	1,7	14,14,15	0.54	0	15,19,21	1.65	2 (13%)
7	NAG	C	306	7	14,14,15	0.52	0	15,19,21	2.12	4 (26%)

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	NAG	A	305	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	306	7	-	0/6/23/26	0/1/1/1
7	NAG	C	305	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	306	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	306	NAG	C4-C3-C2	-3.74	105.42	111.23
7	C	306	NAG	C3-C4-C5	-3.69	103.77	110.20
7	C	305	NAG	C4-C3-C2	2.31	114.82	111.23
7	A	305	NAG	C1-O5-C5	2.51	115.44	112.25
7	C	306	NAG	O3-C3-C2	3.19	115.43	109.11
7	C	306	NAG	C1-O5-C5	3.58	116.79	112.25
7	C	305	NAG	C1-O5-C5	4.89	118.45	112.25
7	A	306	NAG	C1-O5-C5	6.43	120.41	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	305	NAG	1	0

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
5	DB6	A	303	-	53,54,54	0.53	0	59,63,63	0.88	2 (3%)
6	NAG	A	304	1	14,14,15	0.60	0	15,19,21	2.56	1 (6%)
6	NAG	A	307	1	14,14,15	0.42	0	15,19,21	1.33	1 (6%)
5	DB6	C	303	-	53,54,54	0.47	0	59,63,63	1.02	4 (6%)
6	NAG	C	304	1	14,14,15	0.71	0	15,19,21	1.82	2 (13%)
6	NAG	C	307	1	14,14,15	0.53	0	15,19,21	1.10	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	DB6	A	303	-	-	0/52/72/72	0/1/1/1
6	NAG	A	304	1	-	0/6/23/26	0/1/1/1
6	NAG	A	307	1	-	0/6/23/26	0/1/1/1
5	DB6	C	303	-	-	0/52/72/72	0/1/1/1
6	NAG	C	304	1	-	0/6/23/26	0/1/1/1
6	NAG	C	307	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	C	303	DB6	O5A-C6A-C5M	-2.90	101.75	111.33
5	A	303	DB6	O5A-C6A-C5M	-2.28	103.81	111.33
5	C	303	DB6	CAB-CAA-N2	-2.13	112.36	115.83
5	C	303	DB6	C3-C2-N2	2.28	114.82	110.31
5	A	303	DB6	C1A-O6A-C5M	2.60	118.80	113.75
6	C	307	NAG	C1-O5-C5	2.83	115.84	112.25
5	C	303	DB6	O6A-C5M-C4A	2.92	115.16	109.68
6	C	304	NAG	C4-C3-C2	3.32	116.39	111.23
6	A	307	NAG	C1-O5-C5	4.40	117.83	112.25
6	C	304	NAG	C1-O5-C5	5.13	118.75	112.25
6	A	304	NAG	C1-O5-C5	8.96	123.62	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	303	DB6	3	0
5	C	303	DB6	3	0

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	286/302 (94%)	-0.03	2 (0%) 89 88	9, 24, 43, 49	0
1	C	285/302 (94%)	-0.09	2 (0%) 89 88	7, 21, 37, 45	0
2	B	98/99 (98%)	-0.10	1 (1%) 84 83	8, 27, 40, 45	0
2	D	98/99 (98%)	-0.24	0 100 100	7, 19, 31, 38	0
3	E	198/204 (97%)	-0.09	0 100 100	13, 24, 42, 46	0
3	G	198/204 (97%)	-0.04	2 (1%) 84 83	11, 26, 42, 46	0
4	F	236/241 (97%)	-0.20	2 (0%) 87 87	10, 19, 32, 48	0
4	H	236/241 (97%)	-0.17	3 (1%) 79 78	10, 21, 32, 50	0
All	All	1635/1692 (96%)	-0.11	12 (0%) 89 88	7, 22, 40, 50	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	47	GLY	6.0
4	H	195	ALA	3.3
4	F	48	HIS	2.7
4	F	47	GLY	2.5
1	C	108	PRO	2.4
3	G	218	SER	2.3
2	B	75	THR	2.3
4	H	57	TYR	2.2
3	G	63	ARG	2.2
1	A	110	ASN	2.1
1	A	202	GLY	2.0
1	C	109	GLY	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	C	306	14/15	0.86	0.17	-	42,47,50,50	0
7	NAG	C	305	14/15	0.96	0.14	-	22,25,33,36	0
7	NAG	A	305	14/15	0.94	0.14	-	20,24,30,35	0
7	NAG	A	306	14/15	0.89	0.13	-	36,42,44,45	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	DB6	A	303	54/54	0.93	0.17	3.16	12,15,26,28	23
5	DB6	C	303	54/54	0.94	0.17	2.40	8,14,31,32	23
6	NAG	A	307	14/15	0.95	0.10	-0.96	31,33,39,41	0
6	NAG	C	307	14/15	0.95	0.11	-1.59	25,28,33,34	0
6	NAG	A	304	14/15	0.84	0.15	-	32,35,43,43	0
6	NAG	C	304	14/15	0.82	0.15	-	44,49,52,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.