



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:34 am GMT

PDB ID : 2ICF
Title : CRIG bound to C3b
Authors : Wiesmann, C.
Deposited on : 2006-09-12
Resolution : 4.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (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

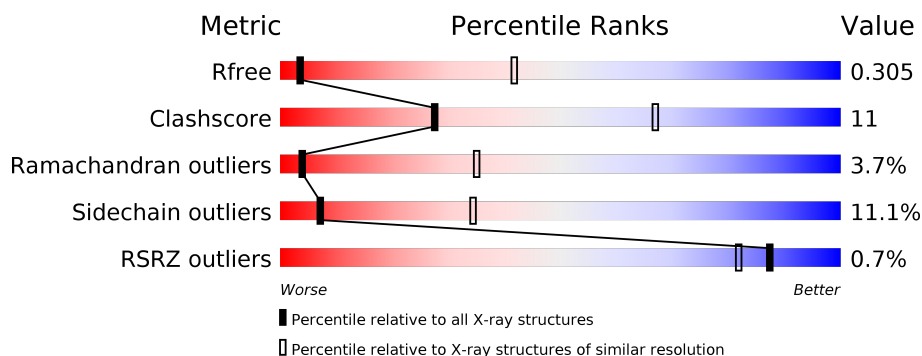
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1153 (4.60-3.60)
Clashscore	112137	1002 (4.54-3.66)
Ramachandran outliers	110173	1000 (4.58-3.62)
Sidechain outliers	110143	1191 (4.60-3.60)
RSRZ outliers	101464	1165 (4.60-3.60)

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	642	 63% 31% 5%
2	B	915	 68% 27% 5% 0%
3	S	119	 71% 26% 3% 0%

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
4	NAG	A	643	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13236 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5008	3188	848	957	15			

- Molecule 2 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	903	Total	C	N	O	S	1161	0	0
			7213	4572	1213	1390	38			

- Molecule 3 is a protein called V-set and immunoglobulin domain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	119	Total	C	N	O	S	0	0	0
			950	595	169	183	3			

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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


- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

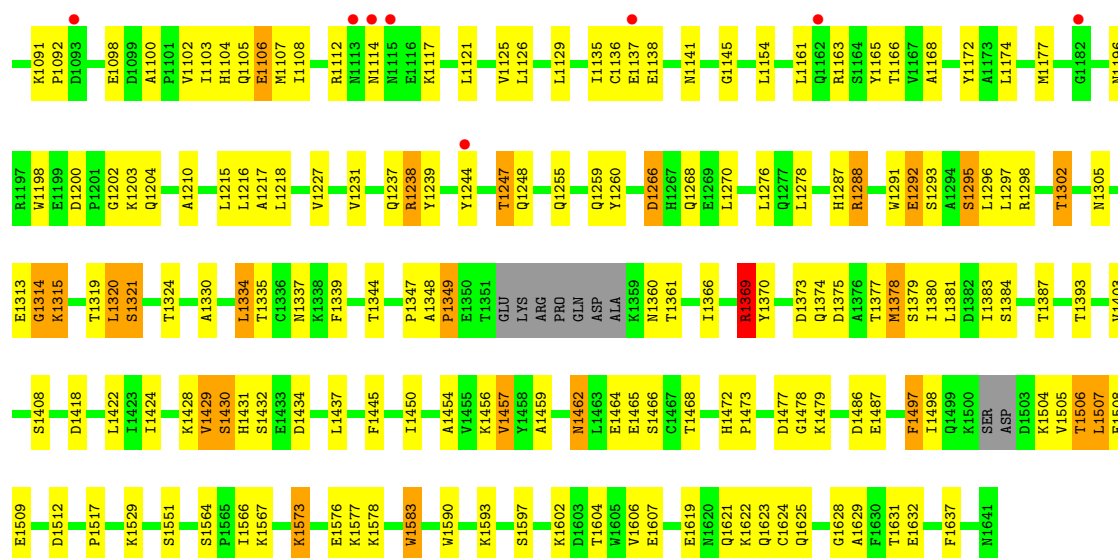
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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.

- Chain A:

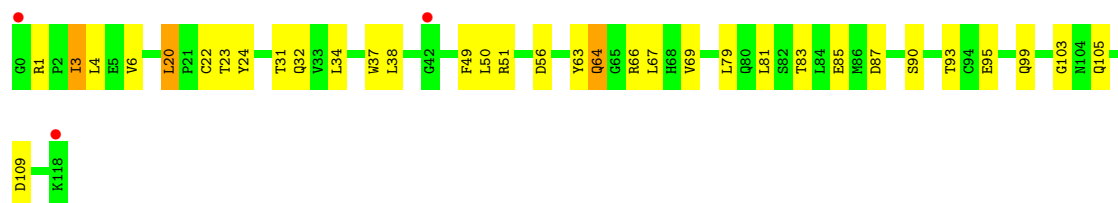
Category	Category	Category	Category	Category	Category	Category	Category	Category	Category
K611	V510	I389	L285	V177	S102	S1	K612	V511	I390
S618	T514	P393	L286	M178	S103	I6	S619	T515	P394
L622	I516	S399	Q289	M179	Q103	I7	L623	I517	S399
T625	Q521	T404	Q290	W182	L108	T8	T626	Q522	T405
S626	R522	R405	Q291	K183	F109	P9	S627	R523	R406
S627	S528	K406	A294	I184	T112	N10	S628	S529	K407
Q630	S529	E408	E295	Y187	D113	N11	Q631	E409	E408
Q631	U530	L409	V298	F196	K114	N12	Q632	U531	L409
Q639	V531	E413	S301	S197	T115	S16	Q640	V532	E414
Q642	D535	Q414	L302	I196	Y117	T19	Q643	D536	Q415
	S536	A415	V303	E199	T118	M20		S537	A416
	C537	T416	V304	T198	S121	V21		C538	T417
	U538	R417	V308	E204	L122	L22		U539	R418
	G539	T426	I309	Y205	V123	V33		G540	T427
	S540	L310	L207	V206	L124	V34		S541	L311
	U541	S437	L208	P208	R126	T36		U542	S438
	V542	E442	S209	F208	I127	V37		V543	E443
	Q547	L443	F210	S209	F128	H38		Q548	L444
	S548	E549	S322	T210	T129	H39		S549	E550
	E549	T448	I324	E211	N131	F40		E550	T449
	D550	R551	Q325	V212	H132	G42		D551	R552
	R551	Q552	R326	W214	K133	K43		R552	Q553
	Q552	U553	V427	E215	L134	K44		Q553	U554
	P553	E462	T328	E218	L135	L45		P554	E463
	V554	A463	S329	K219	T140	V46		V555	A464
	P555	K464	Y331	F220	V141	L47		P556	K465
	N559	T469	Q332	L229	M142	S48		N560	T470
	T560	Y470	I333	E230	V143	E50		T561	Y471
	L561	L471	T336	T233	N144	K51		L562	L472
	D577	M473	K337	F237	P148	V64		D578	M474
	K578	N474	T338	L238	I151	T65		K579	N475
	N587	R477	L350	Y239	P152	T67		N588	R478
	T590	R483	M51	V243	Q155	T68		T591	R484
	Q591	R486	T355	A247	D156	P69		Q592	R487
	I594	E487	S360	F248	S157	A70		I595	E488
	U595	Q490	A361	V249	L158	N71		U596	Q491
	D596	V494	A362	I250	S159	F74		D597	V495
	V597	L495	Y363	T251	S160	N81		V598	L496
	V598	V599	V365	G252	Q161	K32		V599	V600
	K600	L495	V365	G253	Q162	K33		K601	L496
	A601	S498	D373	I253	Q163	V86		A602	S499
	D602	T500	S377	E257	Q164	Q87		D603	T501
	I603	L378	L378	Q258	G185	Q88		I604	L379
	G604	T379	P263	L167	V166	Q89		G605	T380
	P607	F507	L262	P168	P168	E96		P608	F508
	G608	R508	A385	I173	I173	V99		G609	R509

- Chain B: 

SR	ASN	LEU	D730	I733	I734	E735	E736	E737	N738	I739	R742	R743	E744	F745	E746	E747	S748	W751	N752	E758	K761	N762	G763	I764	S765	T766	I771	T778	V785	D789	G792	V795	F799	E800	S801	L813	I825	L829	Y830	N835	Q836		
R841	R846	Q967	M968	D974	A975	L978	L981	T984	C988	I994	V1003	H1004	Q1011	W1012	E1013	L1014	F1015	G1016	L1017	E1018	I1027	F1037	R1038	Q1039	F1040	S1041	A1045	L1052	S1053	L1066	T1067	A1068	V1069	V1060	V1063	F1064	L1066	A1067	V1068	L1069	L1070	Q1076	V1081



• Molecule 3: V-set and immunoglobulin domain-containing protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.61Å 255.75Å 180.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.10 19.98 – 4.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-4.10) 96.0 (19.98-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.252 , 0.330 0.236 , 0.305	Depositor DCC
R_{free} test set	875 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	157.2	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 133.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13236	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, 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	0.58	0/5108	0.71	0/6939
2	B	0.59	5/7356 (0.1%)	0.82	1/9958 (0.0%)
3	S	0.61	0/972	0.66	0/1323
All	All	0.59	5/13436 (0.0%)	0.77	1/18220 (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	2
2	B	0	7
4	A	1	0
All	All	1	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1041	SER	CB-OG	12.37	1.58	1.42
2	B	1607	GLU	CD-OE2	9.88	1.36	1.25
2	B	737	GLU	CD-OE1	6.90	1.33	1.25
2	B	737	GLU	CD-OE2	6.34	1.32	1.25
2	B	1053	SER	CB-OG	6.15	1.50	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1497	PHE	O-C-N	-49.53	43.45	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	643	NAG	C1

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	PHE	Peptide
1	A	599	GLU	Peptide
2	B	1056	LEU	Mainchain
2	B	1335	THR	Peptide
2	B	930	LEU	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	5008	0	5071	143	0
2	B	7213	0	7141	123	99
3	S	950	0	935	15	0
4	A	50	0	43	0	0
5	B	14	0	13	0	0
6	A	1	0	0	0	0
All	All	13236	0	13203	274	99

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 11.

The worst 5 of 274 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)
2:B:1370:TYR:N	2:B:1430:SER:O	2.13	0.81
1:A:507:PHE:CE1	1:A:531:VAL:HB	2.20	0.77
2:B:1383:ILE:HD11	2:B:1424:ILE:HD11	1.69	0.73
1:A:214:VAL:HG12	1:A:233:ILE:HD13	1.70	0.73
2:B:1330:ALA:HB1	2:B:1334:LEU:HD21	1.74	0.69

The worst 5 of 99 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)
2:B:1105:GLN:N	2:B:1508:GLU:CD[5_445]	0.40	1.80
2:B:1203:LYS:NZ	2:B:1622:LYS:C[5_445]	0.42	1.78
2:B:1203:LYS:C	2:B:1622:LYS:NZ[5_445]	0.70	1.50
2:B:1202:GLY:CA	2:B:1621:GLN:CG[5_445]	0.83	1.37
2:B:1203:LYS:CG	2:B:1622:LYS:CB[5_445]	0.90	1.30

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	640/642 (100%)	526 (82%)	93 (14%)	21 (3%)	4	38
2	B	897/915 (98%)	748 (83%)	112 (12%)	37 (4%)	3	32
3	S	117/119 (98%)	99 (85%)	15 (13%)	3 (3%)	6	42
All	All	1654/1676 (99%)	1373 (83%)	220 (13%)	61 (4%)	4	35

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	198	THR
1	A	294	ALA
1	A	549	GLU
1	A	552	GLN

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	566/566 (100%)	491 (87%)	75 (13%)	4	27
2	B	799/810 (99%)	723 (90%)	76 (10%)	10	41
3	S	109/109 (100%)	96 (88%)	13 (12%)	6	31
All	All	1474/1485 (99%)	1310 (89%)	164 (11%)	7	34

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	639	GLN
2	B	959	LEU
3	S	1	ARG
2	B	752	ASN
2	B	836	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	835	ASN
2	B	1004	HIS
2	B	1401	ASN
2	B	897	HIS
2	B	1033	GLN

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](#)

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
4	NAG	A	643	1,4	14,14,15	0.79	0	15,19,21	1.61	2 (13%)
4	NAG	A	644	4	14,14,15	0.46	0	15,19,21	2.09	3 (20%)
4	BMA	A	645	4	11,11,12	0.70	0	13,15,17	1.43	1 (7%)
4	BMA	A	646	4	11,11,12	0.58	0	13,15,17	0.79	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	643	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	644	4	-	0/6/23/26	0/1/1/1
4	BMA	A	645	4	-	0/2/19/22	0/1/1/1
4	BMA	A	646	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	643	NAG	C1-O5-C5	-3.24	107.70	112.17
4	A	644	NAG	C4-C3-C2	-2.51	107.34	111.02
4	A	646	BMA	O5-C1-C2	-2.15	107.42	110.79
4	A	644	NAG	O4-C4-C5	2.96	116.75	109.28
4	A	643	NAG	C4-C3-C2	3.88	116.71	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	643	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	B	5	2	14,14,15	0.60	0	15,19,21	1.29	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	5	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	5	NAG	C1-O5-C5	3.15	116.50	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	642/642 (100%)	-0.59	0 100 100	147, 191, 237, 314	0
2	B	761/915 (83%)	-0.34	8 (1%) 80 72	135, 206, 258, 294	0
3	S	119/119 (100%)	-0.33	3 (2%) 58 47	167, 203, 249, 289	0
All	All	1522/1676 (90%)	-0.44	11 (0%) 87 82	135, 199, 249, 314	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1244	TYR	4.1
2	B	1114	ASN	3.9
2	B	1113	ASN	3.4
2	B	1137	GLU	3.1
2	B	1115	ASN	2.8

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

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

6.3 Carbohydrates [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, 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
4	NAG	A	643	14/15	0.92	0.20	-0.15	207,210,212,214	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BMA	A	645	11/12	0.85	0.47	-	233,236,238,238	0
4	NAG	A	644	14/15	0.87	0.41	-	215,220,226,233	0
4	BMA	A	646	11/12	0.78	0.36	-	222,223,226,228	11

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, 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(\AA^2)	Q<0.9
5	NAG	B	5	14/15	0.92	0.22	0.21	232,236,237,238	0
6	CA	A	647	1/1	0.97	0.08	-3.36	123,123,123,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.