wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:45 AM GMT

PDB ID	:	2Y7Q
Title	:	THE HIGH-AFFINITY COMPLEX BETWEEN IGE AND ITS RECEPTOR FC EPSILON RI
Authors	:	Davies, A.M.; Holdom, M.D.; Nettleship, J.E.; Beavil, A.J.; Owens, R.J.; Sutton, B.J.
Deposited on	:	2011-02-01
Resolution	:	3.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

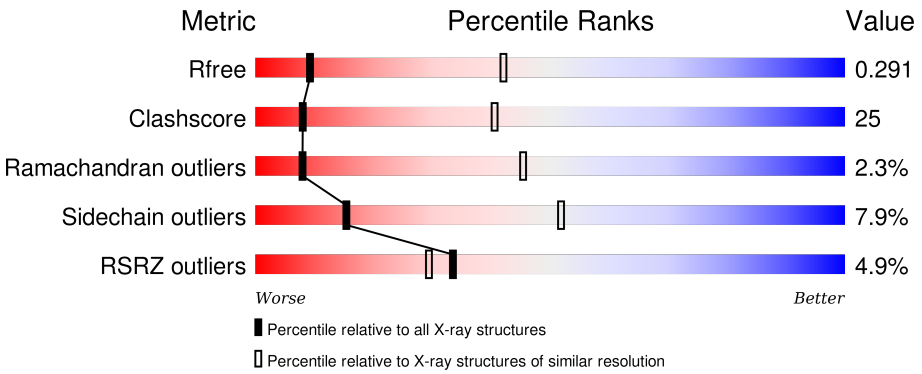
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 <=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	188	5%, 51%, 27%, 6%, 16%
2	B	327	2%, 53%, 32%, •, 12%
2	D	327	6%, 57%, 26%, 5%, 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5355 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 HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	158	1188	773	189	222	4	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLU	-	CLONING ARTIFACT	UNP P12319
A	-1	THR	-	CLONING ARTIFACT	UNP P12319
A	0	GLY	-	CLONING ARTIFACT	UNP P12319
A	74	ALA	ASN	ENGINEERED MUTATION	UNP P12319
A	135	ALA	ASN	ENGINEERED MUTATION	UNP P12319
A	142	ALA	THR	ENGINEERED MUTATION	UNP P12319
A	143	ALA	VAL	CLONING ARTIFACT	UNP P12319
A	177	GLY	-	CLONING ARTIFACT	UNP P12319
A	178	THR	-	CLONING ARTIFACT	UNP P12319
A	179	LYS	-	CLONING ARTIFACT	UNP P12319
A	180	HIS	-	EXPRESSION TAG	UNP P12319
A	181	HIS	-	EXPRESSION TAG	UNP P12319
A	182	HIS	-	EXPRESSION TAG	UNP P12319
A	183	HIS	-	EXPRESSION TAG	UNP P12319
A	184	HIS	-	EXPRESSION TAG	UNP P12319
A	185	HIS	-	EXPRESSION TAG	UNP P12319

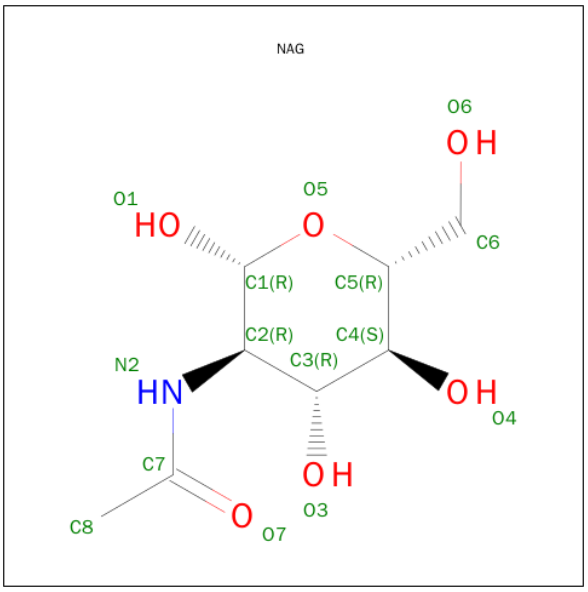
- Molecule 2 is a protein called IG EPSILON CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	287	2043	1290	351	391	11	0	0	0
2	D	290	2032	1287	350	385	10	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	ASP	-	EXPRESSION TAG	UNP P01854
B	223	ILE	-	EXPRESSION TAG	UNP P01854
B	225	ALA	CYS	ENGINEERED MUTATION	UNP P01854
B	265	GLN	ASN	ENGINEERED MUTATION	UNP P01854
B	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
D	222	ASP	-	EXPRESSION TAG	UNP P01854
D	223	ILE	-	EXPRESSION TAG	UNP P01854
D	225	ALA	CYS	ENGINEERED MUTATION	UNP P01854
D	265	GLN	ASN	ENGINEERED MUTATION	UNP P01854
D	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

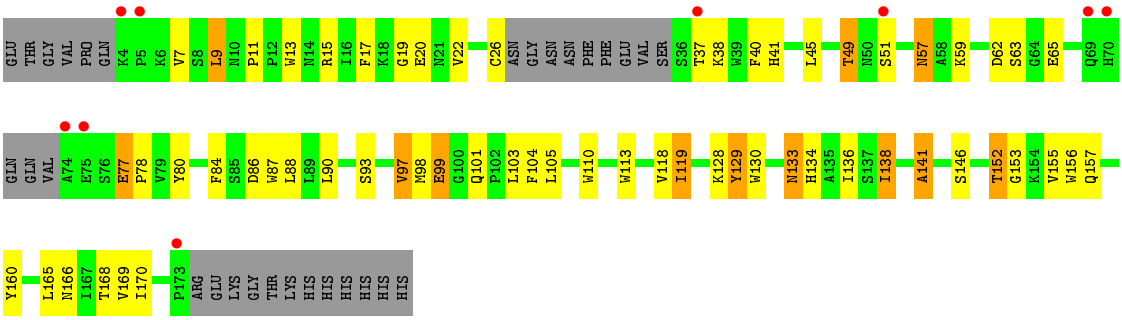
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	4	50	28	2	20	0	0

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.

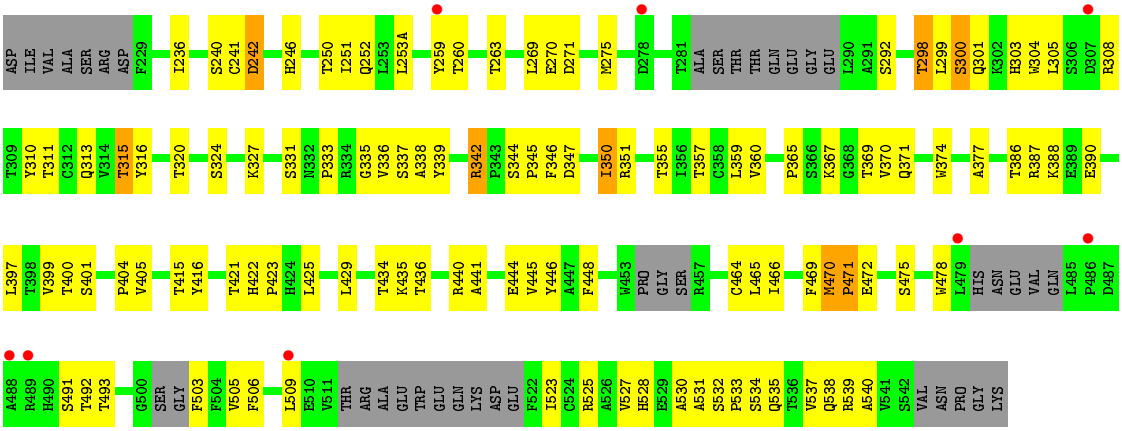
• Molecule 1: HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR SUBUNIT ALPHA

Chain A:



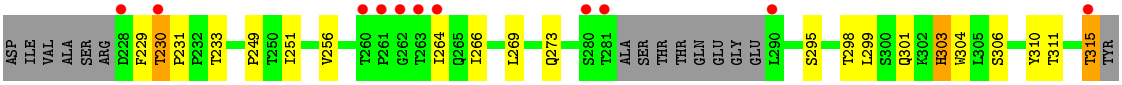
• Molecule 2: IG EPSILON CHAIN C REGION

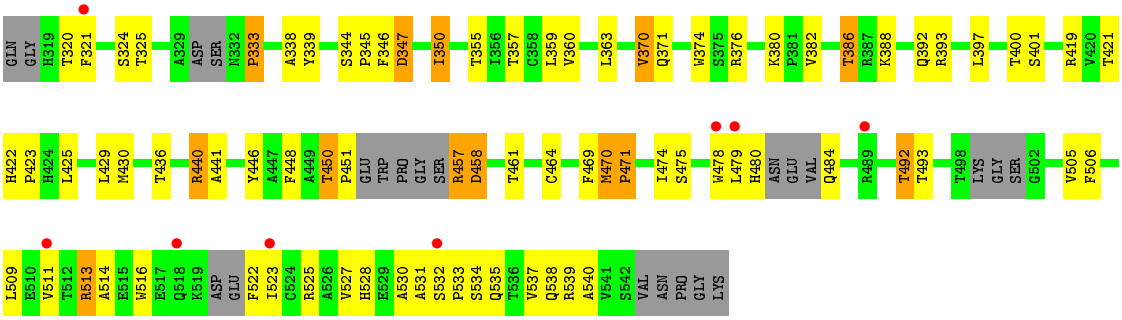
Chain B:



• Molecule 2: IG EPSILON CHAIN C REGION

Chain D:




GLN GLY H319 T320 F321 S324 T325 A329 ASP SER N332 P333 A338 Y339 S344 P345 F346 D347 I350 T355 I356 T357 G358 L359 V360 L363 V370 Q371 W374 S375 R376 K380 P381 V382 T386 R387 K388 Q392 R393 L397 T400 S401 R419 V420 T421
H422 P423 H424 L425 L429 M430 T436 R440 A441 Y446 A447 F448 A449 T450 P451 GLU TRP PRO GLY SER R457 D458 T461 C464 F469 M470 P471 I474 S475 W478 L479 H480 ASN GLU VAL Q484 R489 T492 T493 T498 LYS GLY SER G502 V505 F506
L509 E510 V511 T512 R513 A514 E515 W516 E517 Q518 K519 ASP GLU F522 I523 C524 R525 A526 V527 H528 E529 A530 A531 S532 P533 S534 Q535 T536 V537 Q538 R539 A540 V541 S542 VAL ASN PRO GLY LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.49Å 103.34Å 110.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.68 – 3.40 37.68 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.68-3.40) 99.8 (37.68-3.40)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.245 , 0.292 0.243 , 0.291	Depositor DCC
R_{free} test set	812 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	85.6	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 103.9	EDS
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 16127 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5355	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, MAN

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	0.32	0/1225	0.50	0/1679
2	B	0.30	0/2089	0.55	1/2847 (0.0%)
2	D	0.30	0/2077	0.53	1/2829 (0.0%)
All	All	0.31	0/5391	0.53	2/7355 (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
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	532	SER	C-N-CA	6.14	147.79	122.00
2	D	532	SER	C-N-CA	6.03	147.32	122.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	470	MET	Peptide
2	D	470	MET	Peptide

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	1188	0	1015	52	0
2	B	2043	0	1789	111	0
2	D	2032	0	1769	96	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	D	14	0	13	0	0
4	A	50	0	43	2	0
All	All	5355	0	4655	247	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 25.

The worst 5 of 247 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:342:ARG:HH11	2:B:342:ARG:HG3	1.12	1.06
2:B:471:PRO:HD2	2:B:528:HIS:CE1	1.99	0.97
2:D:471:PRO:HD2	2:D:528:HIS:CE1	1.99	0.97
2:D:344:SER:HB3	2:D:347:ASP:HB2	1.48	0.95
2:B:344:SER:HB3	2:B:347:ASP:HB2	1.50	0.93

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	152/188 (81%)	135 (89%)	13 (9%)	4 (3%)	7	42
2	B	275/327 (84%)	246 (90%)	24 (9%)	5 (2%)	11	50
2	D	274/327 (84%)	244 (89%)	23 (8%)	7 (3%)	7	42
All	All	701/842 (83%)	625 (89%)	60 (9%)	16 (2%)	8	45

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	533	PRO
1	A	57	ASN
1	A	99	GLU
2	B	350	ILE
2	D	458	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	109/167 (65%)	98 (90%)	11 (10%)	9	38
2	B	188/289 (65%)	177 (94%)	11 (6%)	24	64
2	D	182/289 (63%)	166 (91%)	16 (9%)	12	46
All	All	479/745 (64%)	441 (92%)	38 (8%)	15	52

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	351	ARG
2	B	491	SER
2	D	457	ARG
2	B	390	GLU
2	D	233	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	384	HIS
2	B	490	HIS
2	D	417	GLN
2	B	313	GLN
2	D	392	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	1175	1,4	14,14,15	0.59	0	15,19,21	1.00	1 (6%)
4	NAG	A	1176	4	14,14,15	0.53	0	15,19,21	1.45	1 (6%)
4	BMA	A	1177	4	11,11,12	0.86	0	14,15,17	0.89	0
4	MAN	A	1178	4	11,11,12	0.73	0	14,15,17	1.11	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	1175	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1176	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	A	1177	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1178	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1176	NAG	C2-N2-C7	-4.28	117.54	123.04
4	A	1175	NAG	C2-N2-C7	-2.68	119.59	123.04
4	A	1178	MAN	C1-C2-C3	2.65	112.68	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1175	NAG	2	0
4	A	1176	NAG	1	0

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	NAG	A	1174	1	14,14,15	0.46	0	15,19,21	1.67	2 (13%)
3	NAG	B	1543	2	14,14,15	0.60	0	15,19,21	0.77	0
3	NAG	D	1543	2	14,14,15	0.41	0	15,19,21	1.90	3 (20%)

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
3	NAG	A	1174	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1543	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1543	2	-	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(^{o})	Ideal(^{o})
3	D	1543	NAG	C4-C3-C2	-3.61	105.61	111.23
3	D	1543	NAG	C2-N2-C7	-2.39	119.97	123.04
3	A	1174	NAG	C3-C4-C5	2.84	115.15	110.20
3	A	1174	NAG	C1-O5-C5	5.08	118.69	112.25
3	D	1543	NAG	C1-O5-C5	5.42	119.12	112.25

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	158/188 (84%)	0.19	9 (5%)	27	25	28, 64, 114, 146	0
2	B	287/327 (87%)	0.10	8 (2%)	56	52	33, 76, 120, 159	0
2	D	290/327 (88%)	0.38	19 (6%)	22	20	32, 81, 127, 154	0
All	All	735/842 (87%)	0.23	36 (4%)	33	29	28, 76, 124, 159	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	SER	4.4
2	D	479	LEU	4.1
1	A	70	HIS	3.9
2	D	261	PRO	3.8
2	D	518	GLN	3.6

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	MAN	A	1178	11/12	0.86	0.26	-0.69	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	A	1175	14/15	0.97	0.17	-0.69	44,44,44,44	0
4	NAG	A	1176	14/15	0.93	0.17	-0.84	56,56,56,56	0
4	BMA	A	1177	11/12	0.90	0.22	-	104,104,104,104	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, 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
3	NAG	D	1543	14/15	0.91	0.28	0.40	90,90,90,90	0
3	NAG	A	1174	14/15	0.92	0.14	-0.61	83,83,83,83	0
3	NAG	B	1543	14/15	0.89	0.23	-1.11	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.