



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:00 PM GMT

PDB ID : 4NGS
Title : Crystal Structure of Glutamate Carboxypeptidase II in a complex with urea-based inhibitor
Authors : Tykvart, J.; Pachl, P.
Deposited on : 2013-11-02
Resolution : 1.68 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

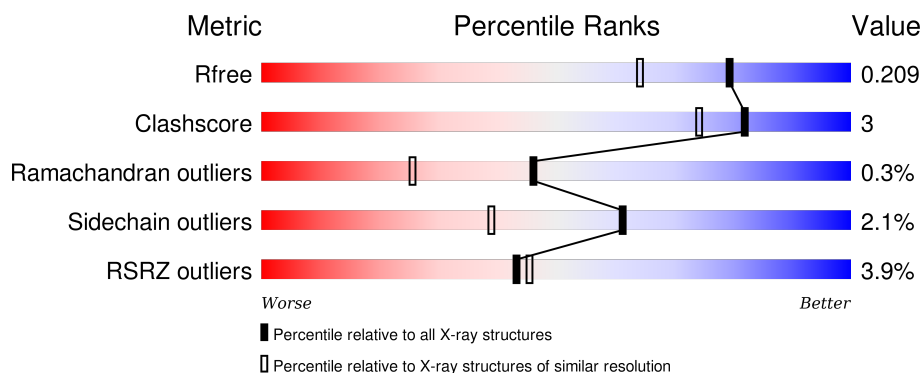
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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	739	

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
2	NAG	A	809	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	814	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6336 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 Glutamate carboxypeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	8	0
			5552	3575	926	1032	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ARG	-	EXPRESSION TAG	UNP Q04609
A	13	SER	-	EXPRESSION TAG	UNP Q04609
A	14	GLY	-	EXPRESSION TAG	UNP Q04609
A	15	LEU	-	EXPRESSION TAG	UNP Q04609
A	16	ASN	-	EXPRESSION TAG	UNP Q04609
A	17	ASP	-	EXPRESSION TAG	UNP Q04609
A	18	ILE	-	EXPRESSION TAG	UNP Q04609
A	19	PHE	-	EXPRESSION TAG	UNP Q04609
A	20	GLU	-	EXPRESSION TAG	UNP Q04609
A	21	ALA	-	EXPRESSION TAG	UNP Q04609
A	22	GLN	-	EXPRESSION TAG	UNP Q04609
A	23	LYS	-	EXPRESSION TAG	UNP Q04609
A	24	ILE	-	EXPRESSION TAG	UNP Q04609
A	25	GLU	-	EXPRESSION TAG	UNP Q04609
A	26	TRP	-	EXPRESSION TAG	UNP Q04609
A	27	HIS	-	EXPRESSION TAG	UNP Q04609
A	28	GLU	-	EXPRESSION TAG	UNP Q04609
A	29	GLY	-	EXPRESSION TAG	UNP Q04609
A	30	SER	-	EXPRESSION TAG	UNP Q04609
A	31	GLY	-	EXPRESSION TAG	UNP Q04609
A	32	SER	-	EXPRESSION TAG	UNP Q04609
A	33	GLY	-	EXPRESSION TAG	UNP Q04609
A	34	SER	-	EXPRESSION TAG	UNP Q04609
A	35	GLU	-	EXPRESSION TAG	UNP Q04609
A	36	ASN	-	EXPRESSION TAG	UNP Q04609
A	37	LEU	-	EXPRESSION TAG	UNP Q04609
A	38	TYR	-	EXPRESSION TAG	UNP Q04609

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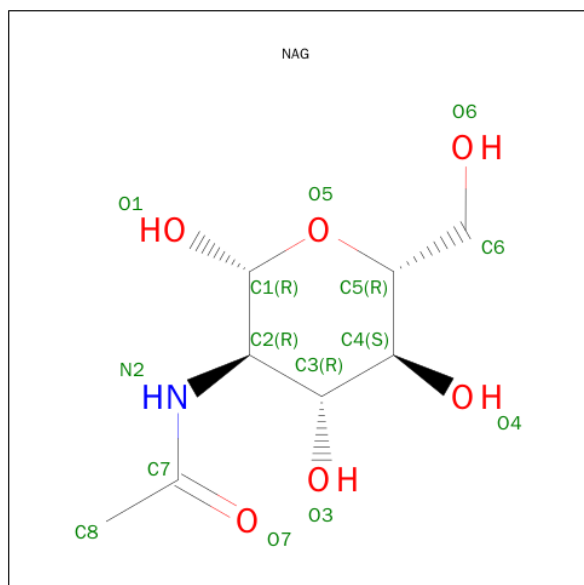
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Chain	Residue	Modelled	Actual	Comment	Reference
A	39	PHE	-	EXPRESSION TAG	UNP Q04609
A	40	GLN	-	EXPRESSION TAG	UNP Q04609
A	41	GLY	-	EXPRESSION TAG	UNP Q04609
A	42	ARG	-	EXPRESSION TAG	UNP Q04609
A	43	SER	-	EXPRESSION TAG	UNP Q04609

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

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

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

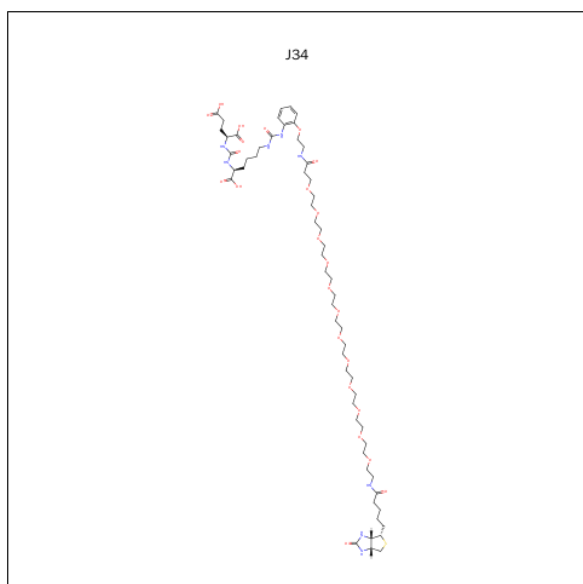


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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 N-{[(1S)-1-CARBOXY-5-({[2-({4,44-DIOXO-48-[(3AS,4S,6AR)-2-OXOHEXAHYDRO-1H-THIENO[3,4-D]IMIDAZOL-4-YL]-7,10,13,16,19,22,25,28,31,34,37,40-DODECAOXA-3,43-DIAZAOCATETRACONT-1-YL}OXY)PHENYL]CARBAMOYL}AMINO)PENTYL]CARBAMOYL}-L-GLUTAMIC ACID (three-letter code: J34) (formula: C₅₈H₉₈N₈O₂₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			38	23	5	10		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Zn	0	0
			2	2		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

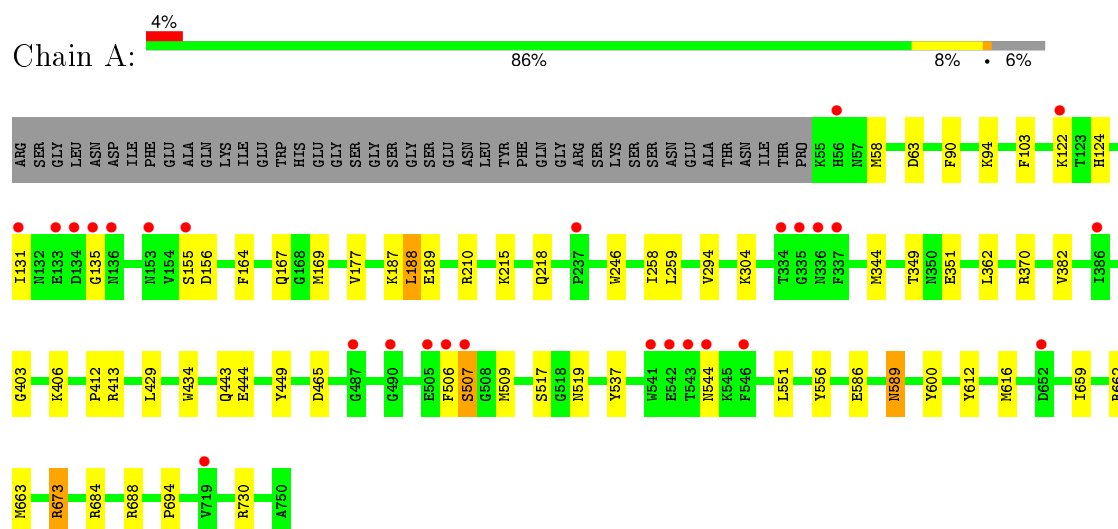
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	551	Total 552	O 552	0	1

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: Glutamate carboxypeptidase 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.44Å 130.05Å 159.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.77 – 1.68 38.09 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.77-1.68) 99.3 (38.09-1.68)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.183 , 0.210 0.182 , 0.209	Depositor DCC
R_{free} test set	5944 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 119022 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6336	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, CA, J34, 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	1.01	1/5730 (0.0%)	0.97	13/7772 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	TRP	CE3-CZ3	5.78	1.48	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	A	673	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	673	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	465	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	688	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	A	662	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	730	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	210	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	63	ASP	CB-CG-OD1	5.37	123.14	118.30
1	A	429	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	A	370	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	449	TYR	CD1-CE1-CZ	-5.07	115.24	119.80
1	A	684	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5552	0	5372	35	0
2	A	112	0	100	1	0
3	A	28	0	26	0	0
4	A	50	0	43	0	0
5	A	38	0	27	2	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	552	0	0	4	0
All	All	6336	0	5568	36	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 3.

All (36) 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)
1:A:443:GLN:HG2	9:A:961:HOH:O	1.73	0.89
1:A:90:PHE:CE2	1:A:94:LYS:HE2	2.16	0.79
1:A:659:ILE:O	1:A:663[B]:MET:HG3	1.83	0.79
1:A:58:MET:CE	1:A:586:GLU:HG2	2.25	0.66
1:A:506:PHE:CB	1:A:509:MET:HG3	2.27	0.65
1:A:215:LYS:HE2	9:A:1108:HOH:O	2.00	0.59
1:A:506:PHE:HB2	1:A:509:MET:HG3	1.84	0.59
1:A:90:PHE:CZ	1:A:94:LYS:HE2	2.39	0.56
1:A:544:ASN:HD21	5:A:815:J34:C15	2.19	0.56
1:A:362:LEU:CD1	1:A:406:LYS:HD2	2.39	0.53
1:A:362:LEU:HD11	1:A:406:LYS:HD2	1.91	0.53
1:A:506:PHE:HB3	1:A:509:MET:HG3	1.91	0.52
1:A:517:SER:HB2	1:A:694:PRO:HG3	1.92	0.51
1:A:58:MET:HE3	1:A:586:GLU:HG2	1.93	0.51
1:A:246:TRP:CD1	2:A:807:NAG:H83	2.46	0.51
1:A:131:ILE:HG12	1:A:135:GLY:HA2	1.92	0.51
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.45	0.51
1:A:413:ARG:H	1:A:589[A]:ASN:HD22	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:MET:HE1	1:A:586:GLU:HG2	1.94	0.49
1:A:169:MET:HA	1:A:344:MET:O	2.14	0.48
5:A:815:J34:H24	5:A:815:J34:O23	2.14	0.48
1:A:412:PRO:HA	1:A:589[A]:ASN:ND2	2.29	0.47
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.97	0.47
1:A:413:ARG:H	1:A:589[A]:ASN:ND2	2.13	0.47
1:A:663[A]:MET:HB2	1:A:663[A]:MET:HE2	1.77	0.46
1:A:155[B]:SER:O	1:A:156:ASP:HB2	2.16	0.45
1:A:177:VAL:HG12	1:A:188:LEU:HD21	1.98	0.45
1:A:507:SER:HA	9:A:1182:HOH:O	2.17	0.45
1:A:443:GLN:CG	9:A:961:HOH:O	2.48	0.44
1:A:258:ILE:HD13	1:A:294:VAL:HB	2.00	0.43
1:A:304:LYS:HE3	1:A:304:LYS:HB3	1.88	0.43
1:A:551:LEU:HA	1:A:551:LEU:HD23	1.88	0.42
1:A:103:PHE:O	1:A:403:GLY:HA3	2.18	0.42
1:A:444:GLU:HA	1:A:444:GLU:OE1	2.19	0.42
1:A:164:PHE:CG	1:A:259:LEU:HD21	2.56	0.40
1:A:167:GLN:NE2	1:A:349:THR:HG22	2.37	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	702/739 (95%)	685 (98%)	15 (2%)	2 (0%)	46 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	SER
1	A	382	VAL

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	589/629 (94%)	576 (98%)	13 (2%)	60 37

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LYS
1	A	124	HIS
1	A	187	LYS
1	A	188	LEU
1	A	189	GLU
1	A	218	GLN
1	A	351	GLU
1	A	519	ASN
1	A	537	TYR
1	A	589[A]	ASN
1	A	589[B]	ASN
1	A	600	TYR
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	620	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 ⓘ

12 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$
2	NAG	A	801	1,2	14,14,15	0.61	0	15,19,21	0.99	1 (6%)
2	NAG	A	802	2	14,14,15	0.49	0	15,19,21	1.24	1 (6%)
2	NAG	A	804	1,2	14,14,15	0.88	2 (14%)	15,19,21	1.01	0
2	NAG	A	805	2	14,14,15	0.49	0	15,19,21	1.19	1 (6%)
2	NAG	A	807	1,2	14,14,15	0.64	0	15,19,21	2.10	6 (40%)
2	NAG	A	808	2	14,14,15	0.61	0	15,19,21	2.69	2 (13%)
2	NAG	A	809	1,2	14,14,15	0.85	1 (7%)	15,19,21	1.23	1 (6%)
2	NAG	A	810	2	14,14,15	0.47	0	15,19,21	1.42	4 (26%)
4	NAG	A	811	1,4	14,14,15	1.00	1 (7%)	15,19,21	1.70	4 (26%)
4	NAG	A	812	4	14,14,15	0.85	1 (7%)	15,19,21	1.23	2 (13%)
4	BMA	A	813	4	11,11,12	0.57	0	14,15,17	1.00	1 (7%)
4	MAN	A	814	4	11,11,12	0.76	0	14,15,17	1.09	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
2	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	NAG	A	804	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	805	2	-	0/6/23/26	0/1/1/1
2	NAG	A	807	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	808	2	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	810	2	-	0/6/23/26	0/1/1/1
4	NAG	A	811	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	812	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	A	813	4	-	0/2/19/22	0/1/1/1
4	MAN	A	814	4	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	812	NAG	O5-C1	-2.35	1.39	1.43
2	A	804	NAG	C4-C5	2.04	1.57	1.53
2	A	809	NAG	C1-C2	2.05	1.55	1.52
2	A	804	NAG	C1-C2	2.13	1.55	1.52
4	A	811	NAG	C1-C2	2.23	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	807	NAG	O3-C3-C4	-3.63	102.17	110.34
2	A	809	NAG	C2-N2-C7	-3.10	119.06	123.04
4	A	811	NAG	C3-C4-C5	-3.08	104.83	110.20
2	A	810	NAG	C3-C4-C5	-3.01	104.94	110.20
4	A	813	BMA	O3-C3-C2	-2.74	105.05	110.00
2	A	810	NAG	C2-N2-C7	-2.66	119.62	123.04
4	A	811	NAG	C1-O5-C5	-2.65	108.88	112.25
2	A	802	NAG	C3-C4-C5	-2.63	105.61	110.20
4	A	812	NAG	C3-C4-C5	-2.54	105.77	110.20
2	A	807	NAG	O7-C7-C8	-2.44	117.59	122.06
4	A	811	NAG	O4-C4-C5	-2.35	103.00	109.24
2	A	807	NAG	C2-N2-C7	-2.29	120.09	123.04
2	A	807	NAG	C3-C4-C5	-2.25	106.28	110.20
4	A	812	NAG	C1-O5-C5	-2.22	109.43	112.25
2	A	801	NAG	C2-N2-C7	-2.14	120.28	123.04
2	A	810	NAG	O6-C6-C5	-2.09	104.43	111.33
2	A	808	NAG	C6-C5-C4	-2.04	107.99	113.02
2	A	807	NAG	O4-C4-C5	2.04	114.64	109.24
2	A	805	NAG	C2-N2-C7	2.05	125.68	123.04
4	A	814	MAN	O5-C5-C6	2.18	112.06	107.35
2	A	810	NAG	O4-C4-C5	2.27	115.25	109.24
4	A	811	NAG	O5-C5-C6	3.66	115.28	107.35
2	A	807	NAG	C1-O5-C5	4.46	117.91	112.25
2	A	808	NAG	C1-O5-C5	9.32	124.08	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
2	A	807	NAG	1	0

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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
3	NAG	A	803	1	14,14,15	0.72	0	15,19,21	1.58	2 (13%)
3	NAG	A	806	1	14,14,15	0.58	0	15,19,21	2.42	3 (20%)
5	J34	A	815	6	29,38,93	0.95	2 (6%)	33,48,110	1.64	9 (27%)

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	803	1	-	0/6/23/26	0/1/1/1
3	NAG	A	806	1	-	0/6/23/26	0/1/1/1
5	J34	A	815	6	-	0/30/40/110	0/1/1/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	815	J34	C13-N3	-2.41	1.37	1.41
5	A	815	J34	C8-C1	2.31	1.56	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	815	J34	C22-C21-N4	-3.67	110.60	116.19
3	A	806	NAG	C6-C5-C4	-3.37	104.71	113.02
5	A	815	J34	O7-C18-C17	-2.69	118.38	124.01
5	A	815	J34	O23-C12-N3	-2.05	120.46	123.58
3	A	803	NAG	C4-C3-C2	2.02	114.37	111.23
5	A	815	J34	C19-O7-C18	2.09	122.78	117.64
5	A	815	J34	C9-C8-C1	2.33	121.06	113.87
5	A	815	J34	N1-C2-N	2.62	119.41	115.08
5	A	815	J34	O22-C21-N4	2.63	126.48	121.79
5	A	815	J34	C20-N4-C21	2.73	126.82	122.36
5	A	815	J34	O7-C18-C13	3.07	120.63	115.05
3	A	803	NAG	O5-C5-C6	3.16	114.20	107.35
3	A	806	NAG	O5-C5-C6	3.37	114.64	107.35
3	A	806	NAG	C1-O5-C5	7.40	121.64	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	815	J34	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	696/739 (94%)	0.03	27 (3%)	43 45	12, 21, 42, 65	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	PHE	6.4
1	A	546	PHE	3.7
1	A	237	PRO	3.2
1	A	155[A]	SER	3.2
1	A	541	TRP	3.1
1	A	507	SER	3.1
1	A	335	GLY	3.0
1	A	487	GLY	2.9
1	A	544	ASN	2.9
1	A	122	LYS	2.8
1	A	543	THR	2.8
1	A	505	GLU	2.8
1	A	336	ASN	2.7
1	A	542	GLU	2.6
1	A	334	THR	2.5
1	A	56	HIS	2.5
1	A	153	ASN	2.5
1	A	134	ASP	2.5
1	A	386	ILE	2.4
1	A	133	GLU	2.4
1	A	337	PHE	2.4
1	A	719	VAL	2.4
1	A	131	ILE	2.3
1	A	490	GLY	2.2
1	A	136	ASN	2.2
1	A	135	GLY	2.1
1	A	652	ASP	2.1

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
2	NAG	A	809	14/15	0.93	0.12	5.31	25,27,30,36	0
4	MAN	A	814	11/12	0.90	0.17	2.34	46,48,51,52	0
4	NAG	A	811	14/15	0.94	0.08	1.87	19,26,36,45	0
2	NAG	A	804	14/15	0.86	0.14	1.86	32,38,41,48	0
2	NAG	A	808	14/15	0.78	0.38	-	61,67,80,80	0
2	NAG	A	802	14/15	0.75	0.24	-	34,48,54,56	0
4	BMA	A	813	11/12	0.89	0.14	-	37,39,44,44	0
2	NAG	A	801	14/15	0.94	0.10	-	27,35,41,44	0
4	NAG	A	812	14/15	0.92	0.18	-	32,39,48,58	0
2	NAG	A	810	14/15	0.92	0.15	-	33,41,47,48	0
2	NAG	A	805	14/15	0.86	0.25	-	43,54,64,70	0
2	NAG	A	807	14/15	0.91	0.11	-	26,43,48,56	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
8	CA	A	819	1/1	1.00	0.07	0.99	13,13,13,13	0
5	J34	A	815	38/91	0.95	0.16	0.73	13,26,56,58	0
6	ZN	A	817	1/1	1.00	0.09	-1.82	15,15,15,15	0
6	ZN	A	816	1/1	1.00	0.08	-3.63	14,14,14,14	0
7	CL	A	818	1/1	0.99	0.08	-3.96	15,15,15,15	0
3	NAG	A	806	14/15	0.72	0.19	-	53,60,66,68	0
3	NAG	A	803	14/15	0.78	0.24	-	42,50,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.