



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2020 – 02:07 PM EDT

PDB ID : 6S1X
Title : X-ray structure of human glutamate carboxypeptidase II (GCP II)-E424M inactive mutant, in complex with a inhibitor KB1160
Authors : Barinka, C.; Kutil, Z.
Deposited on : 2019-06-19
Resolution : 1.76 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.10.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

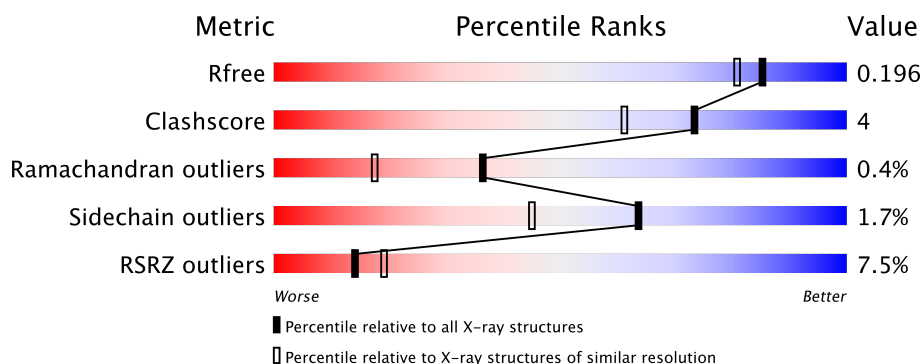
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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}	111664	1952 (1.76-1.76)
Clashscore	122126	2072 (1.76-1.76)
Ramachandran outliers	120053	2050 (1.76-1.76)
Sidechain outliers	120020	2050 (1.76-1.76)
RSRZ outliers	108989	1913 (1.76-1.76)

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 respectively. 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	707	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6776 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.

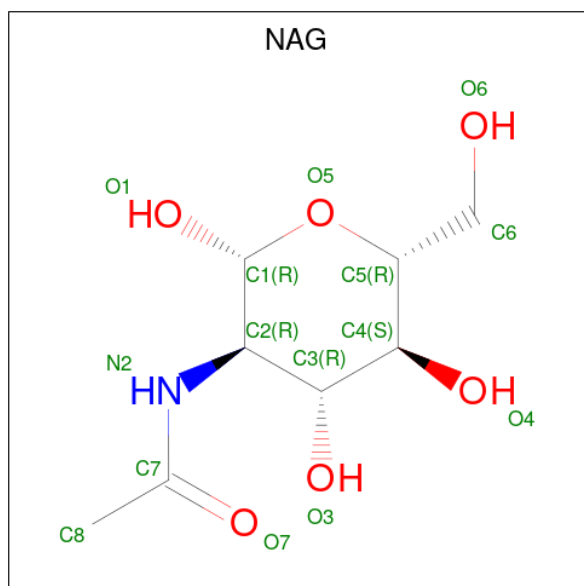
- Molecule 1 is a protein called Glutamate carboxypeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	696	5968	3822	1004	1119	23	0	56	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	424	MET	GLU	engineered mutation	UNP Q04609

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



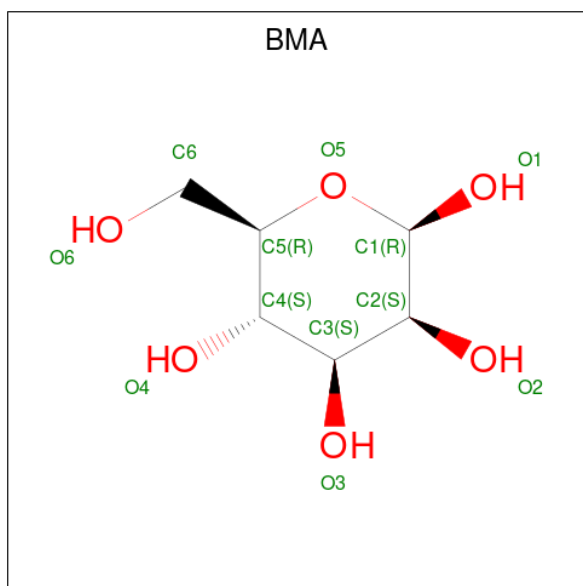
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

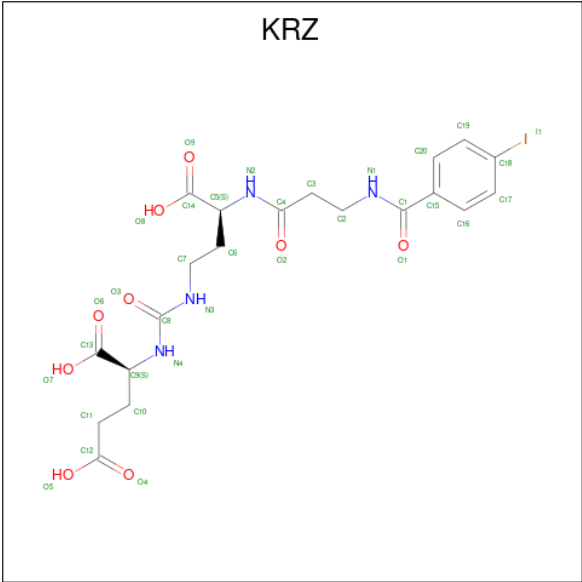
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- 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 (2 {S})-2-[[[(3 {S})-3-[3-[(4-iodophenyl)carbonylamino]propanoylamino]-4-oxidanyl-4-oxidanylidene-butyl]carbamoylamino]pentanedioic acid (three-letter code: KRZ) (formula: C₂₀H₂₅IN₄O₉) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	I	N	O	0	0
			34	20	1	4	9		

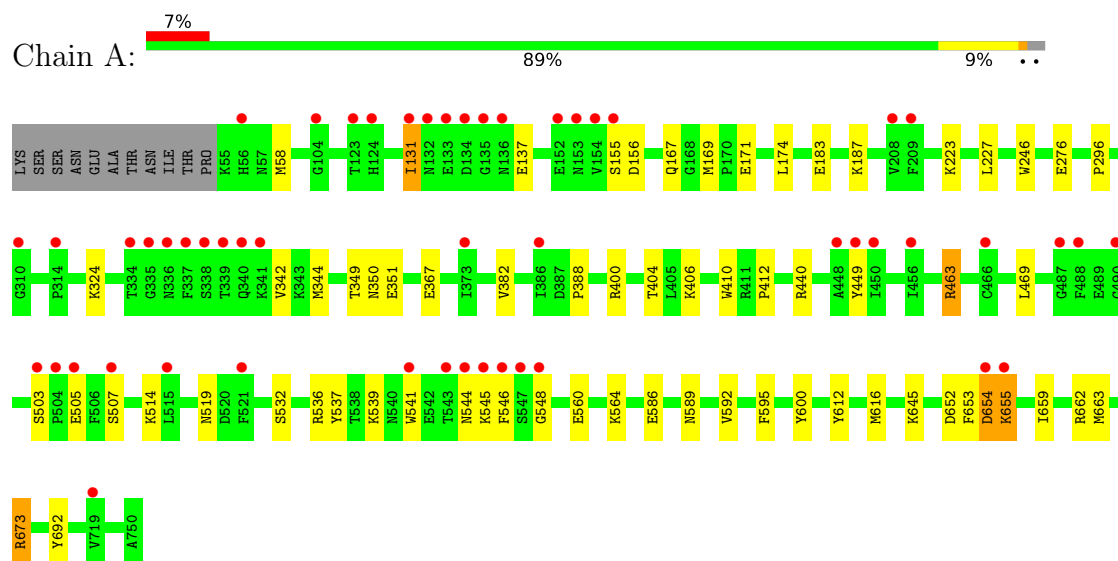
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	572	Total	O	0	0
			572	572		

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 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 ($RSRZ > 2$). 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	101.40Å 130.15Å 159.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 1.76 47.03 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.00-1.76) 99.6 (47.03-1.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.167 , 0.194 0.172 , 0.196	Depositor DCC
R_{free} test set	2100 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.7	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	0.97	EDS
Total number of atoms	6776	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: KRZ, ZN, BMA, NAG, CL, CA, 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	0.55	1/6168 (0.0%)	0.84	6/8347 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	GLU	CD-OE1	5.92	1.32	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652[A]	ASP	CB-CA-C	-6.46	97.47	110.40
1	A	652[B]	ASP	CB-CA-C	-6.46	97.47	110.40
1	A	440	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	673	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	440	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	463	ARG	CG-CD-NE	-5.18	100.93	111.80

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	5968	0	5804	41	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	154	0	137	5	0
3	A	22	0	18	0	1
4	A	22	0	20	0	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	34	0	0	2	0
9	A	572	0	0	5	0
All	All	6776	0	5979	44	1

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 4.

All (44) 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:653[B]:PHE:O	1:A:654[B]:ASP:O	1.79	1.00
1:A:58:MET:CE	1:A:586:GLU:HG2	2.12	0.79
1:A:463:ARG:HD3	8:A:820:KRZ:C17	2.17	0.75
1:A:58:MET:HE2	1:A:586:GLU:HG2	1.73	0.70
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.96	0.65
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.32	0.65
1:A:541:TRP:HZ3	1:A:546:PHE:O	1.80	0.64
1:A:654[B]:ASP:O	1:A:655[B]:LYS:HG3	1.98	0.64
1:A:541:TRP:CZ3	1:A:546:PHE:O	2.53	0.62
1:A:659[B]:ILE:O	1:A:663[B]:MET:HG3	2.00	0.62
1:A:653[B]:PHE:C	1:A:654[B]:ASP:O	2.45	0.55
1:A:58:MET:HE1	1:A:586:GLU:HG2	1.90	0.53
1:A:536:ARG:HG2	8:A:820:KRZ:I1	2.80	0.52
1:A:541:TRP:O	1:A:545:LYS:HG2	2.10	0.51
1:A:412:PRO:HA	1:A:589[A]:ASN:OD1	2.10	0.50
1:A:350:ASN:C	1:A:351[B]:GLU:HG2	2.32	0.50
2:A:809:NAG:H83	9:A:1328:HOH:O	2.12	0.49
1:A:548:GLY:HA3	9:A:1332:HOH:O	2.13	0.49
1:A:174[B]:LEU:HD11	1:A:342:VAL:HG21	1.95	0.48
1:A:171[B]:GLU:O	1:A:223:LYS:NZ	2.41	0.47
1:A:131:ILE:HD11	1:A:171[A]:GLU:HG3	1.96	0.47
2:A:809:NAG:C8	9:A:1328:HOH:O	2.63	0.47
1:A:131:ILE:CG2	1:A:137:GLU:HG2	2.45	0.46
1:A:324:LYS:HD3	1:A:324:LYS:HA	1.79	0.46
1:A:560:GLU:HB3	1:A:564[B]:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLU:OE1	1:A:662[B]:ARG:NH1	2.44	0.45
1:A:246:TRP:CD1	2:A:807:NAG:H83	2.52	0.45
1:A:654[A]:ASP:C	1:A:654[A]:ASP:OD1	2.56	0.43
1:A:406:LYS:HA	1:A:410:TRP:O	2.18	0.43
1:A:469:LEU:O	1:A:595:PHE:HA	2.19	0.43
2:A:803:NAG:H83	9:A:1037:HOH:O	2.18	0.41
1:A:155[A]:SER:O	1:A:156[A]:ASP:HB2	2.20	0.41
1:A:645[C]:LYS:HD3	9:A:1394:HOH:O	2.20	0.41
1:A:169:MET:HA	1:A:344:MET:O	2.20	0.41
1:A:544:ASN:HB3	1:A:546:PHE:CZ	2.55	0.41
1:A:227:LEU:O	1:A:296:PRO:HA	2.21	0.41
1:A:514[A]:LYS:HD2	1:A:692:TYR:HE1	1.84	0.41
1:A:131:ILE:HD11	1:A:171[A]:GLU:CD	2.40	0.41
1:A:167:GLN:NE2	1:A:349:THR:HG22	2.36	0.41
1:A:592:VAL:HG23	1:A:655[B]:LYS:HE2	2.03	0.41
1:A:539:LYS:NZ	1:A:546:PHE:HB2	2.36	0.41
1:A:137:GLU:OE1	2:A:804:NAG:H5	2.21	0.40
1:A:449:TYR:O	1:A:532:SER:HA	2.20	0.40
1:A:131:ILE:HG23	1:A:137:GLU:HG2	2.02	0.40

All (1) 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)
1:A:276[A]:GLU:OE1	3:A:813:BMA:O2[2_565]	2.15	0.05

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	751/707 (106%)	722 (96%)	24 (3%)	5 (1%)	24 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	654[A]	ASP
1	A	654[B]	ASP
1	A	382	VAL
1	A	655[A]	LYS
1	A	655[B]	LYS

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	650/603 (108%)	640 (98%)	10 (2%)	67	52

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ILE
1	A	187	LYS
1	A	388	PRO
1	A	503	SER
1	A	505	GLU
1	A	507	SER
1	A	519	ASN
1	A	537	TYR
1	A	600	TYR
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	BMA	A	813	2,4	11,11,12	0.39	0	15,15,17	1.35	3 (20%)
2	NAG	A	807	1	14,14,15	0.57	0	17,19,21	1.22	3 (17%)
2	NAG	A	805	2	14,14,15	0.49	0	17,19,21	1.11	2 (11%)
2	NAG	A	808	1,2	14,14,15	0.69	0	17,19,21	1.12	2 (11%)
2	NAG	A	801	1,2	14,14,15	0.36	0	17,19,21	1.19	0
2	NAG	A	812	3,2	14,14,15	0.56	0	17,19,21	1.34	1 (5%)
2	NAG	A	806	1	14,14,15	0.53	0	17,19,21	1.68	3 (17%)
2	NAG	A	802	2	14,14,15	0.54	0	17,19,21	0.80	0
2	NAG	A	809	3,2	14,14,15	0.51	0	17,19,21	0.99	1 (5%)
4	MAN	A	815	3	11,11,12	0.64	0	15,15,17	1.10	1 (6%)
2	NAG	A	803	1	14,14,15	0.70	0	17,19,21	1.53	1 (5%)
2	NAG	A	811	1,2	14,14,15	0.55	0	17,19,21	1.51	2 (11%)
2	NAG	A	804	1,2	14,14,15	0.75	0	17,19,21	0.69	0
3	BMA	A	810	2	11,11,12	0.55	0	15,15,17	1.06	1 (6%)
4	MAN	A	814	3	11,11,12	0.46	0	15,15,17	1.24	1 (6%)
8	KRZ	A	820	5	25,34,34	0.43	0	29,44,44	0.93	1 (3%)

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	BMA	A	813	2,4	-	0/2/19/22	0/1/1/1
2	NAG	A	807	1	-	0/6/23/26	0/1/1/1
2	NAG	A	805	2	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	812	3,2	-	3/6/23/26	0/1/1/1
2	NAG	A	806	1	-	4/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	NAG	A	809	3,2	-	2/6/23/26	0/1/1/1
4	MAN	A	815	3	-	0/2/19/22	0/1/1/1
2	NAG	A	803	1	-	4/6/23/26	0/1/1/1
2	NAG	A	811	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	804	1,2	-	0/6/23/26	0/1/1/1
3	BMA	A	810	2	-	0/2/19/22	0/1/1/1
4	MAN	A	814	3	-	0/2/19/22	0/1/1/1
8	KRZ	A	820	5	-	5/27/37/37	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	812	NAG	C1-O5-C5	4.31	118.03	112.19
2	A	803	NAG	O5-C5-C6	4.28	113.91	107.20
2	A	806	NAG	C1-O5-C5	4.22	117.91	112.19
2	A	811	NAG	C1-O5-C5	4.13	117.79	112.19
4	A	814	MAN	O5-C5-C6	3.38	112.50	107.20
2	A	806	NAG	O5-C5-C6	3.31	112.39	107.20
8	A	820	KRZ	C3-C2-N1	2.97	117.89	111.90
4	A	815	MAN	O5-C5-C6	2.97	111.86	107.20
3	A	810	BMA	O5-C5-C6	2.84	111.65	107.20
2	A	805	NAG	O5-C5-C6	2.82	111.62	107.20
2	A	811	NAG	O5-C1-C2	-2.72	106.99	111.29
2	A	808	NAG	O5-C5-C4	-2.60	104.50	110.83
3	A	813	BMA	C1-C2-C3	2.60	112.86	109.67
3	A	813	BMA	O3-C3-C2	-2.52	105.18	109.99
2	A	808	NAG	O4-C4-C3	-2.47	104.64	110.35
2	A	806	NAG	C6-C5-C4	-2.20	107.86	113.00
2	A	809	NAG	C8-C7-N2	2.20	119.82	116.10
2	A	807	NAG	O5-C5-C6	2.14	110.56	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	813	BMA	O6-C6-C5	-2.13	104.00	111.29
2	A	807	NAG	O3-C3-C4	-2.11	105.46	110.35
2	A	805	NAG	O4-C4-C5	2.09	114.47	109.30
2	A	807	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	820	KRZ	N1-C2-C3-C4
8	A	820	KRZ	C6-C5-N2-C4
2	A	806	NAG	C8-C7-N2-C2
2	A	806	NAG	O7-C7-N2-C2
2	A	803	NAG	C8-C7-N2-C2
2	A	806	NAG	O5-C5-C6-O6
2	A	808	NAG	C8-C7-N2-C2
2	A	808	NAG	O7-C7-N2-C2
2	A	812	NAG	C8-C7-N2-C2
2	A	812	NAG	O7-C7-N2-C2
2	A	809	NAG	C8-C7-N2-C2
2	A	809	NAG	O7-C7-N2-C2
2	A	803	NAG	O7-C7-N2-C2
8	A	820	KRZ	C3-C2-N1-C1
2	A	803	NAG	C4-C5-C6-O6
2	A	806	NAG	C4-C5-C6-O6
8	A	820	KRZ	C13-C9-N4-C8
2	A	803	NAG	O5-C5-C6-O6
8	A	820	KRZ	C14-C5-N2-C4
2	A	811	NAG	C4-C5-C6-O6
2	A	811	NAG	O5-C5-C6-O6
2	A	812	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 8 short contacts:

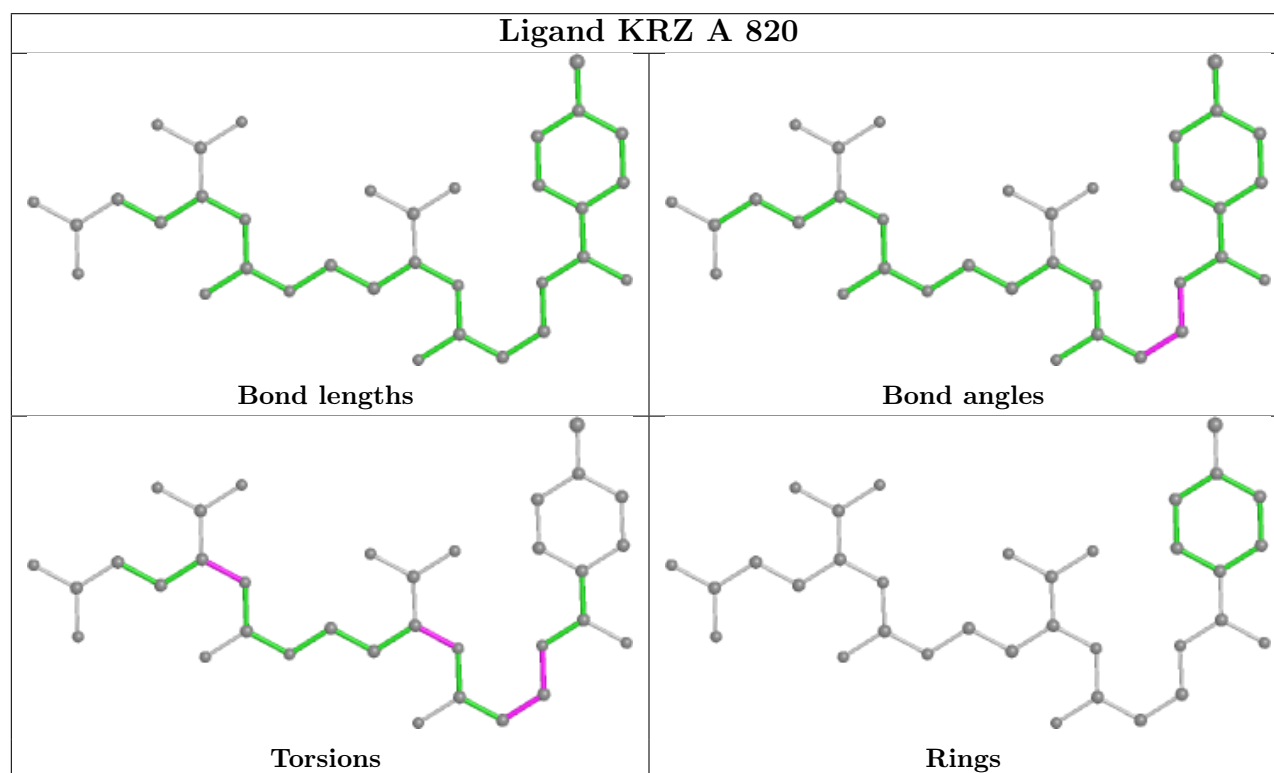
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	813	BMA	0	1
2	A	807	NAG	1	0
2	A	809	NAG	2	0
2	A	803	NAG	1	0
2	A	804	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	820	KRZ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	696/707 (98%)	0.38	52 (7%) 14 19	23, 33, 54, 89	9 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	SER	10.0
1	A	655[A]	LYS	8.4
1	A	541	TRP	7.3
1	A	135	GLY	4.8
1	A	153	ASN	4.7
1	A	507	SER	4.6
1	A	487	GLY	4.4
1	A	719	VAL	4.0
1	A	335	GLY	3.8
1	A	155[A]	SER	3.6
1	A	136	ASN	3.4
1	A	134	ASP	3.3
1	A	546	PHE	3.3
1	A	488	PHE	3.2
1	A	131	ILE	3.2
1	A	56	HIS	3.2
1	A	339	THR	3.0
1	A	490	GLY	3.0
1	A	334	THR	3.0
1	A	132	ASN	3.0
1	A	337	PHE	2.9
1	A	310	GLY	2.9
1	A	505	GLU	2.8
1	A	548	GLY	2.7
1	A	133	GLU	2.7
1	A	456	ILE	2.6
1	A	543	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	504	PRO	2.6
1	A	340	GLN	2.6
1	A	154	VAL	2.6
1	A	336	ASN	2.5
1	A	124	HIS	2.5
1	A	466	CYS	2.5
1	A	544	ASN	2.5
1	A	152	GLU	2.4
1	A	545	LYS	2.4
1	A	515	LEU	2.3
1	A	314	PRO	2.3
1	A	521	PHE	2.3
1	A	341	LYS	2.3
1	A	386	ILE	2.2
1	A	338	SER	2.2
1	A	123	THR	2.2
1	A	208	VAL	2.2
1	A	373	ILE	2.2
1	A	450	ILE	2.2
1	A	209	PHE	2.1
1	A	448	ALA	2.1
1	A	449	TYR	2.1
1	A	104	GLY	2.0
1	A	503	SER	2.0
1	A	654[A]	ASP	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 ⓘ

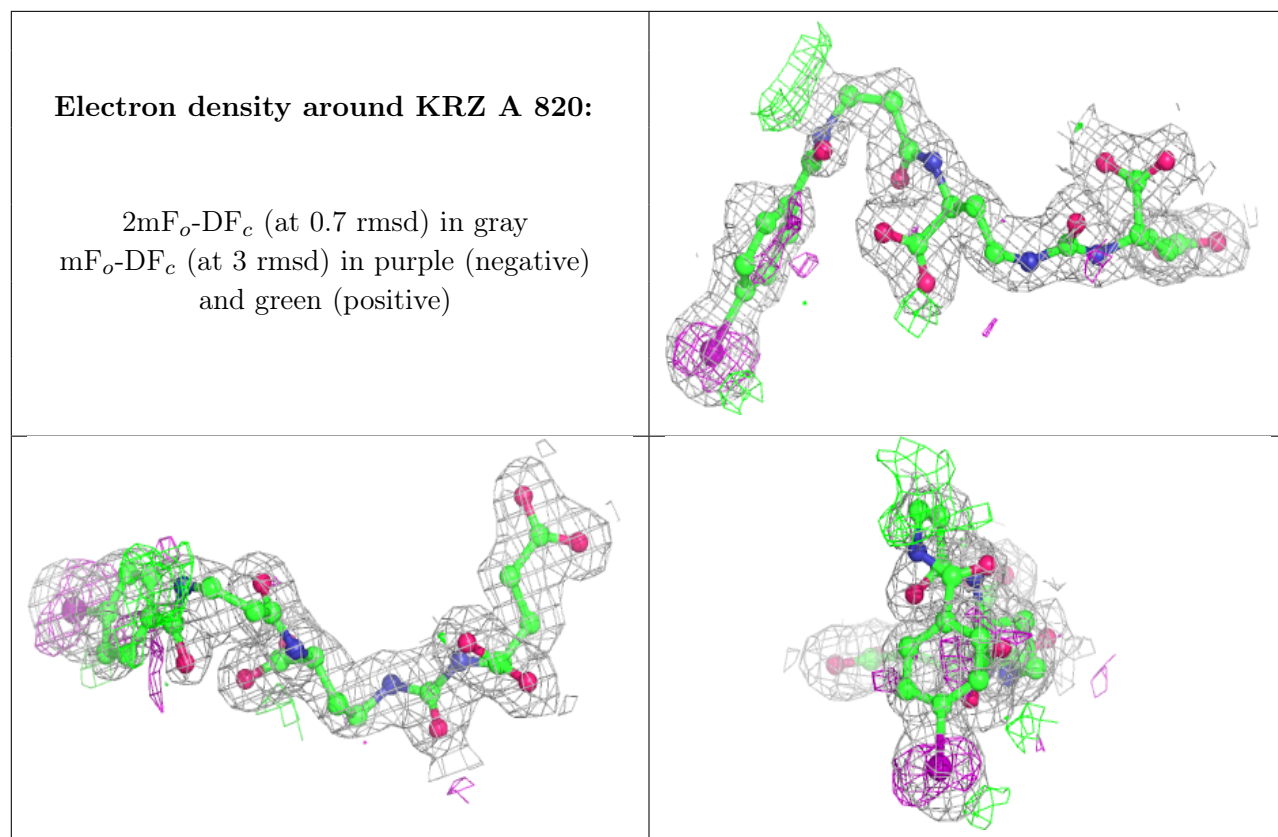
There are no carbohydrates in this entry.

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. 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	B-factors(\AA^2)	Q<0.9
2	NAG	A	802	14/15	0.76	0.34	47,60,67,70	0
2	NAG	A	803	14/15	0.76	0.29	53,62,72,73	0
4	MAN	A	815	11/12	0.77	0.25	61,74,80,84	0
2	NAG	A	806	14/15	0.77	0.26	69,79,86,91	0
3	BMA	A	810	11/12	0.77	0.25	54,65,71,83	0
2	NAG	A	804	14/15	0.82	0.24	44,49,54,58	0
2	NAG	A	805	14/15	0.83	0.34	56,65,75,79	0
2	NAG	A	811	14/15	0.88	0.12	27,37,50,57	0
2	NAG	A	807	14/15	0.88	0.11	37,50,57,63	0
3	BMA	A	813	11/12	0.88	0.13	50,55,63,63	0
4	MAN	A	814	11/12	0.89	0.11	55,59,64,66	0
2	NAG	A	812	14/15	0.89	0.20	49,53,67,74	0
2	NAG	A	801	14/15	0.92	0.17	39,46,53,56	0
2	NAG	A	809	14/15	0.93	0.11	41,47,56,58	0
2	NAG	A	808	14/15	0.94	0.09	33,37,43,47	0
8	KRZ	A	820	34/34	0.96	0.13	25,36,59,60	3
7	CL	A	819	1/1	1.00	0.17	30,30,30,30	0
6	CA	A	818	1/1	1.00	0.10	26,26,26,26	0
5	ZN	A	816	1/1	1.00	0.08	27,27,27,27	0
5	ZN	A	817	1/1	1.00	0.07	26,26,26,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.