



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2016 – 08:26 AM EDT

PDB ID : 5F09
Title : Structure of inactive GCPII mutant in complex with beta-citryl glutamate
Authors : Tykvar, J.; Navratil, M.; Pachl, P.; Konvalinka, J.
Deposited on : 2015-11-27
Resolution : 1.85 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

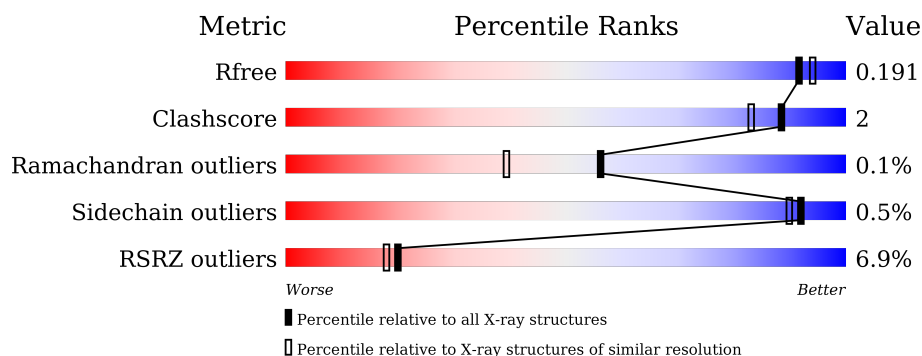
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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
4	MAN	A	814	-	-	-	X
9	PGE	A	820	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6402 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	23	0
			5617	3612	940	1047	18			

There are 33 discrepancies between the modelled and reference sequences:

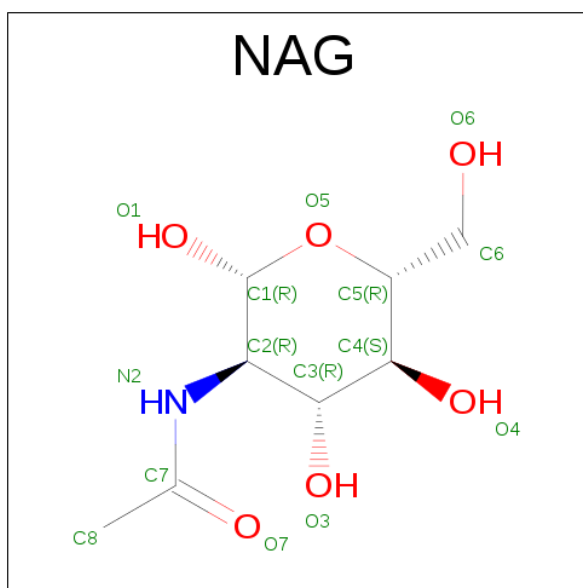
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ARG	-	expression tag	UNP Q04609
A	13	SER	-	expression tag	UNP Q04609
A	14	GLY	-	expression tag	UNP Q04609
A	15	LEU	-	expression tag	UNP Q04609
A	16	ASN	-	expression tag	UNP Q04609
A	17	ASP	-	expression tag	UNP Q04609
A	18	ILE	-	expression tag	UNP Q04609
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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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
A	424	ALA	GLU	engineered mutation	UNP Q04609

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



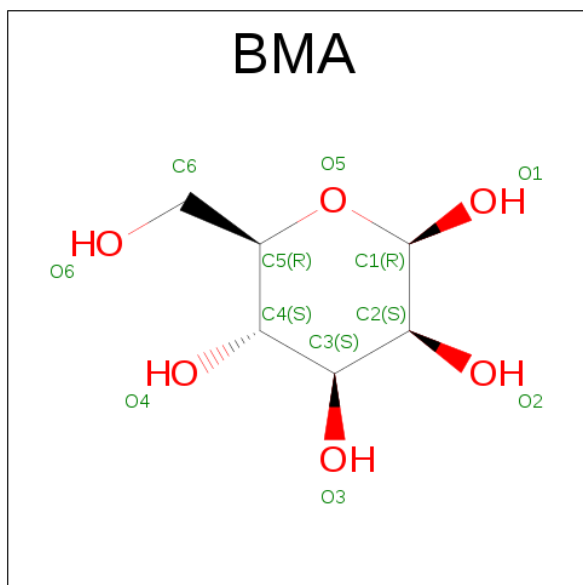
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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		

- 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		

- 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		

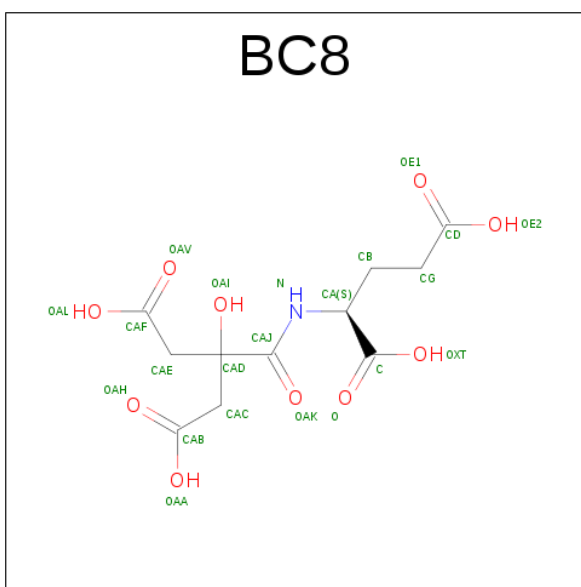
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

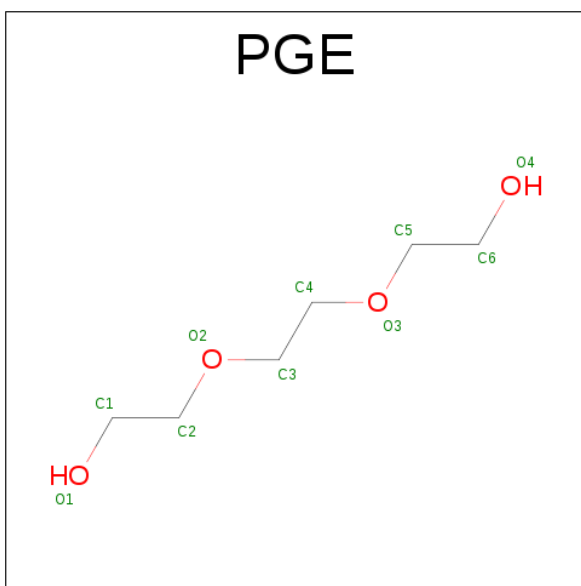
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is beta-citryl-L-glutamic acid (three-letter code: BC8) (formula: C₁₁H₁₅NO₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	1
			22	11	1	10		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		

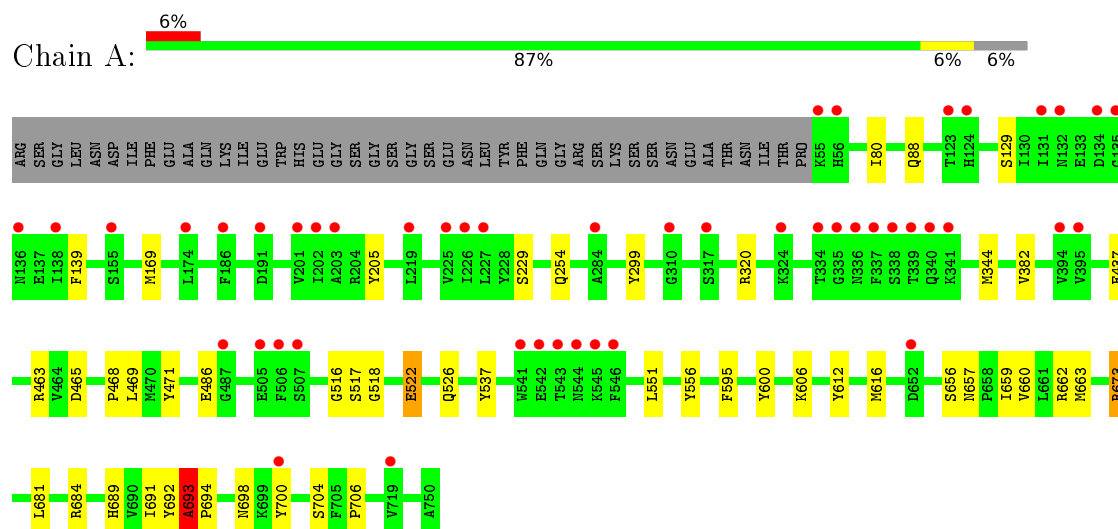
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	561	Total 562	O 562	0	32

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	100.90Å 130.92Å 159.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 29.40 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.85) 99.1 (29.40-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.155 , 0.181 0.167 , 0.191	Depositor DCC
R_{free} test set	4444 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6402	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PGE, NAG, CL, CA, BMA, BC8, 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	0.77	4/5830 (0.1%)	0.86	10/7915 (0.1%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	GLU	CD-OE2	-6.01	1.19	1.25
1	A	437	GLU	CD-OE2	-5.94	1.19	1.25
1	A	656	SER	CA-C	5.40	1.67	1.52
1	A	486	GLU	CD-OE1	5.08	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	ARG	NE-CZ-NH2	14.83	127.72	120.30
1	A	662	ARG	NE-CZ-NH1	-14.06	113.27	120.30
1	A	673	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	463	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	465	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	693[A]	ALA	C-N-CD	5.62	140.21	128.40
1	A	693[B]	ALA	C-N-CD	5.62	140.21	128.40
1	A	463	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	320	ARG	NE-CZ-NH1	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	ARG	CD-NE-CZ	5.12	130.77	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	693[A]	ALA	Mainchain

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	5617	0	5397	26	0
2	A	154	0	137	0	0
3	A	22	0	19	0	0
4	A	11	0	10	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	22	0	0	3	0
9	A	10	0	14	0	2
10	A	562	0	0	3	0
All	All	6402	0	5577	28	2

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 2.

All (28) 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:704[A]:SER:OG	10:A:901[A]:HOH:O	1.94	0.84
1:A:657:ASN:ND2	1:A:660:VAL:HG23	2.02	0.75
1:A:659:ILE:O	1:A:663[B]:MET:HG3	1.93	0.69
1:A:517[A]:SER:OG	1:A:518:GLY:N	2.22	0.68
1:A:516:GLY:O	1:A:526[A]:GLN:NE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ASN:HD22	1:A:660:VAL:HG23	1.65	0.61
1:A:684:ARG:NH2	1:A:694[B]:PRO:O	2.36	0.53
1:A:517[A]:SER:OG	1:A:522:GLU:OE2	2.20	0.53
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.46	0.51
1:A:657:ASN:HD22	1:A:660:VAL:CG2	2.24	0.51
1:A:205:TYR:CE2	1:A:254:GLN:HB3	2.51	0.45
1:A:691:ILE:O	1:A:704[A]:SER:HA	2.17	0.45
1:A:689:HIS:HB3	1:A:692[A]:TYR:O	2.17	0.45
1:A:606:LYS:NZ	10:A:913:HOH:O	2.51	0.43
1:A:681:LEU:HD11	1:A:693[B]:ALA:HB3	1.99	0.42
1:A:698[A]:ASN:OD1	1:A:700[A]:TYR:HB2	2.18	0.42
8:A:819[A]:BC8:CAJ	10:A:902:HOH:O	2.67	0.42
1:A:80:ILE:HD12	1:A:88:GLN:HG2	2.02	0.42
1:A:518:GLY:O	8:A:819[A]:BC8:CAC	2.67	0.42
1:A:129:SER:HA	1:A:139:PHE:O	2.20	0.42
1:A:469:LEU:O	1:A:595:PHE:HA	2.20	0.42
1:A:693[A]:ALA:HB3	1:A:706:PRO:HG3	2.02	0.42
1:A:229:SER:O	1:A:299:TYR:HB3	2.21	0.41
1:A:551:LEU:HD22	1:A:556:TYR:HB2	2.02	0.41
1:A:468:PRO:HA	1:A:471:TYR:CE1	2.56	0.41
1:A:517[A]:SER:HB2	1:A:694[A]:PRO:HG3	2.03	0.41
8:A:819[A]:BC8:OAV	8:A:819[A]:BC8:CAB	2.69	0.41
1:A:169:MET:HA	1:A:344:MET:O	2.22	0.41

All (2) 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)
9:A:820:PGE:O1	9:A:820:PGE:O1[2_555]	1.05	1.15
9:A:820:PGE:C1	9:A:820:PGE:O1[2_555]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	717/739 (97%)	698 (97%)	18 (2%)	1 (0%)	56	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL

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	595/628 (95%)	592 (100%)	3 (0%)	92	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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 ⓘ

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	$\# Z > 2$
2	NAG	A	801	1,2	14,14,15	0.49	0	15,19,21	0.89	1 (6%)
2	NAG	A	802	2	14,14,15	0.54	0	15,19,21	1.43	2 (13%)
2	NAG	A	803	1	14,14,15	0.75	0	15,19,21	1.76	3 (20%)
2	NAG	A	804	1,2	14,14,15	0.59	0	15,19,21	0.95	0
2	NAG	A	805	2	14,14,15	0.52	0	15,19,21	1.75	3 (20%)
2	NAG	A	806	1	14,14,15	0.58	0	15,19,21	2.18	2 (13%)
2	NAG	A	807	1	14,14,15	1.14	1 (7%)	15,19,21	2.29	3 (20%)
2	NAG	A	808	1,2	14,14,15	0.96	1 (7%)	15,19,21	0.85	1 (6%)
2	NAG	A	809	3,2	14,14,15	0.55	0	15,19,21	0.91	0
3	BMA	A	810	2	11,11,12	0.85	0	15,15,17	2.34	5 (33%)
2	NAG	A	811	1,2	14,14,15	0.60	0	15,19,21	1.13	2 (13%)
2	NAG	A	812	3,2	14,14,15	0.70	0	15,19,21	1.81	4 (26%)
3	BMA	A	813	2,4	11,11,12	0.57	0	15,15,17	1.29	1 (6%)
4	MAN	A	814	3	11,11,12	0.64	0	15,15,17	1.22	1 (6%)
8	BC8	A	819[A]	5	9,21,21	0.90	0	13,29,29	3.13	6 (46%)
9	PGE	A	820	-	9,9,9	0.69	0	8,8,8	0.62	0

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	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	806	1	-	0/6/23/26	0/1/1/1
2	NAG	A	807	1	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	809	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	810	2	-	0/2/19/22	0/1/1/1
2	NAG	A	811	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	812	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	813	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	814	3	-	0/2/19/22	0/1/1/1
8	BC8	A	819[A]	5	-	0/19/29/29	0/0/0/0
9	PGE	A	820	-	-	0/7/7/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	807	NAG	O5-C1	-3.19	1.38	1.43
2	A	808	NAG	O5-C1	-2.49	1.39	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	819[A]	BC8	C-CA-N	-6.04	100.88	112.93
8	A	819[A]	BC8	CAE-CAD-CAJ	-4.41	100.18	109.99
3	A	813	BMA	O3-C3-C2	-3.25	104.06	110.01
2	A	812	NAG	C2-N2-C7	-3.07	119.12	123.11
2	A	805	NAG	C4-C3-C2	-2.75	107.06	111.34
2	A	812	NAG	O3-C3-C2	-2.51	104.01	109.37
2	A	811	NAG	C6-C5-C4	-2.32	107.18	112.99
2	A	808	NAG	C4-C3-C2	-2.19	107.94	111.34
2	A	803	NAG	C2-N2-C7	-2.06	120.43	123.11
2	A	801	NAG	O4-C4-C3	-2.04	105.75	110.36
2	A	806	NAG	C4-C3-C2	-2.04	108.17	111.34
2	A	811	NAG	C1-O5-C5	2.04	115.14	112.14
2	A	805	NAG	O4-C4-C5	2.04	114.60	109.23
2	A	802	NAG	O5-C5-C4	2.11	113.62	110.13
3	A	810	BMA	C2-C3-C4	2.15	114.80	111.05
2	A	803	NAG	O5-C5-C4	2.31	113.96	110.13
2	A	812	NAG	O3-C3-C4	2.35	115.66	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	NAG	C2-N2-C7	2.40	126.23	123.11
3	A	810	BMA	O5-C5-C4	2.44	114.18	110.13
4	A	814	MAN	O5-C5-C6	2.93	113.61	107.34
8	A	819[A]	BC8	OAI-CAD-CAE	3.03	114.93	109.21
8	A	819[A]	BC8	CB-CA-N	3.07	114.72	109.92
8	A	819[A]	BC8	CAC-CAD-CAJ	3.12	116.91	109.99
2	A	807	NAG	C3-C4-C5	3.32	116.14	110.23
3	A	810	BMA	C3-C4-C5	3.85	117.08	110.23
2	A	812	NAG	C1-O5-C5	3.87	117.83	112.14
3	A	810	BMA	C1-C2-C3	4.23	114.67	109.55
2	A	803	NAG	C1-O5-C5	4.55	118.83	112.14
2	A	805	NAG	C1-O5-C5	4.68	119.02	112.14
2	A	807	NAG	O5-C5-C4	4.87	118.21	110.13
3	A	810	BMA	C1-O5-C5	5.62	120.41	112.14
2	A	807	NAG	C1-O5-C5	5.91	120.83	112.14
8	A	819[A]	BC8	CAD-CAE-CAF	6.08	124.45	114.95
2	A	806	NAG	C1-O5-C5	7.72	123.49	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	819[A]	BC8	3	0
9	A	820	PGE	0	2

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%)	0.11	48 (6%)	20 18	20, 36, 81, 110	3 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	THR	5.7
1	A	335	GLY	5.5
1	A	541	TRP	5.4
1	A	135	GLY	5.2
1	A	337	PHE	5.1
1	A	546	PHE	5.0
1	A	202	ILE	4.5
1	A	700[A]	TYR	4.4
1	A	543	THR	4.4
1	A	219	LEU	4.3
1	A	138	ILE	4.2
1	A	544	ASN	4.2
1	A	136	ASN	3.8
1	A	226	ILE	3.8
1	A	336	ASN	3.6
1	A	227	LEU	3.5
1	A	338	SER	3.3
1	A	506	PHE	3.3
1	A	719	VAL	3.3
1	A	55	LYS	3.3
1	A	201	VAL	3.3
1	A	134	ASP	3.2
1	A	225	VAL	3.0
1	A	340	GLN	3.0
1	A	339	THR	2.9
1	A	310	GLY	2.9
1	A	132	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	341	LYS	2.8
1	A	545	LYS	2.8
1	A	317	SER	2.7
1	A	124	HIS	2.7
1	A	131	ILE	2.6
1	A	652	ASP	2.6
1	A	394	VAL	2.6
1	A	186	PHE	2.5
1	A	324	LYS	2.5
1	A	174	LEU	2.4
1	A	487	GLY	2.4
1	A	505	GLU	2.3
1	A	56	HIS	2.3
1	A	123	THR	2.3
1	A	507	SER	2.3
1	A	542	GLU	2.1
1	A	395	VAL	2.1
1	A	284	ALA	2.1
1	A	155	SER	2.0
1	A	203	ALA	2.0
1	A	191	ASP	2.0

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](#)

There are no carbohydrates in this entry.

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
9	PGE	A	820	10/10	0.73	0.29	5.60	41,44,51,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MAN	A	814	11/12	0.93	0.15	2.23	72,74,75,79	0
8	BC8	A	819[A]	22/22	0.88	0.19	1.37	25,37,48,50	22
2	NAG	A	804	14/15	0.83	0.23	1.08	67,72,78,82	0
7	CA	A	818	1/1	1.00	0.08	0.55	22,22,22,22	0
2	NAG	A	811	14/15	0.93	0.09	0.36	28,35,45,48	0
5	ZN	A	816	1/1	1.00	0.09	-1.40	26,26,26,26	0
6	CL	A	817	1/1	1.00	0.08	-1.44	29,29,29,29	0
5	ZN	A	815	1/1	1.00	0.08	-6.22	27,27,27,27	0
2	NAG	A	805	14/15	0.79	0.41	-	84,90,98,103	0
2	NAG	A	807	14/15	0.92	0.21	-	43,54,63,64	0
2	NAG	A	809	14/15	0.94	0.21	-	53,59,62,70	0
2	NAG	A	803	14/15	0.75	0.32	-	66,72,80,82	0
2	NAG	A	802	14/15	0.76	0.26	-	53,62,69,71	0
2	NAG	A	808	14/15	0.92	0.10	-	41,43,48,49	0
2	NAG	A	806	14/15	0.84	0.23	-	104,109,111,112	0
2	NAG	A	801	14/15	0.96	0.11	-	45,51,55,56	0
3	BMA	A	810	11/12	0.77	0.31	-	77,82,87,88	0
3	BMA	A	813	11/12	0.83	0.18	-	58,66,69,72	0
2	NAG	A	812	14/15	0.85	0.20	-	48,56,61,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.