



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:04 AM GMT

PDB ID : 3D7D  
Title : A high resolution crystal structure of human glutamate carboxypeptidase II (GCPII) in a complex with DCFBD, a urea-based inhibitor  
Authors : Lubkowski, J.; Barinka, C.  
Deposited on : 2008-05-21  
Resolution : 1.69 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](mailto: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.

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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



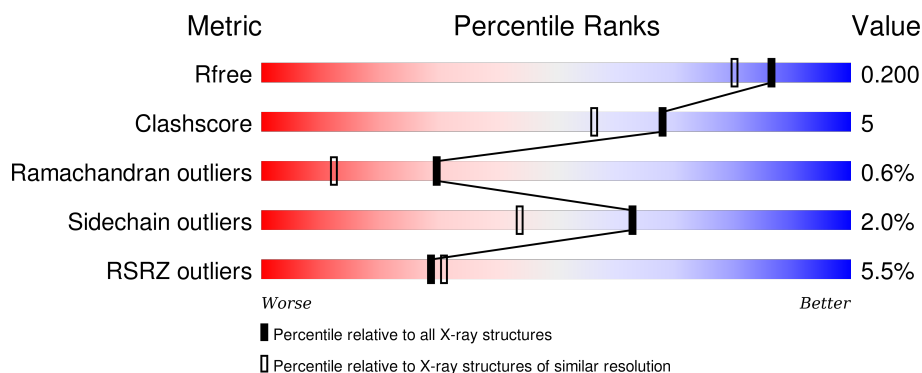
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.69 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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  $\geq 3$ , 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	709	

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	1756	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1758	-	-	-	X
3	NAG	A	1757	-	-	-	X
4	NAG	A	1761	-	-	-	X



## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6580 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	694	Total	C	N	O	S	0	55	0
			5736	3693	955	1066	22			

There are 2 discrepancies between the modelled and reference sequences:

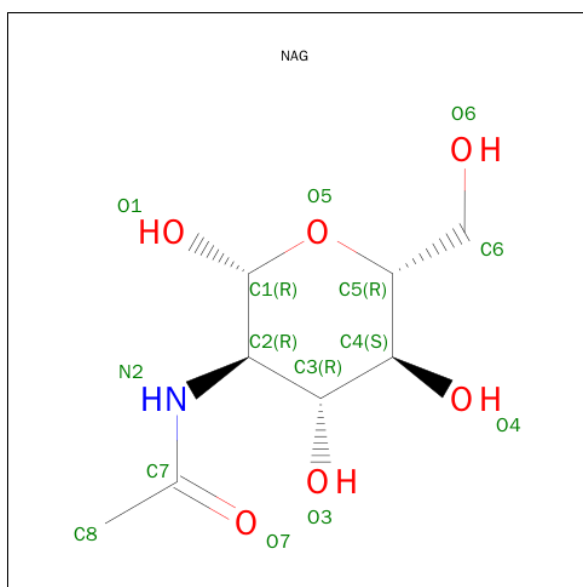
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ARG	-	EXPRESSION TAG	UNP Q04609
A	43	SER	-	EXPRESSION TAG	UNP Q04609

- 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		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





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		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

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

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

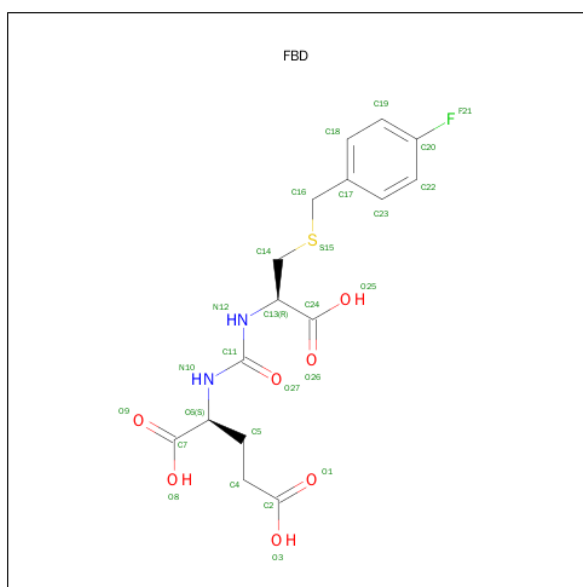


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is N-((1R)-1-CARBOXY-2-[(4-FLUOROBENZYL)SULFANYL]ETHYL)CARBAMOYL)-L-GLUTAMIC ACID (three-letter code: FBD) (formula: C<sub>16</sub>H<sub>19</sub>FN<sub>2</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C F N O S 27 16 1 2 7 1	0	0

- Molecule 10 is water.

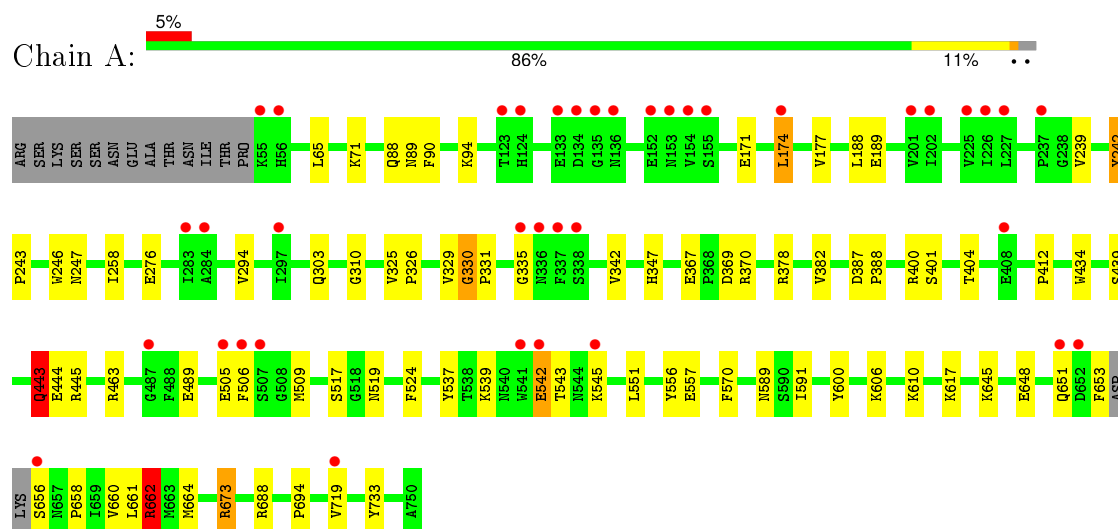
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	626	Total O 626 626	0	3



### 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, $\alpha$ , $\beta$ , $\gamma$	101.93Å 130.50Å 159.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.69 27.55 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-1.69) 98.9 (27.55-1.69)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.02 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.179 , 0.199 0.178 , 0.200	Depositor DCC
$R_{free}$ test set	1730 reflections (1.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 116642 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, CA, FBD, 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	0.97	5/6106 (0.1%)	0.88	9/8266 (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	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443[A]	GLN	CB-CG	-5.74	1.37	1.52
1	A	443[B]	GLN	CB-CG	-5.74	1.37	1.52
1	A	434	TRP	CE3-CZ3	5.40	1.47	1.38
1	A	557	GLU	CB-CG	-5.37	1.42	1.52
1	A	524	PHE	CE1-CZ	5.14	1.47	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	673	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	370	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	174[A]	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	174[B]	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	662[A]	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	662[B]	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	445	ARG	NE-CZ-NH1	5.26	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	PRO	N-CA-C	-5.20	98.58	112.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	TYR	Mainchain,Peptide
1	A	330	GLY	Mainchain,Peptide
1	A	387	ASP	Mainchain,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	5736	0	5620	52	3
2	A	56	0	50	2	0
3	A	42	0	39	1	0
4	A	39	0	34	1	0
5	A	50	0	43	0	1
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	27	0	16	1	0
10	A	626	0	0	19	4
All	All	6580	0	5802	56	5

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 5.

All (56) 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:660[A]:VAL:O	1:A:664[A]:MET:HG2	1.42	1.16
1:A:89[B]:ASN:HD21	1:A:378:ARG:HH21	1.07	0.99
1:A:89[B]:ASN:ND2	1:A:378:ARG:HH21	1.74	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:HA	1:A:589[B]:ASN:HD21	1.41	0.82
1:A:658[A]:PRO:HB3	10:A:2134:HOH:O	1.83	0.78
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.85	0.77
1:A:89[B]:ASN:HD21	1:A:378:ARG:NH2	1.84	0.75
1:A:242:TYR:OH	10:A:2311:HOH:O	2.09	0.71
2:A:1756:NAG:H81	10:A:2022:HOH:O	1.93	0.69
1:A:591[A]:ILE:HG23	1:A:661[A]:LEU:HD21	1.76	0.66
1:A:733:TYR:HE2	10:A:2155:HOH:O	1.80	0.64
1:A:463:ARG:NH2	1:A:545:LYS:HG3	2.16	0.61
1:A:177:VAL:HG12	1:A:188:LEU:HD11	1.84	0.60
1:A:506:PHE:HB2	1:A:509:MET:HG3	1.84	0.59
1:A:463:ARG:NH2	1:A:545:LYS:HE2	2.21	0.56
1:A:539:LYS:CD	10:A:2329:HOH:O	2.55	0.55
1:A:539:LYS:HE2	10:A:2366:HOH:O	2.07	0.53
1:A:239[A]:VAL:HG22	1:A:247:ASN:ND2	2.24	0.52
9:A:1:FBD:H19	10:A:2385:HOH:O	2.09	0.52
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.90	0.52
1:A:517:SER:HB2	1:A:694:PRO:HG3	1.91	0.52
1:A:617:LYS:NZ	10:A:2279:HOH:O	2.43	0.51
1:A:542:GLU:HG2	1:A:543:THR:HG23	1.92	0.51
1:A:463:ARG:HH21	1:A:545:LYS:HE2	1.75	0.50
1:A:653:PHE:HZ	1:A:661[A]:LEU:HD13	1.77	0.50
1:A:539:LYS:HE3	10:A:1859:HOH:O	2.12	0.50
1:A:539:LYS:HD3	10:A:2329:HOH:O	2.11	0.49
1:A:325:VAL:HB	1:A:326:PRO:HD2	1.93	0.49
1:A:246:TRP:CD1	3:A:1760:NAG:H83	2.48	0.48
1:A:610:LYS:CE	10:A:1951:HOH:O	2.60	0.48
1:A:90[B]:PHE:CE2	1:A:94:LYS:HE2	2.48	0.48
1:A:90[B]:PHE:CZ	1:A:94:LYS:HD3	2.49	0.48
1:A:645[A]:LYS:HD2	10:A:2332:HOH:O	2.14	0.48
4:A:1761:NAG:H81	10:A:2095:HOH:O	2.14	0.47
1:A:188:LEU:CD2	1:A:329:VAL:HG11	2.46	0.45
1:A:258:ILE:HD13	1:A:294:VAL:HB	1.98	0.45
1:A:688[B]:ARG:CZ	10:A:1878:HOH:O	2.64	0.45
1:A:506:PHE:CB	1:A:509:MET:HG3	2.46	0.45
1:A:606[A]:LYS:HG2	10:A:1982:HOH:O	2.18	0.44
1:A:310:GLY:O	1:A:330:GLY:HA2	2.18	0.43
2:A:1756:NAG:C8	10:A:2022:HOH:O	2.59	0.43
1:A:65:LEU:HD23	1:A:401[B]:SER:OG	2.19	0.43
1:A:239[A]:VAL:HG22	1:A:247:ASN:CG	2.39	0.42
1:A:648:GLU:O	1:A:651[B]:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:HIS:HE1	10:A:2118:HOH:O	2.01	0.42
1:A:439:SER:O	1:A:443[A]:GLN:HB2	2.19	0.42
1:A:71:LYS:HG3	1:A:570:PHE:CE2	2.54	0.42
1:A:174[B]:LEU:HD11	1:A:342:VAL:HG21	2.02	0.41
1:A:88[B]:GLN:CD	10:A:2138:HOH:O	2.58	0.41
1:A:367:GLU:OE1	1:A:662[A]:ARG:NH1	2.42	0.41
1:A:539:LYS:HD2	10:A:2329:HOH:O	2.20	0.41
1:A:444:GLU:HA	1:A:444:GLU:OE1	2.21	0.41
1:A:369:ASP:OD2	1:A:662[B]:ARG:NH2	2.32	0.40
1:A:489:GLU:H	1:A:489:GLU:CD	2.24	0.40

All (5) 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)
10:A:1990:HOH:O	10:A:2355:HOH:O[2_565]	1.95	0.25
1:A:656[B]:SER:OG	10:A:2134:HOH:O[4_566]	1.99	0.21
10:A:2038:HOH:O	10:A:2170:HOH:O[2_565]	2.08	0.12
1:A:276:GLU:OE1	5:A:1765:BMA:O2[2_565]	2.08	0.12
1:A:656[B]:SER:O	10:A:2134:HOH:O[4_566]	2.10	0.10

## 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	742/709 (105%)	719 (97%)	19 (3%)	4 (0%)	34 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	PRO
1	A	243	PRO

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Mol	Chain	Res	Type
1	A	382	VAL
1	A	335	GLY

### 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	644/605 (106%)	630 (98%)	14 (2%)	60 39

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	GLU
1	A	189	GLU
1	A	303	GLN
1	A	443[A]	GLN
1	A	443[B]	GLN
1	A	505	GLU
1	A	519	ASN
1	A	537	TYR
1	A	542	GLU
1	A	600	TYR
1	A	662[A]	ARG
1	A	662[B]	ARG
1	A	673	ARG
1	A	719	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	136	ASN
1	A	618	HIS



### 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 ⓘ

11 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	1755	1,2	14,14,15	0.50	0	15,19,21	1.22	1 (6%)
2	NAG	A	1756	2	14,14,15	0.65	0	15,19,21	1.61	2 (13%)
2	NAG	A	1758	1,2	14,14,15	0.72	0	15,19,21	0.97	0
4	NAG	A	1761	1,4	14,14,15	1.08	2 (14%)	15,19,21	0.93	0
4	NAG	A	1762	4	14,14,15	0.57	0	15,19,21	1.03	2 (13%)
5	NAG	A	1763	1,5	14,14,15	0.83	1 (7%)	15,19,21	1.33	3 (20%)
5	NAG	A	1764	5	14,14,15	0.58	0	15,19,21	1.16	2 (13%)
5	BMA	A	1765	5	11,11,12	0.67	0	14,15,17	1.22	0
5	MAN	A	1766	5	11,11,12	0.48	0	14,15,17	1.05	0
2	NAG	A	1767	2	14,14,15	0.38	0	15,19,21	1.05	1 (6%)
4	BMA	A	1768	4	11,11,12	0.63	0	14,15,17	1.38	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	1755	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1756	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1758	1,2	-	0/6/23/26	0/1/1/1
4	NAG	A	1761	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1762	4	-	0/6/23/26	0/1/1/1
5	NAG	A	1763	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1764	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1765	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1766	5	-	0/2/19/22	0/1/1/1
2	NAG	A	1767	2	-	0/6/23/26	0/1/1/1
4	BMA	A	1768	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1763	NAG	C1-C2	2.03	1.55	1.52
4	A	1761	NAG	C1-C2	2.25	1.55	1.52
4	A	1761	NAG	O7-C7	2.54	1.29	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1763	NAG	O4-C4-C5	-2.67	102.15	109.24
2	A	1755	NAG	C2-N2-C7	-2.51	119.82	123.04
4	A	1762	NAG	O7-C7-C8	-2.29	117.85	122.06
5	A	1763	NAG	C6-C5-C4	-2.20	107.59	113.02
5	A	1764	NAG	O7-C7-C8	-2.09	118.22	122.06
5	A	1764	NAG	C3-C4-C5	-2.04	106.65	110.20
4	A	1762	NAG	C8-C7-N2	2.08	120.09	116.11
2	A	1767	NAG	O5-C5-C6	2.27	112.25	107.35
5	A	1763	NAG	C1-O5-C5	2.43	115.33	112.25
2	A	1756	NAG	C2-N2-C7	3.24	127.20	123.04
4	A	1768	BMA	C1-O5-C5	3.66	116.90	112.25
2	A	1756	NAG	C1-O5-C5	4.22	117.61	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1756	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1761	NAG	1	0
5	A	1765	BMA	0	1

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z  > 2$
9	FBD	A	1	-	18,27,27	1.18	2 (11%)	21,35,35	1.61	2 (9%)
3	NAG	A	1757	1	14,14,15	0.62	0	15,19,21	2.18	3 (20%)
3	NAG	A	1759	1	14,14,15	0.43	0	15,19,21	1.83	1 (6%)
3	NAG	A	1760	1	14,14,15	0.59	0	15,19,21	1.56	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
9	FBD	A	1	-	-	0/17/27/27	0/1/1/1
3	NAG	A	1757	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1759	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1760	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1	FBD	C16-S15	-2.21	1.78	1.82
9	A	1	FBD	C19-C20	2.33	1.41	1.37

All (9) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1	FBD	C14-C13-N12	-4.77	99.10	110.81
3	A	1760	NAG	C2-N2-C7	-2.57	119.74	123.04
3	A	1757	NAG	O5-C5-C6	2.28	112.28	107.35
3	A	1760	NAG	O5-C5-C6	2.28	112.29	107.35
3	A	1757	NAG	C3-C4-C5	2.58	114.69	110.20
9	A	1	FBD	F21-C20-C19	2.64	122.94	118.52
3	A	1760	NAG	C1-O5-C5	3.33	116.47	112.25
3	A	1759	NAG	C1-O5-C5	6.45	120.43	112.25
3	A	1757	NAG	C1-O5-C5	7.17	121.35	112.25

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
9	A	1	FBD	1	0
3	A	1760	NAG	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	694/709 (97%)	0.14	38 (5%)	29 31	15, 25, 43, 59	3 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	LYS	4.7
1	A	153	ASN	4.3
1	A	506	PHE	4.3
1	A	155[A]	SER	3.8
1	A	719	VAL	3.8
1	A	226	ILE	3.7
1	A	336	ASN	3.7
1	A	542	GLU	3.6
1	A	227	LEU	3.5
1	A	154	VAL	3.5
1	A	507	SER	3.5
1	A	652	ASP	3.5
1	A	135	GLY	3.4
1	A	237	PRO	3.3
1	A	134	ASP	3.2
1	A	335	GLY	3.2
1	A	505	GLU	3.1
1	A	656[A]	SER	3.1
1	A	541	TRP	3.0
1	A	201[A]	VAL	2.9
1	A	487	GLY	2.8
1	A	123	THR	2.7
1	A	152	GLU	2.6
1	A	174[A]	LEU	2.6
1	A	56	HIS	2.5
1	A	337	PHE	2.5
1	A	283[A]	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	225	VAL	2.3
1	A	284	ALA	2.3
1	A	136	ASN	2.3
1	A	202	ILE	2.2
1	A	545	LYS	2.2
1	A	651[A]	GLN	2.2
1	A	338	SER	2.1
1	A	297	ILE	2.1
1	A	124	HIS	2.1
1	A	133	GLU	2.1
1	A	408	GLU	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	A	1756	14/15	0.62	0.26	7.70	42,50,55,56	0
2	NAG	A	1758	14/15	0.84	0.17	4.13	38,43,46,52	0
4	NAG	A	1761	14/15	0.91	0.12	3.33	27,29,34,39	0
5	NAG	A	1763	14/15	0.91	0.09	1.07	21,27,36,45	0
5	MAN	A	1766	11/12	0.92	0.14	0.78	42,44,49,50	0
5	NAG	A	1764	14/15	0.92	0.18	-	35,38,46,49	0
5	BMA	A	1765	11/12	0.94	0.14	-	34,36,38,40	0
4	BMA	A	1768	11/12	0.74	0.30	-	52,54,59,61	0
2	NAG	A	1755	14/15	0.92	0.10	-	33,38,43,46	0
4	NAG	A	1762	14/15	0.86	0.18	-	33,40,47,49	0
2	NAG	A	1767	14/15	0.79	0.25	-	56,59,64,64	0



## 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	1757	14/15	0.69	0.26	2.10	46,52,58,58	0
3	NAG	A	1760	14/15	0.83	0.13	1.57	30,45,52,55	0
9	FBD	A	1	27/27	0.92	0.11	0.15	18,22,43,46	0
7	CA	A	1753	1/1	1.00	0.05	-1.76	16,16,16,16	0
8	CL	A	1754	1/1	1.00	0.03	-2.13	24,24,24,24	0
6	ZN	A	1752	1/1	1.00	0.04	-2.32	19,19,19,19	0
6	ZN	A	1751	1/1	1.00	0.06	-2.70	20,20,20,20	0
3	NAG	A	1759	14/15	0.83	0.21	-	61,66,67,68	0

## 6.5 Other polymers

There are no such residues in this entry.