



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:58 PM GMT

PDB ID : 1Z8L  
Title : Crystal structure of prostate-specific membrane antigen, a tumor marker and peptidase  
Authors : Davis, M.I.; Bennett, M.J.; Thomas, L.M.; Bjorkman, P.J.  
Deposited on : 2005-03-30  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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.

---

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

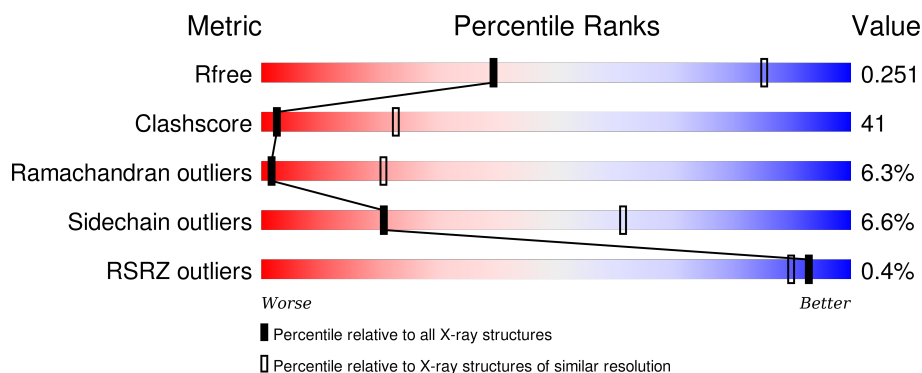
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	695	<div> <div>39%</div> <div>52%</div> <div>9%</div> </div>
1	B	695	<div> <div>40%</div> <div>51%</div> <div>9%</div> </div>
1	C	695	<div> <div>39%</div> <div>52%</div> <div>9%</div> </div>
1	D	695	<div> <div>39%</div> <div>51%</div> <div>9%</div> </div>

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
5	NAG	C	3759	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 22836 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			
1	B	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			
1	C	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			
1	D	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			

- 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	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

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

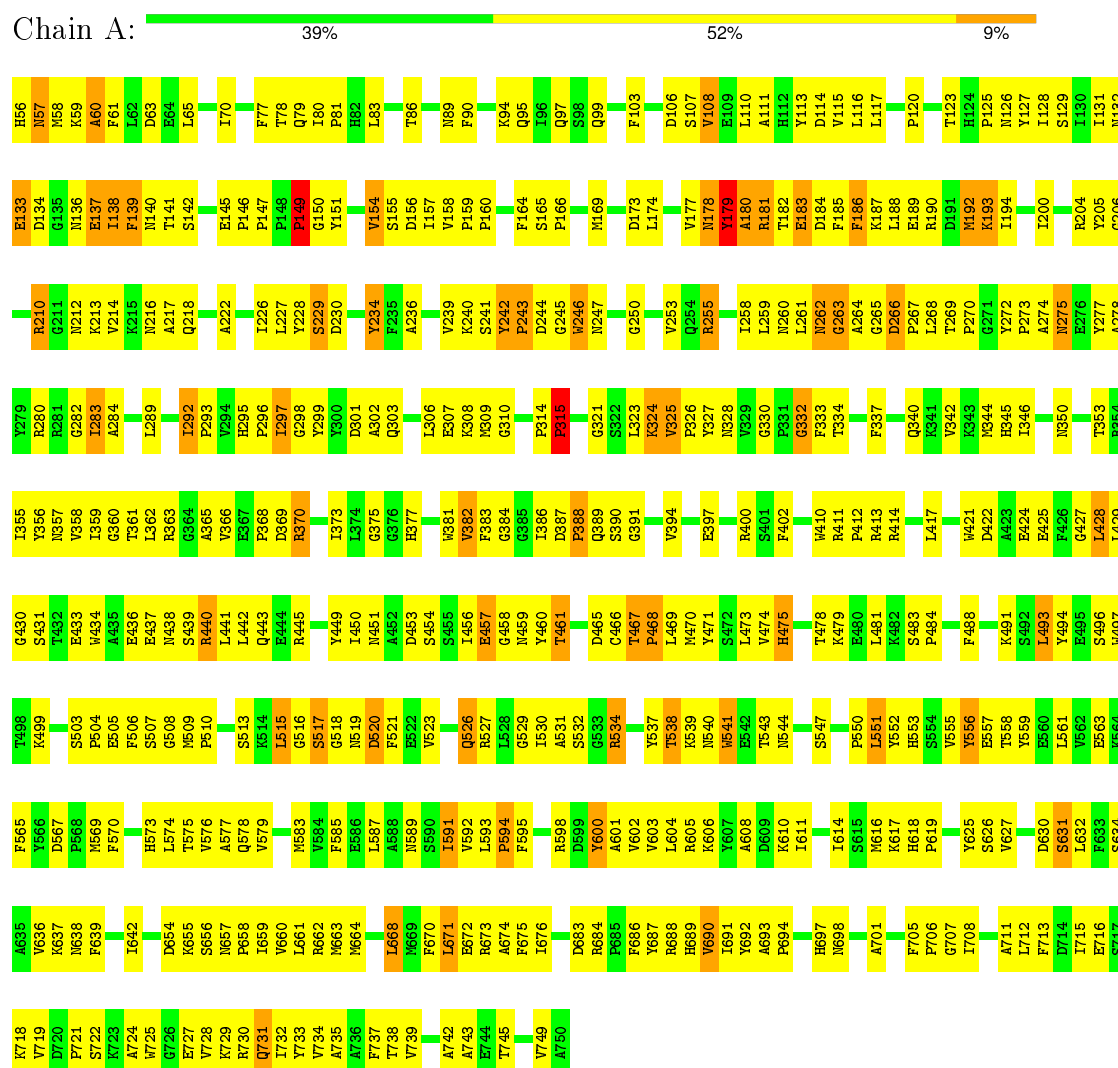
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total 3	O 3	0	0
7	B	3	Total 3	O 3	0	0
7	C	4	Total 4	O 4	0	0
7	D	2	Total 2	O 2	0	0

### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

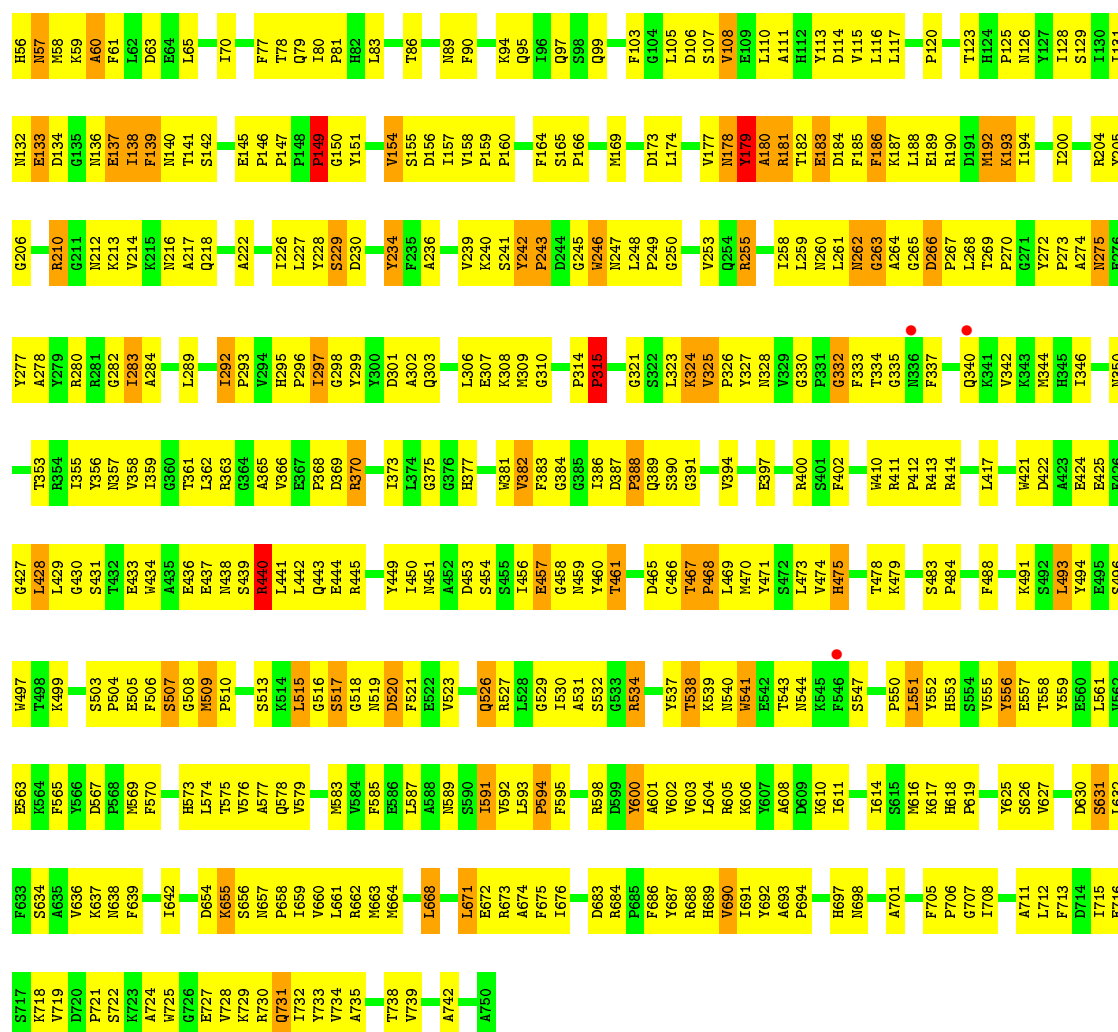
#### • Molecule 1: Glutamate carboxypeptidase II



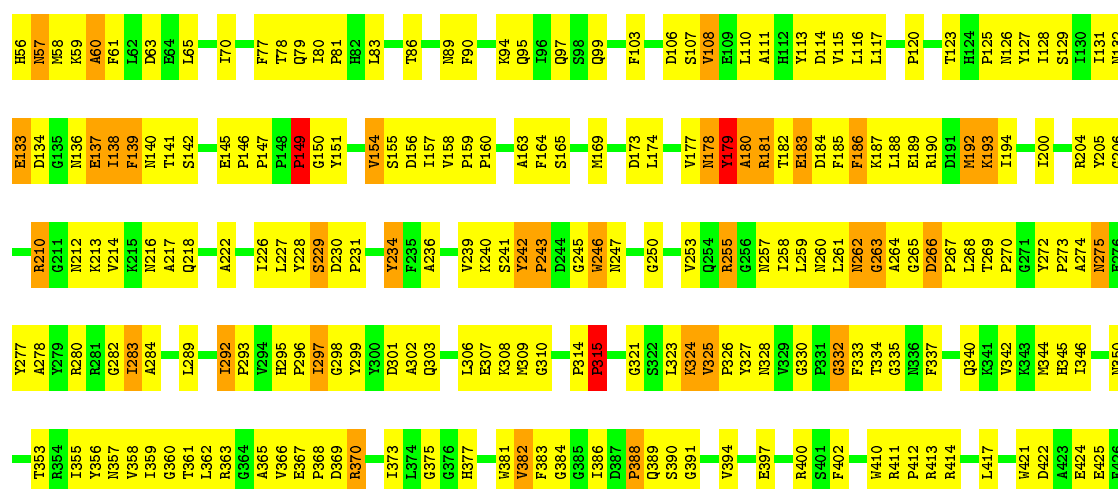
#### • Molecule 1: Glutamate carboxypeptidase II







Chain C: 39% 52% 9%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.86Å 157.76Å 133.84Å 90.00° 93.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 30.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.50) 98.7 (30.00-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.252 , 0.284 0.258 , 0.251	Depositor DCC
$R_{free}$ test set	1977 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.0	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 80077 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	22836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.34% 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, NAG, NDG

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	0.42	0/5693	0.69	0/7720
1	B	0.41	0/5693	0.69	0/7720
1	C	0.42	0/5693	0.69	0/7720
1	D	0.41	0/5693	0.69	0/7720
All	All	0.42	0/22772	0.69	0/30880

There are no bond length outliers.

There are no bond angle outliers.

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	5536	0	5373	458	11
1	B	5536	0	5373	467	9
1	C	5536	0	5373	468	14
1	D	5536	0	5373	468	16
2	A	28	0	25	2	0
2	B	28	0	25	2	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	A	84	0	75	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	84	0	75	6	1
3	C	84	0	75	6	0
3	D	84	0	75	6	0
4	A	28	0	25	1	1
4	B	28	0	25	1	0
4	C	28	0	25	1	0
4	D	28	0	25	1	0
5	A	28	0	26	5	0
5	B	28	0	26	6	0
5	C	28	0	26	5	0
5	D	28	0	26	5	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
7	C	4	0	0	0	0
7	D	2	0	0	0	0
All	All	22836	0	22096	1840	26

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 41.

The worst 5 of 1840 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:140:ASN:HB2	5:A:1760:NAG:H62	1.33	1.10
1:C:140:ASN:HB2	5:C:3760:NAG:H62	1.33	1.10
1:D:128:ILE:HD13	1:D:226:ILE:HD12	1.33	1.08
1:C:128:ILE:HD13	1:C:226:ILE:HD12	1.33	1.07
1:A:128:ILE:HD13	1:A:226:ILE:HD12	1.33	1.07

The worst 5 of 26 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:C:507:SER:OG	1:D:506:PHE:CE2[1_455]	0.99	1.21
1:C:507:SER:CB	1:D:506:PHE:CZ[1_455]	1.07	1.13
1:C:505:GLU:CA	1:D:507:SER:OG[1_455]	1.09	1.11

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:PHE:CZ	1:B:507:SER:OG[1_455]	1.18	1.02
1:C:505:GLU:N	1:D:507:SER:OG[1_455]	1.23	0.97

## 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	693/695 (100%)	534 (77%)	115 (17%)	44 (6%)	2	21
1	B	693/695 (100%)	533 (77%)	116 (17%)	44 (6%)	2	21
1	C	693/695 (100%)	533 (77%)	116 (17%)	44 (6%)	2	21
1	D	693/695 (100%)	532 (77%)	117 (17%)	44 (6%)	2	21
All	All	2772/2780 (100%)	2132 (77%)	464 (17%)	176 (6%)	2	21

5 of 176 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	GLU
1	A	138	ILE
1	A	149	PRO
1	A	179	TYR
1	A	183	GLU

### 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	592/592 (100%)	553 (93%)	39 (7%)	21	61
1	B	592/592 (100%)	553 (93%)	39 (7%)	21	61
1	C	592/592 (100%)	552 (93%)	40 (7%)	20	60
1	D	592/592 (100%)	553 (93%)	39 (7%)	21	61
All	All	2368/2368 (100%)	2211 (93%)	157 (7%)	21	61

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	541	TRP
1	C	260	ASN
1	D	523	VAL
1	B	600	TYR
1	C	149	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	618	HIS
1	C	178	ASN
1	D	438	ASN
1	B	689	HIS
1	C	82	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

40 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	1754	1,2	14,14,15	0.76	0	15,19,21	1.14	2 (13%)
3	NAG	A	1755	1,3	14,14,15	0.72	1 (7%)	15,19,21	0.83	1 (6%)
4	NDG	A	1756	1,4	14,14,15	0.63	0	15,19,21	0.89	0
3	NAG	A	1757	1,3	14,14,15	0.61	0	15,19,21	1.01	2 (13%)
3	NAG	A	1758	1,3	14,14,15	0.59	0	15,19,21	1.04	1 (6%)
2	NDG	A	1761	2	14,14,15	0.72	1 (7%)	15,19,21	0.75	0
3	NAG	A	1762	3	14,14,15	0.75	0	15,19,21	0.89	1 (6%)
4	NDG	A	1763	4	14,14,15	0.65	0	15,19,21	0.62	0
3	NAG	A	1764	3	14,14,15	0.58	0	15,19,21	0.79	1 (6%)
3	NAG	A	1765	3	14,14,15	0.50	0	15,19,21	0.72	1 (6%)
2	NAG	B	2754	1,2	14,14,15	0.76	0	15,19,21	1.15	2 (13%)
3	NAG	B	2755	1,3	14,14,15	0.72	1 (7%)	15,19,21	0.83	1 (6%)
4	NDG	B	2756	1,4	14,14,15	0.63	0	15,19,21	0.89	0
3	NAG	B	2757	1,3	14,14,15	0.60	0	15,19,21	1.02	2 (13%)
3	NAG	B	2758	1,3	14,14,15	0.59	0	15,19,21	1.04	1 (6%)
2	NDG	B	2761	2	14,14,15	0.72	0	15,19,21	0.74	0
3	NAG	B	2762	3	14,14,15	0.76	0	15,19,21	0.89	1 (6%)
4	NDG	B	2763	4	14,14,15	0.65	0	15,19,21	0.62	0
3	NAG	B	2764	3	14,14,15	0.58	0	15,19,21	0.80	1 (6%)
3	NAG	B	2765	3	14,14,15	0.50	0	15,19,21	0.73	1 (6%)
2	NAG	C	3754	1,2	14,14,15	0.76	0	15,19,21	1.14	2 (13%)
3	NAG	C	3755	1,3	14,14,15	0.72	0	15,19,21	0.83	1 (6%)
4	NDG	C	3756	1,4	14,14,15	0.63	0	15,19,21	0.89	0
3	NAG	C	3757	1,3	14,14,15	0.59	0	15,19,21	1.02	2 (13%)
3	NAG	C	3758	1,3	14,14,15	0.59	0	15,19,21	1.04	1 (6%)
2	NDG	C	3761	2	14,14,15	0.73	1 (7%)	15,19,21	0.74	0
3	NAG	C	3762	3	14,14,15	0.77	0	15,19,21	0.89	1 (6%)
4	NDG	C	3763	4	14,14,15	0.64	0	15,19,21	0.62	0
3	NAG	C	3764	3	14,14,15	0.57	0	15,19,21	0.81	1 (6%)
3	NAG	C	3765	3	14,14,15	0.51	0	15,19,21	0.74	1 (6%)
2	NAG	D	4754	1,2	14,14,15	0.77	0	15,19,21	1.14	2 (13%)
3	NAG	D	4755	1,3	14,14,15	0.71	0	15,19,21	0.83	0
4	NDG	D	4756	1,4	14,14,15	0.64	0	15,19,21	0.89	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	D	4757	1,3	14,14,15	0.60	0	15,19,21	1.02	2 (13%)
3	NAG	D	4758	1,3	14,14,15	0.59	0	15,19,21	1.04	1 (6%)
2	NDG	D	4761	2	14,14,15	0.72	0	15,19,21	0.74	0
3	NAG	D	4762	3	14,14,15	0.77	0	15,19,21	0.89	1 (6%)
4	NDG	D	4763	4	14,14,15	0.65	0	15,19,21	0.62	0
3	NAG	D	4764	3	14,14,15	0.57	0	15,19,21	0.81	1 (6%)
3	NAG	D	4765	3	14,14,15	0.50	0	15,19,21	0.74	1 (6%)

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	1754	1,2	-	0/6/23/26	0/1/1/1
3	NAG	A	1755	1,3	-	0/6/23/26	0/1/1/1
4	NDG	A	1756	1,4	-	0/6/23/26	0/1/1/1
3	NAG	A	1757	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	1758	1,3	-	0/6/23/26	0/1/1/1
2	NDG	A	1761	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1762	3	-	0/6/23/26	0/1/1/1
4	NDG	A	1763	4	-	1/6/23/26	0/1/1/1
3	NAG	A	1764	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1765	3	-	0/6/23/26	0/1/1/1
2	NAG	B	2754	1,2	-	0/6/23/26	0/1/1/1
3	NAG	B	2755	1,3	-	0/6/23/26	0/1/1/1
4	NDG	B	2756	1,4	-	0/6/23/26	0/1/1/1
3	NAG	B	2757	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2758	1,3	-	0/6/23/26	0/1/1/1
2	NDG	B	2761	2	-	0/6/23/26	0/1/1/1
3	NAG	B	2762	3	-	0/6/23/26	0/1/1/1
4	NDG	B	2763	4	-	1/6/23/26	0/1/1/1
3	NAG	B	2764	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2765	3	-	0/6/23/26	0/1/1/1
2	NAG	C	3754	1,2	-	0/6/23/26	0/1/1/1
3	NAG	C	3755	1,3	-	0/6/23/26	0/1/1/1
4	NDG	C	3756	1,4	-	0/6/23/26	0/1/1/1
3	NAG	C	3757	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	3758	1,3	-	0/6/23/26	0/1/1/1
2	NDG	C	3761	2	-	0/6/23/26	0/1/1/1
3	NAG	C	3762	3	-	0/6/23/26	0/1/1/1

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDG	C	3763	4	-	1/6/23/26	0/1/1/1
3	NAG	C	3764	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3765	3	-	0/6/23/26	0/1/1/1
2	NAG	D	4754	1,2	-	0/6/23/26	0/1/1/1
3	NAG	D	4755	1,3	-	0/6/23/26	0/1/1/1
4	NDG	D	4756	1,4	-	0/6/23/26	0/1/1/1
3	NAG	D	4757	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	4758	1,3	-	0/6/23/26	0/1/1/1
2	NDG	D	4761	2	-	0/6/23/26	0/1/1/1
3	NAG	D	4762	3	-	0/6/23/26	0/1/1/1
4	NDG	D	4763	4	-	1/6/23/26	0/1/1/1
3	NAG	D	4764	3	-	0/6/23/26	0/1/1/1
3	NAG	D	4765	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1761	NDG	C1-C2	2.01	1.55	1.52
2	C	3761	NDG	C1-C2	2.02	1.55	1.52
3	B	2755	NAG	C1-C2	2.02	1.55	1.52
3	A	1755	NAG	C1-C2	2.04	1.55	1.52

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1758	NAG	C2-N2-C7	-3.49	118.56	123.04
3	C	3758	NAG	C2-N2-C7	-3.48	118.56	123.04
3	B	2758	NAG	C2-N2-C7	-3.48	118.57	123.04
3	D	4758	NAG	C2-N2-C7	-3.47	118.59	123.04
2	B	2754	NAG	C2-N2-C7	-2.87	119.35	123.04

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4763	NDG	O7-C7-N2-C2
4	A	1763	NDG	O7-C7-N2-C2
4	C	3763	NDG	O7-C7-N2-C2
4	B	2763	NDG	O7-C7-N2-C2
3	A	1757	NAG	O7-C7-N2-C2

There are no ring outliers.

29 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1754	NAG	2	0
3	A	1755	NAG	1	0
4	A	1756	NDG	1	0
3	A	1757	NAG	5	0
2	A	1761	NDG	2	0
3	A	1762	NAG	1	0
4	A	1763	NDG	1	1
2	B	2754	NAG	2	0
3	B	2755	NAG	1	0
4	B	2756	NDG	1	0
3	B	2757	NAG	5	0
2	B	2761	NDG	2	0
3	B	2762	NAG	1	0
4	B	2763	NDG	1	0
3	B	2764	NAG	0	1
2	C	3754	NAG	1	0
3	C	3755	NAG	1	0
4	C	3756	NDG	1	0
3	C	3757	NAG	5	0
2	C	3761	NDG	1	0
3	C	3762	NAG	1	0
4	C	3763	NDG	1	0
2	D	4754	NAG	1	0
3	D	4755	NAG	1	0
4	D	4756	NDG	1	0
3	D	4757	NAG	5	0
2	D	4761	NDG	1	0
3	D	4762	NAG	1	0
4	D	4763	NDG	1	0

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
5	NAG	A	1759	1	14,14,15	0.80	0	15,19,21	0.70	0
5	NAG	A	1760	1	14,14,15	0.92	1 (7%)	15,19,21	0.76	0
5	NAG	B	2759	1	14,14,15	0.80	0	15,19,21	0.70	0
5	NAG	B	2760	1	14,14,15	0.92	1 (7%)	15,19,21	0.77	0
5	NAG	C	3759	1	14,14,15	0.80	0	15,19,21	0.70	0
5	NAG	C	3760	1	14,14,15	0.93	1 (7%)	15,19,21	0.78	0
5	NAG	D	4759	1	14,14,15	0.80	0	15,19,21	0.69	0
5	NAG	D	4760	1	14,14,15	0.93	1 (7%)	15,19,21	0.78	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
5	NAG	A	1759	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1760	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2759	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2760	1	-	0/6/23/26	0/1/1/1
5	NAG	C	3759	1	-	0/6/23/26	0/1/1/1
5	NAG	C	3760	1	-	0/6/23/26	0/1/1/1
5	NAG	D	4759	1	-	0/6/23/26	0/1/1/1
5	NAG	D	4760	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1760	NAG	C1-C2	2.77	1.56	1.52
5	B	2760	NAG	C1-C2	2.77	1.56	1.52
5	C	3760	NAG	C1-C2	2.79	1.56	1.52
5	D	4760	NAG	C1-C2	2.82	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1760	NAG	5	0
5	B	2759	NAG	1	0
5	B	2760	NAG	5	0
5	C	3760	NAG	5	0
5	D	4760	NAG	5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	695/695 (100%)	-0.35	0 100 100	2, 51, 143, 197	0
1	B	695/695 (100%)	-0.33	3 (0%) 93 90	2, 51, 143, 197	0
1	C	695/695 (100%)	-0.40	1 (0%) 95 94	2, 51, 143, 197	0
1	D	695/695 (100%)	-0.30	8 (1%) 81 72	2, 51, 143, 197	0
All	All	2780/2780 (100%)	-0.35	12 (0%) 93 90	2, 51, 144, 197	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	ASN	4.1
1	D	307	GLU	3.8
1	D	308	LYS	3.2
1	D	319	TRP	3.1
1	D	336	ASN	3.1

### 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, 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1757	14/15	0.84	0.22	0.03	117,117,117,117	0
3	NAG	B	2757	14/15	0.83	0.23	-0.48	117,117,117,117	0
3	NAG	D	4757	14/15	0.89	0.19	-0.75	117,117,117,117	0
3	NAG	C	3757	14/15	0.84	0.19	-0.89	117,117,117,117	0
3	NAG	D	4764	14/15	0.66	0.34	-	197,197,197,197	0
3	NAG	A	1758	14/15	0.91	0.19	-	88,88,88,88	0
3	NAG	C	3755	14/15	0.76	0.24	-	173,173,173,173	0
3	NAG	B	2765	14/15	0.83	0.27	-	111,111,111,111	0
2	NAG	C	3754	14/15	0.93	0.14	-	77,77,77,77	0
3	NAG	C	3758	14/15	0.93	0.17	-	88,88,88,88	0
4	NDG	D	4756	14/15	0.23	0.57	-	197,197,197,197	0
2	NAG	D	4754	14/15	0.88	0.18	-	77,77,77,77	0
4	NDG	B	2756	14/15	0.25	0.67	-	197,197,197,197	0
3	NAG	D	4762	14/15	0.51	0.34	-	196,196,196,196	0
3	NAG	B	2758	14/15	0.89	0.18	-	88,88,88,88	0
4	NDG	A	1756	14/15	0.68	0.31	-	197,197,197,197	0
4	NDG	D	4763	14/15	0.32	0.38	-	189,189,189,189	0
2	NAG	B	2754	14/15	0.85	0.17	-	77,77,77,77	0
4	NDG	B	2763	14/15	0.77	0.35	-	189,189,189,189	0
3	NAG	A	1755	14/15	0.76	0.26	-	173,173,173,173	0
3	NAG	A	1764	14/15	0.71	0.53	-	197,197,197,197	0
3	NAG	A	1765	14/15	0.89	0.26	-	111,111,111,111	0
3	NAG	B	2762	14/15	0.61	0.36	-	196,196,196,196	0
2	NDG	D	4761	14/15	0.77	0.28	-	142,142,142,142	0
2	NDG	B	2761	14/15	0.80	0.30	-	142,142,142,142	0
3	NAG	B	2764	14/15	0.44	0.35	-	197,197,197,197	0
3	NAG	C	3762	14/15	0.58	0.37	-	196,196,196,196	0
3	NAG	D	4765	14/15	0.86	0.23	-	111,111,111,111	0
2	NDG	C	3761	14/15	0.82	0.25	-	142,142,142,142	0
3	NAG	B	2755	14/15	0.78	0.18	-	173,173,173,173	0
3	NAG	A	1762	14/15	0.74	0.28	-	196,196,196,196	0
2	NAG	A	1754	14/15	0.86	0.17	-	77,77,77,77	0
4	NDG	A	1763	14/15	0.74	0.37	-	189,189,189,189	0
2	NDG	A	1761	14/15	0.83	0.21	-	142,142,142,142	0
4	NDG	C	3756	14/15	0.69	0.50	-	197,197,197,197	0
3	NAG	C	3764	14/15	0.79	0.24	-	197,197,197,197	0
4	NDG	C	3763	14/15	0.69	0.33	-	189,189,189,189	0
3	NAG	C	3765	14/15	0.81	0.27	-	111,111,111,111	0
3	NAG	D	4758	14/15	0.93	0.17	-	88,88,88,88	0
3	NAG	D	4755	14/15	0.70	0.23	-	173,173,173,173	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
5	NAG	C	3759	14/15	0.84	0.26	3.81	57,57,57,57	0
5	NAG	D	4759	14/15	0.84	0.22	1.25	57,57,57,57	0
5	NAG	B	2759	14/15	0.89	0.19	1.08	57,57,57,57	0
5	NAG	A	1759	14/15	0.89	0.20	0.76	57,57,57,57	0
6	ZN	C	3752	1/1	0.89	0.15	0.04	52,52,52,52	0
6	ZN	B	2752	1/1	0.95	0.13	-0.24	52,52,52,52	0
6	ZN	B	2751	1/1	0.95	0.13	-0.30	52,52,52,52	0
6	ZN	A	1752	1/1	0.96	0.08	-1.49	52,52,52,52	0
6	ZN	C	3751	1/1	0.89	0.07	-1.51	52,52,52,52	0
6	ZN	A	1751	1/1	0.97	0.06	-1.82	52,52,52,52	0
6	ZN	D	4752	1/1	0.93	0.07	-2.51	52,52,52,52	0
6	ZN	D	4751	1/1	0.90	0.06	-3.08	52,52,52,52	0
5	NAG	A	1760	14/15	0.62	0.35	-	155,155,155,155	0
5	NAG	B	2760	14/15	0.54	0.32	-	155,155,155,155	0
5	NAG	D	4760	14/15	0.50	0.40	-	155,155,155,155	0
5	NAG	C	3760	14/15	0.60	0.35	-	155,155,155,155	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.