



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:34 pm GMT

PDB ID : 2Y1K  
Title : STRUCTURE OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED  
BY CBDP (12H SOAK): PHOSPHOSERINE ADDUCT  
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Deposited on : 2010-12-08  
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

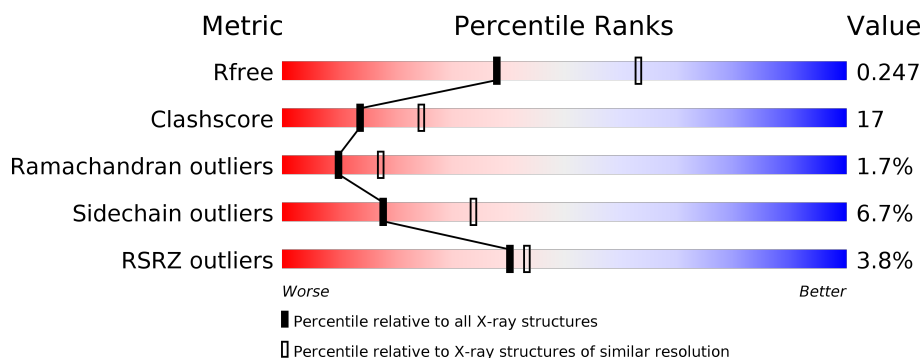
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	529	

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	SO4	A	605	-	X	-	-
4	CL	A	603	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	617	-	-	-	X
6	NAG	A	618	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4597 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.

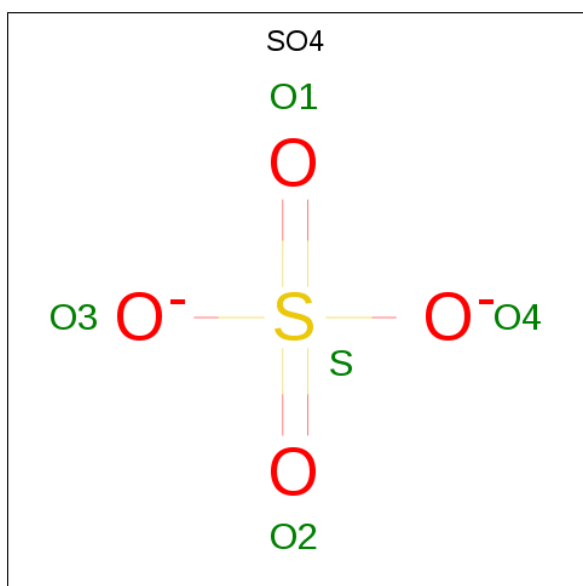
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	526	4193	2704	706	767	1	15	0	2	1

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

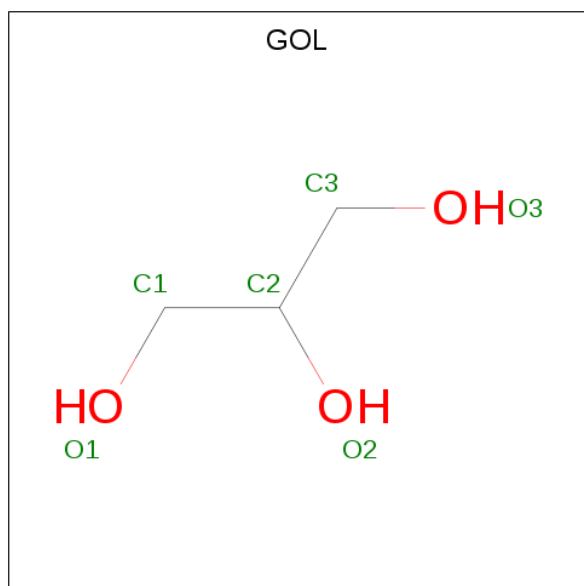
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is 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
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



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

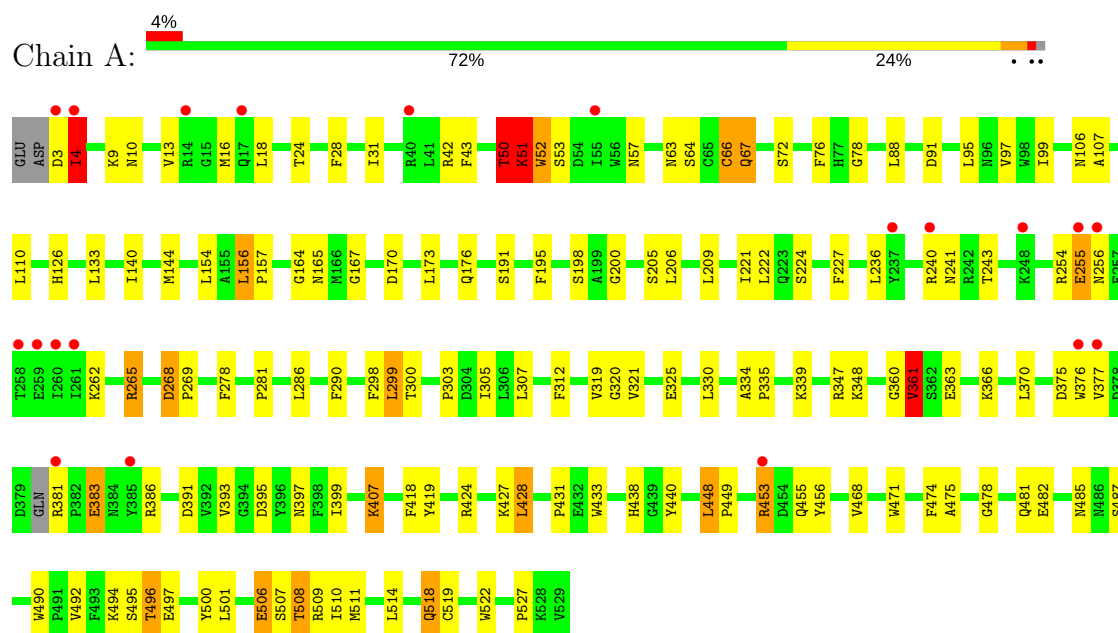
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	229	Total	O	0	0
			229	229		

### 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: CHOLINESTERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.77Å 153.77Å 127.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.38 – 2.50 41.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (41.38-2.50) 94.8 (41.38-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.76 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0093	Depositor
R, $R_{free}$	0.183 , 0.247 0.183 , 0.247	Depositor DCC
$R_{free}$ test set	760 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4597	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, 0.333 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: GOL, NAG, SEP, NA, CL, FUC, SO4

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	0.90	1/4306 (0.0%)	0.86	4/5843 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CYS	CB-SG	-5.11	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	361	VAL	N-CA-C	5.39	125.55	111.00
1	A	265	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	448	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	LEU	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4093	138	0
2	A	25	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	3	0
5	A	6	0	8	0	0
6	A	112	0	103	22	0
7	A	30	0	30	3	0
8	A	229	0	0	38	3
All	All	4597	0	4234	146	3

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 17.

All (146) 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:300:THR:HG22	8:A:880:HOH:O	1.22	1.31
1:A:391:ASP:O	8:A:701:HOH:O	1.52	1.26
1:A:475:ALA:HB3	8:A:711:HOH:O	1.42	1.17
1:A:527:PRO:HD3	8:A:702:HOH:O	1.46	1.16
1:A:522:TRP:O	8:A:702:HOH:O	1.66	1.10
6:A:606:NAG:O4	6:A:609:NAG:C1	2.00	1.09
1:A:475:ALA:CB	8:A:711:HOH:O	1.98	1.04
1:A:518:GLN:H	1:A:518:GLN:HE21	1.04	1.01
1:A:495:SER:HA	8:A:707:HOH:O	1.58	1.00
4:A:603:CL:CL	8:A:920:HOH:O	2.18	0.98
1:A:241:ASN:HD21	6:A:617:NAG:H4	1.26	0.97
1:A:509:ARG:HH11	1:A:509:ARG:HG2	1.32	0.93
6:A:606:NAG:HO4	6:A:609:NAG:C1	1.77	0.93
1:A:522:TRP:C	8:A:702:HOH:O	2.06	0.92
1:A:381:ARG:N	8:A:708:HOH:O	2.01	0.92
1:A:424:ARG:NH1	1:A:428:LEU:HD12	1.86	0.92
1:A:514:LEU:O	8:A:703:HOH:O	1.89	0.91
6:A:606:NAG:O4	6:A:609:NAG:O5	1.86	0.91
1:A:485:ASN:ND2	6:A:615:NAG:H2	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:TYR:O	8:A:704:HOH:O	1.89	0.90
1:A:501:LEU:HA	8:A:704:HOH:O	1.70	0.89
1:A:240:ARG:HG3	8:A:775:HOH:O	1.75	0.87
1:A:485:ASN:HD21	6:A:615:NAG:H2	1.39	0.86
1:A:99:ILE:HG22	1:A:140:ILE:HG12	1.59	0.83
1:A:395:ASP:N	8:A:701:HOH:O	1.82	0.82
1:A:510:ILE:O	8:A:706:HOH:O	1.96	0.81
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.16	0.80
1:A:256:ASN:ND2	6:A:616:NAG:C1	2.45	0.80
1:A:347:ARG:NH1	8:A:705:HOH:O	1.93	0.79
1:A:106:ASN:HD21	6:A:612:NAG:C1	1.97	0.78
6:A:614:NAG:H61	8:A:872:HOH:O	1.85	0.77
6:A:612:NAG:O6	7:A:613:FUC:C1	2.33	0.76
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.69	0.73
1:A:518:GLN:H	1:A:518:GLN:NE2	1.84	0.72
1:A:496:THR:N	8:A:707:HOH:O	2.01	0.72
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.25	0.72
1:A:495:SER:CA	8:A:707:HOH:O	2.24	0.71
1:A:485:ASN:HD21	6:A:615:NAG:H62	1.54	0.70
1:A:485:ASN:HD21	6:A:615:NAG:C2	2.05	0.70
1:A:51:LYS:O	1:A:52:TRP:HB3	1.93	0.68
1:A:241:ASN:ND2	6:A:617:NAG:H4	2.06	0.68
1:A:107:ALA:HB3	1:A:140:ILE:HD12	1.74	0.68
1:A:106:ASN:CG	6:A:612:NAG:H83	2.16	0.66
1:A:485:ASN:ND2	6:A:615:NAG:H62	2.12	0.65
1:A:157:PRO:O	8:A:709:HOH:O	2.14	0.65
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.78	0.64
1:A:330:LEU:O	1:A:334:ALA:HB3	1.97	0.64
1:A:509:ARG:NH1	1:A:509:ARG:HG2	2.10	0.64
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.79	0.63
1:A:50:THR:O	1:A:51:LYS:HB3	1.99	0.63
1:A:256:ASN:HD21	6:A:616:NAG:C1	2.11	0.62
1:A:510:ILE:HA	8:A:704:HOH:O	2.01	0.61
1:A:361:VAL:O	1:A:366:LYS:NZ	2.33	0.61
1:A:106:ASN:ND2	6:A:612:NAG:H83	2.16	0.60
1:A:28:PHE:HB3	1:A:31:ILE:HD11	1.82	0.60
1:A:64:SER:O	1:A:88:LEU:HA	2.02	0.59
1:A:383:GLU:CD	1:A:383:GLU:H	2.05	0.59
1:A:198:SEP:HA	1:A:224:SER:O	2.01	0.59
1:A:509:ARG:HH11	1:A:509:ARG:CG	2.07	0.59
6:A:618:NAG:H5	7:A:619:FUC:O2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TRP:HD1	1:A:53:SER:O	1.86	0.58
1:A:205:SER:HB3	1:A:222:LEU:CD2	2.33	0.57
1:A:508:THR:HB	8:A:771:HOH:O	2.04	0.57
1:A:424:ARG:CZ	1:A:428:LEU:HD12	2.33	0.57
1:A:66:CYS:O	1:A:67:GLN:HB3	2.05	0.57
1:A:95:LEU:HD12	1:A:95:LEU:C	2.25	0.57
1:A:240:ARG:HA	8:A:775:HOH:O	2.05	0.57
6:A:606:NAG:O3	6:A:609:NAG:H61	2.04	0.56
1:A:518:GLN:HE21	1:A:518:GLN:N	1.89	0.56
1:A:319:VAL:O	1:A:418:PHE:HA	2.06	0.55
1:A:126:HIS:HB2	8:A:916:HOH:O	2.05	0.55
1:A:222:LEU:N	1:A:222:LEU:HD12	2.22	0.55
1:A:10:ASN:HB3	1:A:52:TRP:CZ3	2.42	0.54
1:A:492:VAL:CG2	1:A:494:LYS:HE2	2.37	0.54
1:A:508:THR:HG21	4:A:603:CL:CL	2.45	0.54
1:A:255:GLU:HG2	1:A:256:ASN:H	1.73	0.53
1:A:509:ARG:CG	1:A:509:ARG:NH1	2.70	0.53
1:A:320:GLY:HA3	1:A:419:TYR:CD2	2.44	0.53
1:A:254:ARG:NE	8:A:713:HOH:O	2.27	0.52
1:A:227:PHE:CD1	1:A:303:PRO:HB2	2.45	0.51
1:A:347:ARG:NH2	1:A:370:LEU:HD21	2.24	0.51
1:A:3:ASP:C	1:A:4:ILE:HG13	2.31	0.51
1:A:485:ASN:ND2	6:A:615:NAG:C2	2.65	0.51
1:A:154:LEU:HD12	1:A:290:PHE:CE1	2.45	0.51
1:A:471:TRP:O	8:A:711:HOH:O	2.20	0.50
1:A:221:ILE:C	1:A:222:LEU:HD12	2.31	0.50
1:A:339:LYS:O	1:A:431:PRO:HG3	2.11	0.50
1:A:508:THR:CG2	4:A:603:CL:CL	2.97	0.49
1:A:255:GLU:CD	1:A:255:GLU:H	2.15	0.49
1:A:106:ASN:ND2	6:A:612:NAG:C1	2.72	0.49
1:A:482:GLU:OE1	1:A:487:SER:OG	2.31	0.48
1:A:321:VAL:HG11	1:A:399:ILE:HA	1.95	0.48
1:A:133:LEU:HD23	1:A:468:VAL:HG13	1.94	0.48
1:A:455:GLN:N	8:A:735:HOH:O	2.46	0.48
1:A:18:LEU:O	1:A:24:THR:HA	2.14	0.48
1:A:449:PRO:HA	1:A:456:TYR:CD2	2.48	0.48
1:A:4:ILE:N	1:A:4:ILE:HD12	2.29	0.48
1:A:206:LEU:HB3	1:A:298:PHE:HE2	1.79	0.47
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.79	0.47
1:A:97:VAL:HG12	1:A:99:ILE:HG23	1.96	0.47
1:A:506:GLU:HB2	1:A:507:SER:H	1.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLY:O	1:A:165:ASN:HB2	2.15	0.47
1:A:424:ARG:HH12	1:A:428:LEU:HD12	1.76	0.47
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.51	0.46
1:A:13:VAL:HG12	1:A:52:TRP:HZ2	1.81	0.46
1:A:386:ARG:CZ	1:A:433:TRP:HB2	2.46	0.46
1:A:173:LEU:HD12	1:A:173:LEU:HA	1.71	0.46
1:A:325:GLU:O	1:A:438:HIS:HB2	2.15	0.46
1:A:377:VAL:HG23	8:A:739:HOH:O	2.16	0.46
1:A:527:PRO:CD	8:A:702:HOH:O	2.29	0.46
1:A:227:PHE:CD1	1:A:227:PHE:C	2.88	0.46
1:A:299:LEU:HD21	1:A:303:PRO:HD3	1.99	0.45
1:A:492:VAL:HG23	1:A:494:LYS:HE2	1.99	0.45
1:A:395:ASP:CB	8:A:701:HOH:O	2.65	0.44
1:A:448:LEU:N	1:A:449:PRO:CD	2.80	0.44
1:A:76:PHE:CE2	1:A:78:GLY:HA3	2.52	0.44
1:A:42:ARG:NH2	1:A:269:PRO:HD3	2.32	0.44
1:A:474:PHE:O	1:A:478:GLY:N	2.51	0.44
1:A:393:VAL:O	1:A:397:ASN:HB2	2.16	0.44
1:A:191:SER:HB2	7:A:613:FUC:H3	1.99	0.43
1:A:57:ASN:HD21	6:A:614:NAG:C1	2.31	0.43
1:A:198:SEP:C	1:A:200:GLY:N	2.79	0.43
1:A:519:CYS:HB3	8:A:800:HOH:O	2.18	0.43
1:A:334:ALA:HA	1:A:335:PRO:HD3	1.84	0.43
1:A:265:ARG:NE	8:A:723:HOH:O	2.37	0.43
1:A:487:SER:HB2	8:A:769:HOH:O	2.17	0.43
1:A:481:GLN:HA	8:A:743:HOH:O	2.19	0.42
1:A:42:ARG:O	1:A:43:PHE:HB2	2.19	0.42
1:A:240:ARG:CA	8:A:775:HOH:O	2.66	0.42
1:A:427:LYS:O	1:A:428:LEU:C	2.56	0.42
1:A:227:PHE:HZ	1:A:307:LEU:HB2	1.85	0.42
1:A:419:TYR:HB3	1:A:490:TRP:CZ2	2.55	0.42
1:A:492:VAL:HG21	1:A:494:LYS:HE2	2.02	0.42
1:A:407:LYS:HE3	1:A:407:LYS:HB2	1.41	0.42
1:A:255:GLU:HG2	1:A:256:ASN:N	2.32	0.41
1:A:50:THR:O	1:A:51:LYS:CB	2.65	0.41
1:A:300:THR:CG2	8:A:880:HOH:O	2.10	0.41
1:A:268:ASP:O	1:A:269:PRO:C	2.59	0.41
1:A:428:LEU:HD23	1:A:440:TYR:CD2	2.56	0.41
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.56	0.41
1:A:167:GLY:O	1:A:170:ASP:HB2	2.21	0.41
1:A:347:ARG:HH22	1:A:370:LEU:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLU:CG	1:A:256:ASN:H	2.34	0.41
1:A:475:ALA:HB2	8:A:711:HOH:O	1.94	0.40
1:A:63:ASN:HB2	1:A:91:ASP:O	2.22	0.40
1:A:453:ARG:H	1:A:453:ARG:HG2	1.43	0.40

All (3) 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)
8:A:907:HOH:O	8:A:914:HOH:O[7_556]	1.50	0.70
8:A:706:HOH:O	8:A:774:HOH:O[7_556]	1.56	0.64
8:A:844:HOH:O	8:A:897:HOH:O[7_556]	2.11	0.09

## 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	523/529 (99%)	480 (92%)	34 (6%)	9 (2%)	<b>10</b> <b>17</b>

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	281	PRO
1	A	361	VAL
1	A	496	THR
1	A	4	ILE
1	A	50	THR
1	A	52	TRP
1	A	67	GLN
1	A	360	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	449/453 (99%)	418 (93%)	31 (7%)	17	32

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	16	MET
1	A	50	THR
1	A	51	LYS
1	A	72	SER
1	A	110	LEU
1	A	144	MET
1	A	176	GLN
1	A	195	PHE
1	A	236	LEU
1	A	255	GLU
1	A	262	LYS
1	A	268	ASP
1	A	278	PHE
1	A	286	LEU
1	A	299	LEU
1	A	305	ILE
1	A	348	LYS
1	A	363[A]	GLU
1	A	363[B]	GLU
1	A	375	ASP
1	A	376	TRP
1	A	383	GLU
1	A	407	LYS
1	A	428	LEU
1	A	453	ARG
1	A	497	GLU
1	A	506	GLU
1	A	508	THR

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Mol	Chain	Res	Type
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	241	ASN
1	A	485	ASN
1	A	518	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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
1	SEP	A	198	1	9,9,10	3.27	4 (44%)	9,12,14	2.14	3 (33%)

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
1	SEP	A	198	1	-	0/5/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	CA-C	3.08	1.54	1.50
1	A	198	SEP	P-O1P	3.10	1.61	1.50
1	A	198	SEP	P-O2P	3.17	1.67	1.54
1	A	198	SEP	P-OG	8.08	1.86	1.60

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	P-OG-CB	-3.92	107.51	118.30
1	A	198	SEP	O-C-CA	-2.60	117.82	124.96
1	A	198	SEP	O3P-P-OG	-2.24	100.77	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	SO4	A	601	-	4,4,4	0.57	0	6,6,6	0.36	0
5	GOL	A	604	-	5,5,5	0.83	0	5,5,5	1.04	0
2	SO4	A	605	-	4,4,4	0.69	0	6,6,6	3.23	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	606	1,7	14,14,15	0.95	0	17,19,21	2.30	7 (41%)
7	FUC	A	607	6	9,10,11	0.88	0	13,14,16	1.70	3 (23%)
2	SO4	A	608	-	4,4,4	0.61	0	6,6,6	0.30	0
6	NAG	A	609	-	14,14,15	0.61	0	17,19,21	1.62	3 (17%)
2	SO4	A	610	-	4,4,4	0.61	0	6,6,6	0.29	0
2	SO4	A	611	-	4,4,4	0.62	0	6,6,6	0.91	0
6	NAG	A	612	-	14,14,15	0.58	0	17,19,21	1.53	4 (23%)
7	FUC	A	613	-	9,10,11	0.71	0	13,14,16	0.91	1 (7%)
6	NAG	A	614	-	14,14,15	0.45	0	17,19,21	1.67	6 (35%)
6	NAG	A	615	-	14,14,15	0.93	1 (7%)	17,19,21	3.80	10 (58%)
6	NAG	A	616	-	14,14,15	0.85	0	17,19,21	1.87	4 (23%)
6	NAG	A	617	-	14,14,15	0.66	0	17,19,21	1.63	4 (23%)
6	NAG	A	618	-	14,14,15	0.69	0	17,19,21	1.45	4 (23%)
7	FUC	A	619	-	9,10,11	0.82	0	13,14,16	1.19	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	SO4	A	601	-	-	0/0/0/0	0/0/0/0
5	GOL	A	604	-	-	0/4/4/4	0/0/0/0
2	SO4	A	605	-	-	0/0/0/0	0/0/0/0
6	NAG	A	606	1,7	-	0/6/23/26	0/1/1/1
7	FUC	A	607	6	-	0/0/17/20	0/1/1/1
2	SO4	A	608	-	-	0/0/0/0	0/0/0/0
6	NAG	A	609	-	-	0/6/23/26	0/1/1/1
2	SO4	A	610	-	-	0/0/0/0	0/0/0/0
2	SO4	A	611	-	-	0/0/0/0	0/0/0/0
6	NAG	A	612	-	-	0/6/23/26	0/1/1/1
7	FUC	A	613	-	-	0/0/17/20	0/1/1/1
6	NAG	A	614	-	-	0/6/23/26	0/1/1/1
6	NAG	A	615	-	-	0/6/23/26	0/1/1/1
6	NAG	A	616	-	-	0/6/23/26	0/1/1/1
6	NAG	A	617	-	-	0/6/23/26	0/1/1/1
6	NAG	A	618	-	-	0/6/23/26	0/1/1/1
7	FUC	A	619	-	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	615	NAG	C1-C2	2.18	1.55	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	SO4	O4-S-O3	-5.08	86.23	108.83
6	A	606	NAG	C1-C2-N2	-4.44	102.90	110.49
2	A	605	SO4	O3-S-O2	-4.00	87.60	109.24
6	A	612	NAG	O5-C1-C2	-3.88	106.17	111.52
6	A	615	NAG	C8-C7-N2	-3.61	109.78	116.10
6	A	609	NAG	C1-C2-N2	-3.55	104.43	110.49
6	A	615	NAG	C1-C2-N2	-3.49	104.52	110.49
2	A	605	SO4	O3-S-O1	-3.20	91.92	109.24
6	A	615	NAG	C4-C3-C2	-2.74	107.00	111.02
6	A	615	NAG	O7-C7-C8	-2.70	117.19	122.07
6	A	614	NAG	O7-C7-C8	-2.69	117.21	122.07
6	A	612	NAG	O7-C7-C8	-2.61	117.36	122.07
6	A	617	NAG	O3-C3-C4	-2.40	104.73	110.34
6	A	606	NAG	O5-C5-C4	-2.32	105.19	110.83
6	A	614	NAG	O5-C1-C2	-2.28	108.38	111.52
6	A	614	NAG	C4-C3-C2	-2.19	107.80	111.02
6	A	618	NAG	C1-C2-N2	-2.19	106.75	110.49
6	A	606	NAG	C3-C4-C5	-2.10	106.48	110.24
6	A	618	NAG	C3-C4-C5	2.14	114.06	110.24
6	A	615	NAG	C3-C4-C5	2.14	114.07	110.24
6	A	614	NAG	C1-C2-N2	2.21	114.26	110.49
6	A	617	NAG	C3-C4-C5	2.21	114.19	110.24
7	A	613	FUC	C3-C4-C5	2.29	113.27	109.72
6	A	612	NAG	C1-C2-N2	2.35	114.49	110.49
6	A	618	NAG	O5-C5-C6	2.35	110.87	107.15
6	A	612	NAG	C8-C7-N2	2.36	120.23	116.10
6	A	615	NAG	O5-C1-C2	2.37	114.79	111.52
2	A	605	SO4	O4-S-O2	2.46	122.55	109.24
7	A	607	FUC	C1-O5-C5	2.48	117.88	112.39
6	A	614	NAG	C8-C7-N2	2.52	120.52	116.10
6	A	616	NAG	C2-N2-C7	2.61	126.75	122.94
6	A	616	NAG	C3-C4-C5	2.72	115.10	110.24
6	A	606	NAG	C6-C5-C4	2.78	119.56	112.99
6	A	617	NAG	C1-O5-C5	2.90	116.17	112.19
6	A	617	NAG	C2-N2-C7	2.91	127.19	122.94
6	A	609	NAG	C4-C3-C2	3.00	115.42	111.02
6	A	606	NAG	O5-C5-C6	3.21	112.24	107.15
6	A	616	NAG	O5-C1-C2	3.24	116.00	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	609	NAG	O5-C5-C6	3.29	112.35	107.15
7	A	607	FUC	C2-C3-C4	3.39	116.75	110.87
6	A	614	NAG	C1-O5-C5	3.40	116.86	112.19
7	A	607	FUC	C1-C2-C3	3.41	113.98	109.66
6	A	606	NAG	C8-C7-N2	3.43	122.10	116.10
6	A	615	NAG	O5-C5-C6	3.46	112.63	107.15
6	A	606	NAG	C2-N2-C7	3.47	128.00	122.94
6	A	615	NAG	C1-O5-C5	3.50	117.00	112.19
6	A	618	NAG	C4-C3-C2	3.80	116.59	111.02
6	A	616	NAG	C4-C3-C2	4.50	117.61	111.02
6	A	615	NAG	O7-C7-N2	5.86	133.00	121.94
6	A	615	NAG	C2-N2-C7	11.32	139.45	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	606	NAG	4	0
6	A	609	NAG	4	0
6	A	612	NAG	5	0
7	A	613	FUC	2	0
6	A	614	NAG	2	0
6	A	615	NAG	6	0
6	A	616	NAG	2	0
6	A	617	NAG	2	0
6	A	618	NAG	1	0
7	A	619	FUC	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 [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	525/529 (99%)	0.11	20 (3%)	40 43	33, 56, 95, 147	10 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	5.9
1	A	376	TRP	4.4
1	A	377	VAL	3.7
1	A	40	ARG	3.7
1	A	259	GLU	3.6
1	A	255	GLU	3.5
1	A	4	ILE	3.5
1	A	381	ARG	3.3
1	A	261	ILE	3.2
1	A	237	TYR	3.1
1	A	256	ASN	3.0
1	A	17	GLN	2.9
1	A	55	ILE	2.9
1	A	258	THR	2.7
1	A	240	ARG	2.6
1	A	14	ARG	2.5
1	A	453	ARG	2.4
1	A	385	TYR	2.3
1	A	260	ILE	2.0
1	A	248	LYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SEP	A	198	10/11	0.99	0.19	36,40,42,52	0

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	617	14/15	0.66	0.53	81,133,148,149	0
6	NAG	A	618	14/15	0.73	0.56	89,106,135,135	0
6	NAG	A	616	14/15	0.79	0.36	75,97,112,118	0
7	FUC	A	613	10/11	0.80	0.42	36,46,58,76	10
2	SO4	A	610	5/5	0.84	0.17	61,68,72,95	5
6	NAG	A	615	14/15	0.87	0.18	51,89,107,108	0
6	NAG	A	609	14/15	0.89	0.19	76,94,113,114	0
6	NAG	A	614	14/15	0.90	0.33	64,88,99,121	0
2	SO4	A	611	5/5	0.90	0.17	56,58,71,82	5
6	NAG	A	612	14/15	0.91	0.17	50,87,99,102	0
7	FUC	A	619	10/11	0.92	0.51	64,99,120,122	0
5	GOL	A	604	6/6	0.93	0.24	54,60,66,79	0
3	NA	A	602	1/1	0.93	0.66	70,70,70,70	1
2	SO4	A	601	5/5	0.93	0.24	80,83,111,112	0
7	FUC	A	607	10/11	0.94	0.28	74,83,92,99	0
2	SO4	A	605	5/5	0.95	0.23	57,60,66,76	5
2	SO4	A	608	5/5	0.95	0.13	78,82,91,97	0
4	CL	A	603	1/1	0.96	0.11	73,73,73,73	0
6	NAG	A	606	14/15	0.97	0.14	47,57,68,68	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.