



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 03:56 pm BST

PDB ID : 5A2D
Title : CRYSTAL STRUCTURE OF BETAIN ALDEHYDE DEHYDROGENASE
FROM SPINACH SHOWING A THIOHEMIACETAL WITH BETAIN
ALDEHYDE
Authors : Zarate-Romero, A.; Munoz-Clares, R.A.
Deposited on : 2015-05-17
Resolution : 1.98 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

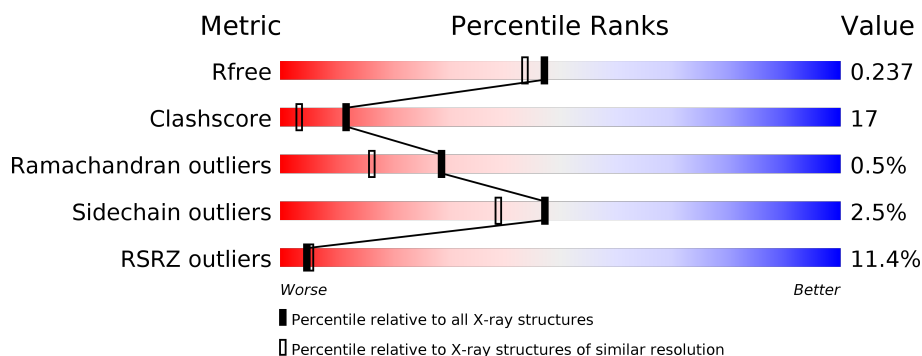
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	<div> <div>4%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	B	497	<div> <div>10%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
2	C	497	<div> <div>23%</div> <div>59%</div> <div>36%</div> <div>..</div> </div>
3	D	497	<div> <div>8%</div> <div>81%</div> <div>16%</div> <div>..</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ETX	D	1498	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16066 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 BETAINES ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	7	0
			3841	2458	641	724	18			
1	B	493	Total	C	N	O	S	0	11	0
			3874	2479	647	731	17			

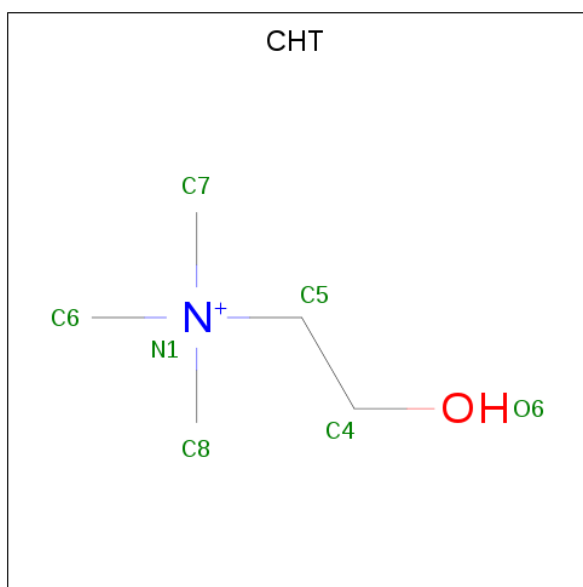
- Molecule 2 is a protein called BETAINES ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	492	Total	C	N	O	S	0	3	0
			3806	2437	636	717	16			

- Molecule 3 is a protein called BETAINES ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC.

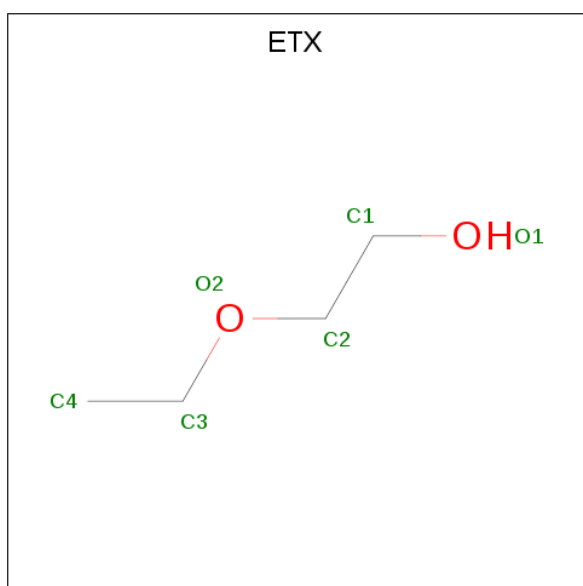
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	493	Total	C	N	O	S	0	3	0
			3817	2447	635	719	16			

- Molecule 4 is CHOLINE ION (three-letter code: CHT) (formula: C₅H₁₄NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			7	5	1	1		
4	B	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 5 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: $C_4H_{10}O_2$).

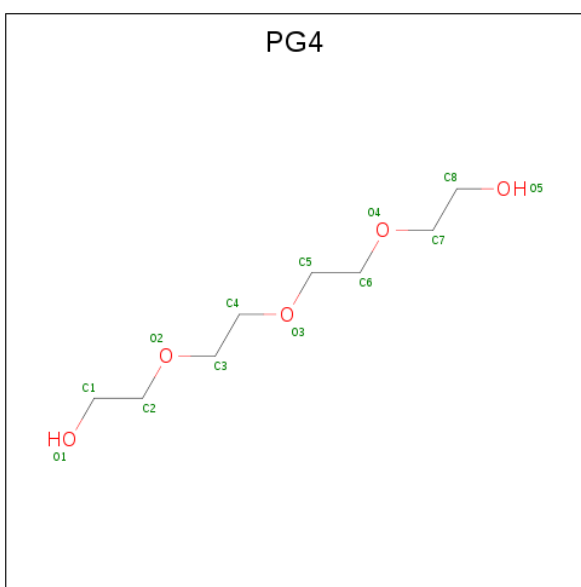


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

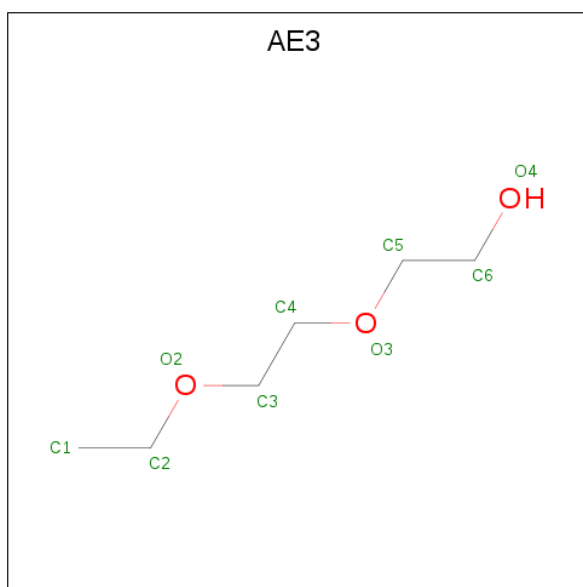
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0
6	A	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 12 8 4	0	0

- Molecule 8 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula: C₆H₁₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			9	6	3		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

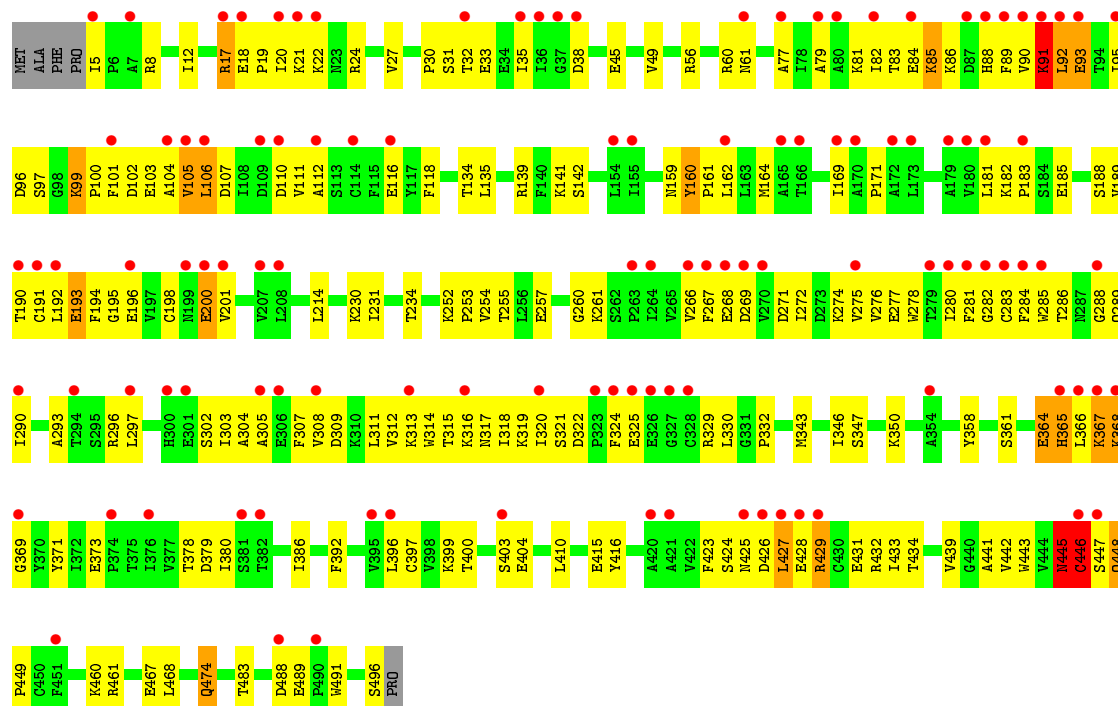
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	239	Total 239	O 239	0	0
10	B	150	Total 150	O 150	0	0
10	C	103	Total 103	O 103	0	0
10	D	179	Total 179	O 179	0	0

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

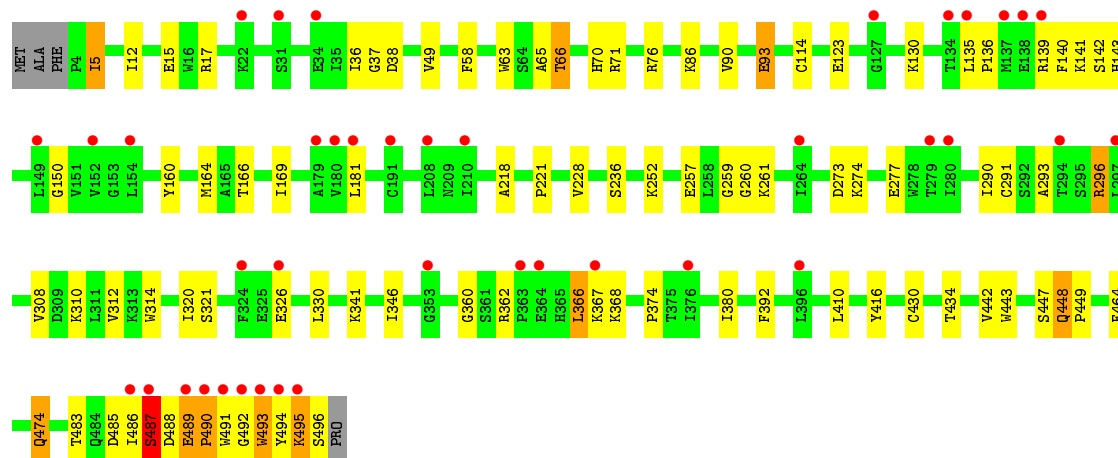
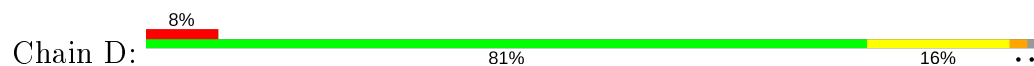
- Chain A:
-
- | Amino Acid | Percentage |
|------------|------------|
| MET | 0.01 |
| ALA | 0.01 |
| PHE | 0.01 |
| P4 | 0.01 |
| I5 | 0.01 |
| R8 | 0.01 |
| K22 | 0.01 |
| T32 | 0.01 |
| E33 | 0.01 |
| E34 | 0.01 |
| R76 | 0.01 |
| K81 | 0.01 |
| K85 | 0.01 |
| E93 | 0.01 |
| T94 | 0.01 |
| I95 | 0.01 |
| E123 | 0.01 |
| R139 | 0.01 |
| S142 | 0.01 |
| R146 | 0.01 |
| P157 | 0.01 |
| Y160 | 0.01 |
| P161 | 0.01 |
| L162 | 0.01 |
| L163 | 0.01 |
| M164 | 0.01 |
| A165 | 0.01 |
| T166 | 0.01 |
| M167 | 0.01 |
| K168 | 0.01 |
| I169 | 0.01 |
| L181 | 0.01 |
| K182 | 0.01 |
| C191 | 0.01 |
| L192 | 0.01 |
| I210 | 0.01 |
| K230 | 0.01 |
| T234 | 0.01 |
| V251 | 0.01 |
| P367 | 0.01 |
| L258 | 0.01 |
| G259 | 0.01 |
| G260 | 0.01 |
| T262 | 0.01 |
| V263 | 0.01 |
| D269 | 0.01 |
| K274 | 0.01 |
| T280 | 0.01 |
| T281 | 0.01 |
| F284 | 0.01 |
| V285 | 0.01 |
| T290 | 0.01 |
| A293 | 0.01 |
| R296 | 0.01 |
| L297 | 0.01 |
| A304 | 0.01 |
| A305 | 0.01 |
| E306 | 0.01 |
| F307 | 0.01 |
| V308 | 0.01 |
| D309 | 0.01 |
| K310 | 0.01 |
| L311 | 0.01 |
| V312 | 0.01 |
| K313 | 0.01 |
| K314 | 0.01 |
| K319 | 0.01 |
| E326 | 0.01 |
| L330 | 0.01 |
| K344 | 0.01 |
| S351 | 0.01 |
| R362 | 0.01 |
| P363 | 0.01 |
| E364 | 0.01 |
| K367 | 0.01 |
| K368 | 0.01 |
| G369 | 0.01 |
| P374 | 0.01 |
| I376 | 0.01 |
| T380 | 0.01 |
| G381 | 0.01 |

- Chain B:
-
- 10% 79% 19%

- Chain C:  23% 59% 36%



• Molecule 3: BETAINES ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.72Å 82.29Å 87.72Å 79.41° 84.75° 77.40°	Depositor
Resolution (Å)	28.70 – 1.98 28.70 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.8 (28.70-1.98) 96.8 (28.70-1.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.194 , 0.237 0.195 , 0.237	Depositor DCC
R_{free} test set	6195 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16066	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSO, ETX, AE3, PG4, CHT, K

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	0.51	0/3934	0.61	2/5350 (0.0%)
1	B	0.48	0/3964	0.59	1/5390 (0.0%)
2	C	0.57	0/3890	0.72	7/5289 (0.1%)
3	D	0.52	0/3891	0.66	3/5291 (0.1%)
All	All	0.52	0/15679	0.65	13/21320 (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
1	B	0	2
2	C	0	3
All	All	0	6

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	487	SER	CB-CA-C	-18.03	75.85	110.10
2	C	446	CYS	C-N-CA	11.58	150.65	121.70
1	A	448	GLN	N-CA-C	8.54	134.06	111.00
2	C	91	LYS	CB-CA-C	-8.46	93.48	110.40
2	C	445	ASN	O-C-N	-8.37	109.31	122.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	396	LEU	Mainchain
1	B	24	ARG	Mainchain
2	C	21	LYS	Mainchain
2	C	445	ASN	Mainchain
2	C	446	CYS	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	3841	0	3834	62	2
1	B	3874	0	3867	83	2
2	C	3806	0	3804	328	0
3	D	3817	0	3819	88	0
4	A	7	0	12	0	0
4	B	7	0	12	1	0
5	A	6	0	10	0	0
5	D	6	0	10	4	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	B	12	0	15	1	0
8	C	9	0	14	1	0
9	D	6	0	8	1	0
10	A	239	0	0	0	0
10	B	150	0	0	3	0
10	C	103	0	0	6	0
10	D	179	0	0	2	0
All	All	16066	0	15405	536	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 17.

The worst 5 of 536 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)
2:C:278:TRP:CA	2:C:281:PHE:CE2	1.82	1.60
2:C:278:TRP:HE3	2:C:281:PHE:CZ	1.24	1.54
2:C:5:ILE:HD11	2:C:95:ILE:CD1	1.16	1.52
2:C:314:TRP:HA	2:C:317:ASN:ND2	1.29	1.41
2:C:278:TRP:HA	2:C:281:PHE:CE2	0.88	1.41

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)
1:A:326:GLU:OE2	1:B:313:LYS:NZ[1_465]	1.81	0.39
1:A:326:GLU:OE2	1:B:313:LYS:CE[1_465]	1.87	0.33

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	498/497 (100%)	482 (97%)	15 (3%)	1 (0%)	47	38
1	B	502/497 (101%)	474 (94%)	26 (5%)	2 (0%)	34	22
2	C	492/497 (99%)	447 (91%)	40 (8%)	5 (1%)	15	6
3	D	492/497 (99%)	474 (96%)	16 (3%)	2 (0%)	34	22
All	All	1984/1988 (100%)	1877 (95%)	97 (5%)	10 (0%)	29	16

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	GLN
1	B	367	LYS
1	B	448	GLN
2	C	365	HIS
2	C	448	GLN

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	414/410 (101%)	407 (98%)	7 (2%)	60	53
1	B	417/410 (102%)	411 (99%)	6 (1%)	67	62
2	C	408/409 (100%)	389 (95%)	19 (5%)	26	13
3	D	408/408 (100%)	396 (97%)	12 (3%)	42	31
All	All	1647/1637 (101%)	1603 (97%)	44 (3%)	47	35

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	116	GLU
2	C	367	LYS
3	D	487	SER
2	C	160	TYR
2	C	200	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	61	ASN
2	C	88	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	CSO	D	291	3	3,6,7	0.98	0	0,6,8	0.00	-
2	CSO	C	291	2	3,6,7	0.55	0	0,6,8	0.00	-
3	CSO	D	450	3	3,6,7	0.78	0	0,6,8	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CSO	D	291	3	-	0/1/5/7	-
2	CSO	C	291	2	-	0/1/5/7	-
3	CSO	D	450	3	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	291	CSO	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	GOL	D	1500	-	5,5,5	0.35	0	5,5,5	0.30	0
5	ETX	D	1498	-	5,5,5	0.39	0	4,4,4	0.51	0
7	PG4	B	1498	-	11,11,12	0.75	0	10,10,11	0.45	0
4	CHT	B	1497	1	6,6,6	1.98	1 (16%)	8,8,8	1.10	1 (12%)
4	CHT	A	1497	1	6,6,6	1.97	1 (16%)	8,8,8	1.20	1 (12%)
8	AE3	C	1497	-	8,8,8	0.71	0	7,7,7	0.38	0
5	ETX	A	1498	-	5,5,5	0.44	0	4,4,4	0.29	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
9	GOL	D	1500	-	-	0/4/4/4	-
5	ETX	D	1498	-	-	1/3/3/3	-
7	PG4	B	1498	-	-	7/9/9/10	-
4	CHT	B	1497	1	-	1/4/4/4	-
4	CHT	A	1497	1	-	0/4/4/4	-
8	AE3	C	1497	-	-	3/6/6/6	-
5	ETX	A	1498	-	-	2/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1497	CHT	O6-C4	-3.82	1.22	1.42
4	A	1497	CHT	O6-C4	-3.70	1.23	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1497	CHT	C8-N1-C5	2.29	119.29	109.92
4	B	1497	CHT	C8-N1-C5	2.00	118.10	109.92

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1497	AE3	C4-C3-O2-C2
8	C	1497	AE3	O3-C5-C6-O4
5	A	1498	ETX	O1-C1-C2-O2
7	B	1498	PG4	O2-C3-C4-O3
7	B	1498	PG4	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	1500	GOL	1	0
5	D	1498	ETX	4	0
7	B	1498	PG4	1	0
4	B	1497	CHT	1	0
8	C	1497	AE3	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, 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	493/497 (99%)	0.24	20 (4%) 37 39	20, 38, 67, 97	0
1	B	493/497 (99%)	0.58	49 (9%) 7 8	24, 48, 79, 118	0
2	C	491/497 (98%)	1.29	115 (23%) 0 0	30, 68, 109, 194	0
3	D	491/497 (98%)	0.35	40 (8%) 12 13	23, 41, 78, 183	0
All	All	1968/1988 (98%)	0.61	224 (11%) 5 5	20, 46, 92, 194	0

The worst 5 of 224 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	281	PHE	11.5
2	C	313	LYS	6.7
2	C	427	LEU	6.7
2	C	106	LEU	6.1
2	C	324	PHE	6.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CSO	D	450	7/8	0.88	0.15	38,43,61,89	0
2	CSO	C	291	7/8	0.90	0.15	54,59,75,80	0
3	CSO	D	291	7/8	0.96	0.12	29,30,62,92	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ETX	D	1498	6/6	0.64	0.35	55,63,66,68	0
9	GOL	D	1500	6/6	0.72	0.21	54,60,62,63	0
8	AE3	C	1497	9/9	0.82	0.14	50,53,56,59	0
5	ETX	A	1498	6/6	0.84	0.18	57,58,60,62	0
4	CHT	A	1497	7/7	0.90	0.40	53,55,61,61	7
6	K	B	1499	1/1	0.92	0.10	45,45,45,45	1
7	PG4	B	1498	12/13	0.93	0.11	35,40,48,51	0
4	CHT	B	1497	7/7	0.94	0.26	59,60,65,66	7
6	K	C	1498	1/1	0.95	0.11	48,48,48,48	1
6	K	D	1499	1/1	0.96	0.13	43,43,43,43	1
6	K	A	1499	1/1	0.97	0.07	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.