



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:25 AM BST

PDB ID : 6BJP  
Title : Apo form of the E124S mutant of betaine aldehyde dehydrogenase from *Pseudomonas aeruginosa*  
Authors : Carrizosa-Carbajal, E.I.; Gonzalez-Segura, L.; Munoz-Clares, R.A.  
Deposited on : 2017-11-06  
Resolution : 2.10 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.

---

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 : 2.13.1  
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) : 2.13.1

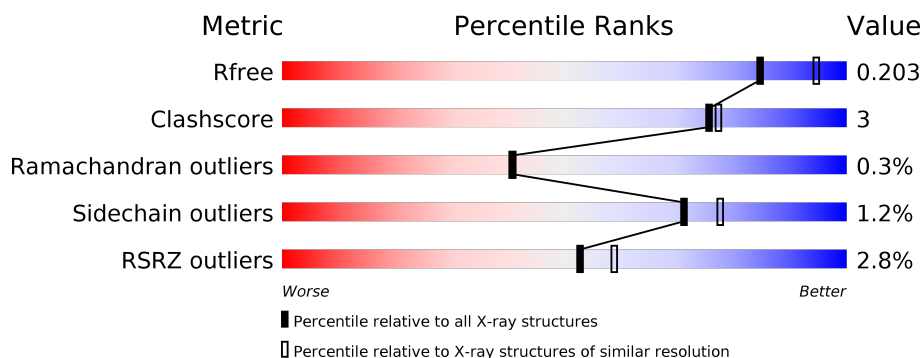
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	491	<div> <div>0%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>
1	B	491	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>5%</div> </div> </div>
2	C	490	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
2	D	490	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15154 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 NAD/NADP-dependent betaine aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	4	0
			3574	2243	635	683	13			
1	B	466	Total	C	N	O	S	0	6	0
			3636	2286	644	693	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	SER	GLU	engineered mutation	UNP Q9HTJ1
B	124	SER	GLU	engineered mutation	UNP Q9HTJ1

- Molecule 2 is a protein called NAD/NADP-dependent betaine aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	463	Total	C	N	O	S	0	3	0
			3597	2262	637	686	12			
2	D	461	Total	C	N	O	S	0	4	0
			3579	2249	633	684	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	124	SER	GLU	engineered mutation	UNP Q9HTJ1
D	124	SER	GLU	engineered mutation	UNP Q9HTJ1

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

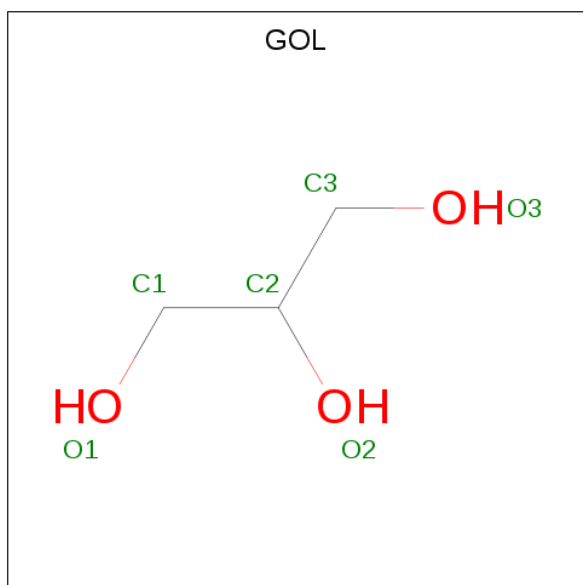
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

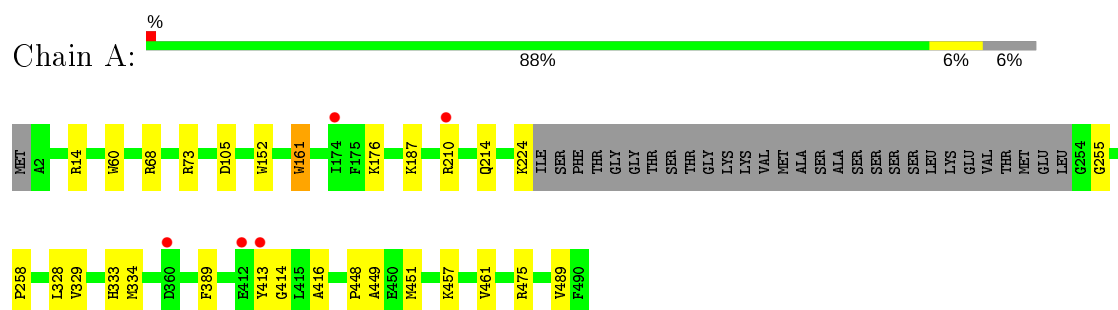
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	251	Total O 251 251	0	0
6	B	170	Total O 170 170	0	0
6	C	196	Total O 196 196	0	0
6	D	97	Total O 97 97	0	0

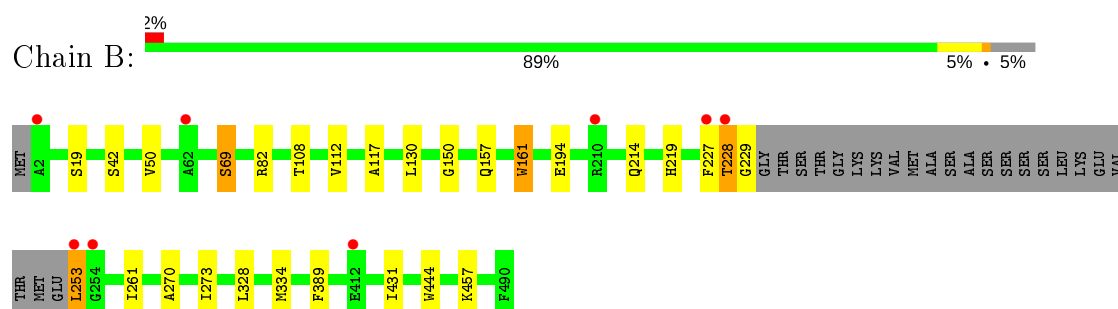
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

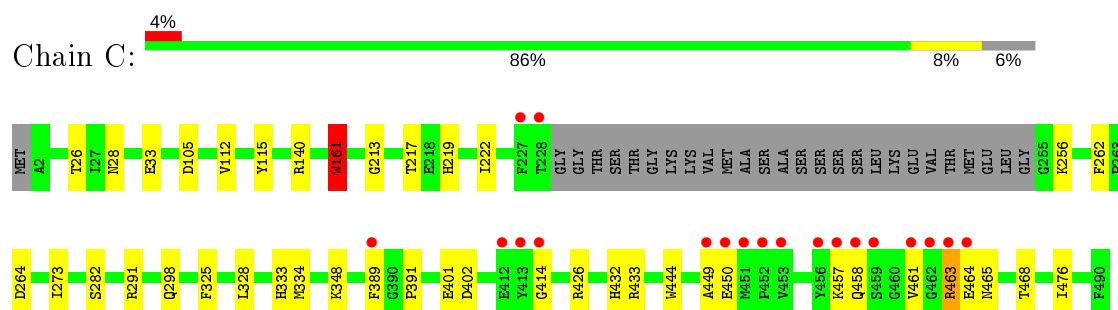
- Molecule 1: NAD/NADP-dependent betaine aldehyde dehydrogenase



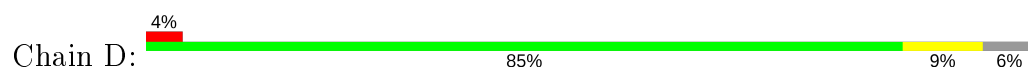
- Molecule 1: NAD/NADP-dependent betaine aldehyde dehydrogenase

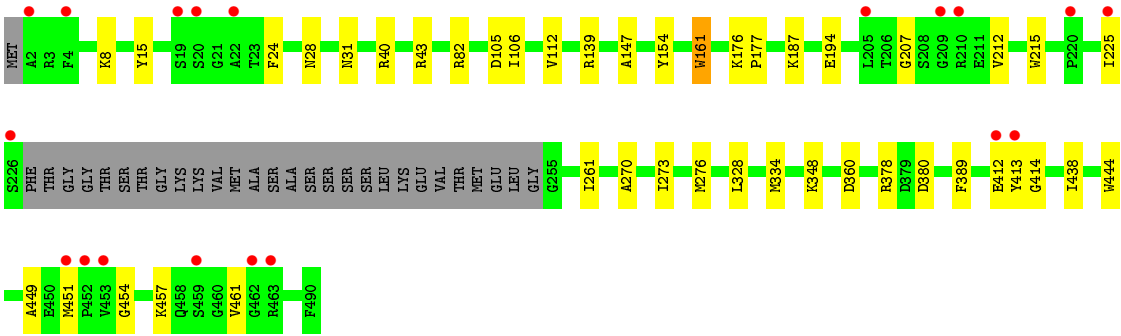


- Molecule 2: NAD/NADP-dependent betaine aldehyde dehydrogenase



- Molecule 2: NAD/NADP-dependent betaine aldehyde dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.22Å 96.54Å 280.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.10 19.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.83-2.10) 99.6 (19.83-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.11Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.164 , 0.204 0.165 , 0.203	Depositor DCC
$R_{free}$ test set	6772 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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 [i](#)

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

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

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	0.43	0/3632	0.54	0/4921
1	B	0.41	0/3695	0.53	0/5007
2	C	0.46	1/3665 (0.0%)	0.52	0/4969
2	D	0.34	0/3645	0.49	0/4942
All	All	0.41	1/14637 (0.0%)	0.52	0/19839

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	161	TRP	CB-CG	-11.07	1.30	1.50

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	3574	0	3533	17	0
1	B	3636	0	3600	19	0
2	C	3597	0	3556	31	0
2	D	3579	0	3543	24	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	24	0	0
5	A	12	0	18	1	0
5	B	20	0	30	1	0
6	A	251	0	0	1	1
6	B	170	0	0	1	0
6	C	196	0	0	1	1
6	D	97	0	0	1	0
All	All	15154	0	14304	88	1

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 3.

All (88) 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:112:VAL:HG21	2:C:161:TRP:CH2	2.11	0.86
1:B:19:SER:OG	1:B:42:SER:OG	2.11	0.69
2:D:161:TRP:CZ2	2:D:457:LYS:HE2	2.29	0.68
2:D:82:ARG:NH2	2:D:194:GLU:OE1	2.26	0.68
2:C:465:ASN:HA	2:C:468:THR:HB	1.78	0.63
2:C:112:VAL:HG21	2:C:161:TRP:CZ2	2.33	0.63
2:C:450:GLU:HB3	2:C:465:ASN:OD1	1.99	0.61
1:B:161:TRP:CZ2	1:B:457:LYS:HE2	2.37	0.59
2:D:176:LYS:NZ	2:D:177:PRO:O	2.36	0.59
1:A:255:GLY:HA2	1:A:413:TYR:CD1	2.39	0.58
2:D:328:LEU:HD12	2:D:334:MET:HA	1.85	0.57
1:A:73[B]:ARG:NH1	6:A:602:HOH:O	2.38	0.56
1:B:261[A]:ILE:HD12	1:B:270:ALA:HB1	1.87	0.56
1:A:161:TRP:CZ2	1:A:457:LYS:HE2	2.41	0.56
2:D:43:ARG:HG2	2:D:215:TRP:CE2	2.41	0.55
2:D:161:TRP:CH2	2:D:457:LYS:HG3	2.41	0.55
1:A:449:ALA:HB3	1:A:461:VAL:HG22	1.88	0.55
2:C:328:LEU:HD12	2:C:334:MET:HA	1.89	0.54
1:B:82:ARG:NH2	1:B:194:GLU:OE1	2.40	0.54
2:C:333[A]:HIS:NE2	2:C:389:PHE:O	2.36	0.53
1:B:108:THR:OG1	1:B:157:GLN:NE2	2.42	0.52
2:C:264:ASP:OD2	2:C:426:ARG:NH1	2.43	0.52
2:C:298:GLN:NE2	6:C:601:HOH:O	2.32	0.52
1:A:60:TRP:CE2	1:A:68:ARG:HD2	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:HIS:NE2	1:A:389:PHE:O	2.40	0.50
1:A:448:PRO:HB2	1:A:451:MET:HG3	1.94	0.50
2:C:463:ARG:C	2:C:465:ASN:H	2.15	0.49
1:B:19:SER:HG	1:B:42:SER:HG	1.41	0.49
1:A:176:LYS:O	1:A:176:LYS:HE3	2.12	0.49
2:D:378:ARG:NH1	2:D:380:ASP:OD1	2.46	0.49
1:B:69:SER:HB2	1:B:117:ALA:O	2.13	0.48
2:D:112[B]:VAL:HG21	2:D:161:TRP:CZ2	2.49	0.48
2:C:219:HIS:HB3	2:C:222:ILE:HD12	1.95	0.48
2:D:106:ILE:HD12	2:D:106:ILE:H	1.79	0.48
1:B:161:TRP:CD1	5:B:503:EDO:H12	2.48	0.48
2:D:147:ALA:HB3	2:D:225:ILE:HG13	1.96	0.47
2:C:115:TYR:CZ	2:C:461:VAL:HB	2.49	0.47
2:D:261:ILE:HD12	2:D:270:ALA:HB1	1.95	0.47
1:A:328:LEU:HD12	1:A:334:MET:HA	1.97	0.47
1:B:130:LEU:HD21	2:C:458[B]:GLN:HB2	1.95	0.47
2:D:139:ARG:NH1	6:D:606:HOH:O	2.48	0.46
2:C:28:ASN:HB3	2:C:33:GLU:HG2	1.97	0.46
2:D:24:PHE:HB3	2:D:40:ARG:NH1	2.31	0.46
1:B:130:LEU:HD21	2:C:458[A]:GLN:HB3	1.97	0.46
1:A:210:ARG:NH1	1:A:214:GLN:OE1	2.49	0.45
2:C:112:VAL:CG2	2:C:161:TRP:CH2	2.93	0.45
2:C:457:LYS:HA	2:C:457:LYS:HD2	1.82	0.45
2:D:449:ALA:HB3	2:D:461:VAL:HG13	1.98	0.45
1:B:82:ARG:HH22	1:B:194:GLU:CD	2.19	0.45
6:B:657:HOH:O	2:C:432:HIS:HE1	2.00	0.45
1:B:161:TRP:CH2	1:B:457:LYS:HG3	2.52	0.45
1:A:152:TRP:CE3	1:A:329:VAL:HG11	2.52	0.44
2:C:262:PHE:HE1	2:C:401:GLU:HG3	1.82	0.44
1:A:187:LYS:NZ	5:A:506:EDO:H12	2.33	0.44
2:D:154:TYR:CD2	2:D:454:GLY:HA3	2.52	0.44
1:B:227:PHE:O	1:B:228:THR:OG1	2.33	0.43
1:A:161:TRP:CH2	1:A:457:LYS:HG3	2.53	0.43
2:C:402:ASP:OD1	2:C:433:ARG:NH2	2.51	0.43
2:D:8:LYS:HE2	2:D:15:TYR:HB3	2.00	0.43
2:D:187:LYS:HD3	2:D:187:LYS:HA	1.85	0.43
2:D:207:GLY:HA3	2:D:212:VAL:HG21	2.01	0.43
1:B:431:ILE:HD13	1:B:431:ILE:HA	1.88	0.43
2:C:140:ARG:CZ	2:C:476:ILE:HD11	2.49	0.43
2:C:256:LYS:HG3	2:C:291:ARG:HG3	2.00	0.43
1:B:273:ILE:HG23	1:B:444:TRP:HB2	2.00	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:273:ILE:HG23	2:D:444:TRP:HB2	2.01	0.42
1:B:328:LEU:HD12	1:B:334:MET:HA	2.01	0.42
1:B:50:VAL:HG11	1:B:219:HIS:CE1	2.54	0.42
2:C:273:ILE:HG23	2:C:444:TRP:HB2	2.01	0.42
2:C:112:VAL:HG21	2:C:161:TRP:CZ3	2.54	0.42
2:C:348:LYS:HD3	2:C:348:LYS:HA	1.85	0.42
2:C:449:ALA:HB3	2:C:461:VAL:HG22	2.01	0.42
1:A:489:VAL:HG22	2:D:276:MET:SD	2.60	0.42
2:C:213:GLY:O	2:C:217:THR:HG23	2.20	0.42
2:C:328:LEU:HD21	2:C:391:PRO:HD3	2.02	0.41
2:D:438:ILE:HD11	2:D:451:MET:SD	2.60	0.41
2:C:282:SER:HA	2:C:325:PHE:CE2	2.55	0.41
1:A:255:GLY:HA2	1:A:413:TYR:CG	2.55	0.41
1:A:258:PRO:HD2	1:A:416:ALA:O	2.20	0.41
2:C:463:ARG:O	2:C:465:ASN:N	2.49	0.41
2:D:28:ASN:HB3	2:D:31:ASN:OD1	2.20	0.41
1:B:150:GLY:O	1:B:229:GLY:HA3	2.21	0.41
1:B:253:LEU:HD12	1:B:253:LEU:HA	1.96	0.41
2:C:449:ALA:HB2	2:C:458[B]:GLN:HG3	2.03	0.41
1:A:224:LYS:HE3	1:A:224:LYS:HB3	1.88	0.40
2:D:348:LYS:HA	2:D:348:LYS:HD3	1.90	0.40
2:D:412:GLU:HG3	2:D:413:TYR:N	2.35	0.40
2:C:449:ALA:CB	2:C:461:VAL:HG22	2.52	0.40

All (1) 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)
6:A:713:HOH:O	6:C:737:HOH:O[3_454]	2.19	0.01

## 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	458/491 (93%)	449 (98%)	8 (2%)	1 (0%)	47	49
1	B	466/491 (95%)	457 (98%)	8 (2%)	1 (0%)	47	49
2	C	462/490 (94%)	447 (97%)	13 (3%)	2 (0%)	34	32
2	D	461/490 (94%)	451 (98%)	9 (2%)	1 (0%)	47	49
All	All	1847/1962 (94%)	1804 (98%)	38 (2%)	5 (0%)	41	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	THR
2	C	464	GLU
2	C	414	GLY
2	D	414	GLY
1	A	414	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	369/391 (94%)	365 (99%)	4 (1%)	73	79
1	B	376/391 (96%)	370 (98%)	6 (2%)	62	69
2	C	373/391 (95%)	369 (99%)	4 (1%)	73	79
2	D	372/391 (95%)	368 (99%)	4 (1%)	73	79
All	All	1490/1564 (95%)	1472 (99%)	18 (1%)	71	77

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	105	ASP
1	A	161	TRP
1	A	475	ARG
1	B	69	SER
1	B	112	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	161	TRP
1	B	214	GLN
1	B	253	LEU
1	B	389	PHE
2	C	26	THR
2	C	105	ASP
2	C	161	TRP
2	C	463	ARG
2	D	105	ASP
2	D	161	TRP
2	D	360	ASP
2	D	389	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	432	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z  > 2$
1	CSO	B	286[A]	1	3,6,7	0.77	0	0,6,8	0.00	-
1	CSO	A	286[A]	1	3,6,7	0.65	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
1	CSO	B	286[A]	1	-	1/1/5/7	-
1	CSO	A	286[A]	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	286[A]	CSO	N-CA-CB-SG
1	A	286[A]	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	EDO	B	504	-	3,3,3	0.48	0	2,2,2	0.31	0
5	EDO	B	505	-	3,3,3	0.52	0	2,2,2	0.24	0
5	EDO	A	507	-	3,3,3	0.51	0	2,2,2	0.31	0
4	GOL	A	503	-	5,5,5	0.38	0	5,5,5	0.34	0
5	EDO	B	502	-	3,3,3	0.47	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	502	-	5,5,5	0.32	0	5,5,5	0.42	0
5	EDO	B	506	-	3,3,3	0.56	0	2,2,2	0.07	0
5	EDO	B	503	-	3,3,3	0.48	0	2,2,2	0.26	0
4	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.26	0
5	EDO	A	505	-	3,3,3	0.48	0	2,2,2	0.35	0
5	EDO	A	506	-	3,3,3	0.44	0	2,2,2	0.44	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	EDO	B	504	-	-	0/1/1/1	-
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	A	507	-	-	0/1/1/1	-
4	GOL	A	503	-	-	2/4/4/4	-
5	EDO	B	502	-	-	0/1/1/1	-
4	GOL	A	502	-	-	0/4/4/4	-
5	EDO	B	506	-	-	0/1/1/1	-
5	EDO	B	503	-	-	0/1/1/1	-
4	GOL	A	504	-	-	2/4/4/4	-
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	A	506	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	C1-C2-C3-O3
4	A	504	GOL	O1-C1-C2-C3
4	A	504	GOL	O1-C1-C2-O2
4	A	503	GOL	O2-C2-C3-O3
5	A	506	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	EDO	1	0
5	A	506	EDO	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	459/491 (93%)	-0.37	5 (1%) 80 84	13, 22, 46, 84	0
1	B	465/491 (94%)	-0.27	8 (1%) 70 74	13, 28, 54, 70	0
2	C	463/490 (94%)	-0.12	19 (4%) 37 43	13, 29, 62, 120	0
2	D	461/490 (94%)	0.04	19 (4%) 37 43	15, 39, 69, 102	0
All	All	1848/1962 (94%)	-0.18	51 (2%) 53 59	13, 30, 61, 120	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	413	TYR	5.9
2	C	227	PHE	5.5
2	D	413	TYR	5.4
2	C	451	MET	5.2
1	A	413	TYR	5.2
2	C	453	VAL	5.1
2	C	462	GLY	4.4
2	D	452	PRO	4.3
2	C	456	TYR	4.3
2	C	459	SER	4.2
2	C	228	THR	4.1
1	B	210	ARG	4.0
2	D	210	ARG	4.0
2	C	414	GLY	3.8
2	C	412	GLU	3.8
1	A	210	ARG	3.7
2	D	412	GLU	3.7
2	D	226	SER	3.6
1	B	227	PHE	3.5
2	C	463	ARG	3.4
2	D	451	MET	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	412	GLU	3.2
2	C	389	PHE	3.2
1	A	412	GLU	3.1
2	D	19	SER	3.0
2	D	2	ALA	2.9
1	B	228	THR	2.9
2	C	464	GLU	2.8
1	B	2	ALA	2.8
2	D	459	SER	2.8
2	D	22	ALA	2.7
2	D	209	GLY	2.7
2	C	452	PRO	2.7
2	C	461	VAL	2.7
1	B	254	GLY	2.6
2	D	20	SER	2.4
2	D	225	ILE	2.3
2	C	458[A]	GLN	2.2
2	D	205	LEU	2.2
2	C	449	ALA	2.2
1	A	174	ILE	2.2
2	C	457	LYS	2.2
1	A	360	ASP	2.1
2	D	4	PHE	2.1
2	D	462	GLY	2.1
1	B	62	ALA	2.1
2	C	450	GLU	2.1
2	D	463	ARG	2.0
2	D	220	PRO	2.0
2	D	453	VAL	2.0
1	B	253	LEU	2.0

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

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(Å <sup>2</sup> )	Q<0.9
1	CSO	A	286[A]	7/8	0.92	0.10	21,22,30,54	7
1	CSO	B	286[A]	7/8	0.96	0.08	13,19,21,49	7

### 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 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. 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(Å <sup>2</sup> )	Q<0.9
5	EDO	B	505	4/4	0.67	0.18	48,50,52,53	0
5	EDO	A	507	4/4	0.80	0.17	51,51,52,54	0
5	EDO	B	504	4/4	0.83	0.17	50,55,55,56	0
5	EDO	A	506	4/4	0.85	0.12	53,53,57,61	0
5	EDO	B	506	4/4	0.86	0.17	32,42,47,53	0
4	GOL	A	502	6/6	0.89	0.16	37,41,43,48	0
5	EDO	B	503	4/4	0.91	0.18	34,41,48,50	0
4	GOL	A	503	6/6	0.93	0.10	45,48,49,50	0
5	EDO	B	502	4/4	0.93	0.13	47,49,49,50	0
4	GOL	A	504	6/6	0.94	0.13	47,52,57,58	0
5	EDO	A	505	4/4	0.95	0.08	40,50,56,60	0
3	K	D	501	1/1	0.95	0.10	46,46,46,46	0
3	K	C	501	1/1	0.99	0.11	26,26,26,26	0
3	K	A	501	1/1	0.99	0.06	20,20,20,20	0
3	K	B	501	1/1	0.99	0.07	26,26,26,26	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.