



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2023 – 11:58 AM EST

PDB ID : 2FG7  
Title : N-succinyl-L-ornithine transcarbamylase from *B. fragilis* complexed with carbamoyl phosphate and N-succinyl-L-norvaline  
Authors : Shi, D.; Yu, X.; Malamy, M.H.; Allewell, N.M.; Tuchman, M.  
Deposited on : 2005-12-21  
Resolution : 2.90 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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 : 2.36  
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) : 2.36

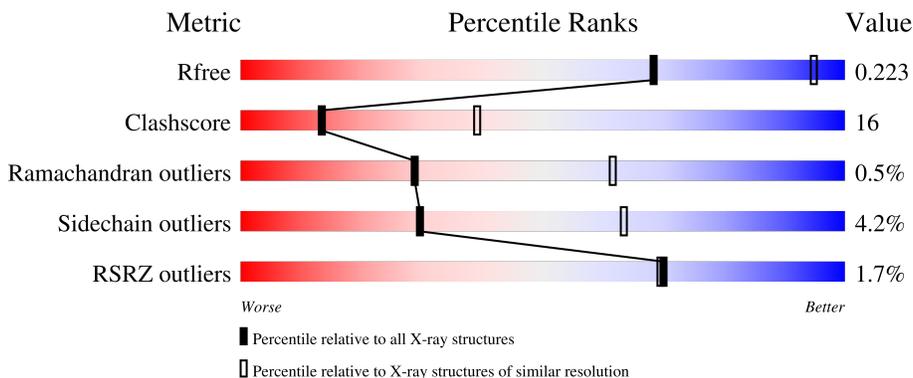
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of 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	C	338	 4% 65% 27% • 5%
1	D	338	 3% 63% 28% • 5%
1	E	338	 % 67% 25% • 5%
1	X	338	 66% 27% • 5%
1	Y	338	 67% 25% • 5%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	Z	338	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment labeled '68%', a yellow segment labeled '24%', and a red segment labeled '5%'. A small red square is positioned at the start of the bar, and a small black dot is at the end of the red segment. A '%' symbol is located above the start of the bar.</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15889 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 putative ornithine carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	321	2582	1645	444	477	16	0	0	0
1	Y	321	2582	1645	444	477	16	0	0	0
1	Z	320	2578	1643	443	476	16	0	0	0
1	C	320	2578	1643	443	476	16	0	0	0
1	D	320	2578	1643	443	476	16	0	0	0
1	E	320	2578	1643	443	476	16	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-19	MET	-	expression tag	UNP Q5LI27
X	-18	GLY	-	expression tag	UNP Q5LI27
X	-17	SER	-	expression tag	UNP Q5LI27
X	-16	SER	-	expression tag	UNP Q5LI27
X	-15	HIS	-	expression tag	UNP Q5LI27
X	-14	HIS	-	expression tag	UNP Q5LI27
X	-13	HIS	-	expression tag	UNP Q5LI27
X	-12	HIS	-	expression tag	UNP Q5LI27
X	-11	HIS	-	expression tag	UNP Q5LI27
X	-10	HIS	-	expression tag	UNP Q5LI27
X	-9	SER	-	expression tag	UNP Q5LI27
X	-8	SER	-	expression tag	UNP Q5LI27
X	-7	GLY	-	expression tag	UNP Q5LI27
X	-6	LEU	-	expression tag	UNP Q5LI27
X	-5	VAL	-	expression tag	UNP Q5LI27
X	-4	PRO	-	expression tag	UNP Q5LI27
X	-3	ARG	-	expression tag	UNP Q5LI27

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	GLY	-	expression tag	UNP Q5LI27
X	-1	SER	-	expression tag	UNP Q5LI27
X	0	HIS	-	expression tag	UNP Q5LI27
X	242	LEU	THR	engineered mutation	UNP Q5LI27
Y	-19	MET	-	expression tag	UNP Q5LI27
Y	-18	GLY	-	expression tag	UNP Q5LI27
Y	-17	SER	-	expression tag	UNP Q5LI27
Y	-16	SER	-	expression tag	UNP Q5LI27
Y	-15	HIS	-	expression tag	UNP Q5LI27
Y	-14	HIS	-	expression tag	UNP Q5LI27
Y	-13	HIS	-	expression tag	UNP Q5LI27
Y	-12	HIS	-	expression tag	UNP Q5LI27
Y	-11	HIS	-	expression tag	UNP Q5LI27
Y	-10	HIS	-	expression tag	UNP Q5LI27
Y	-9	SER	-	expression tag	UNP Q5LI27
Y	-8	SER	-	expression tag	UNP Q5LI27
Y	-7	GLY	-	expression tag	UNP Q5LI27
Y	-6	LEU	-	expression tag	UNP Q5LI27
Y	-5	VAL	-	expression tag	UNP Q5LI27
Y	-4	PRO	-	expression tag	UNP Q5LI27
Y	-3	ARG	-	expression tag	UNP Q5LI27
Y	-2	GLY	-	expression tag	UNP Q5LI27
Y	-1	SER	-	expression tag	UNP Q5LI27
Y	0	HIS	-	expression tag	UNP Q5LI27
Y	242	LEU	THR	engineered mutation	UNP Q5LI27
Z	-19	MET	-	expression tag	UNP Q5LI27
Z	-18	GLY	-	expression tag	UNP Q5LI27
Z	-17	SER	-	expression tag	UNP Q5LI27
Z	-16	SER	-	expression tag	UNP Q5LI27
Z	-15	HIS	-	expression tag	UNP Q5LI27
Z	-14	HIS	-	expression tag	UNP Q5LI27
Z	-13	HIS	-	expression tag	UNP Q5LI27
Z	-12	HIS	-	expression tag	UNP Q5LI27
Z	-11	HIS	-	expression tag	UNP Q5LI27
Z	-10	HIS	-	expression tag	UNP Q5LI27
Z	-9	SER	-	expression tag	UNP Q5LI27
Z	-8	SER	-	expression tag	UNP Q5LI27
Z	-7	GLY	-	expression tag	UNP Q5LI27
Z	-6	LEU	-	expression tag	UNP Q5LI27
Z	-5	VAL	-	expression tag	UNP Q5LI27
Z	-4	PRO	-	expression tag	UNP Q5LI27
Z	-3	ARG	-	expression tag	UNP Q5LI27

*Continued on next page...*

*Continued from previous page...*

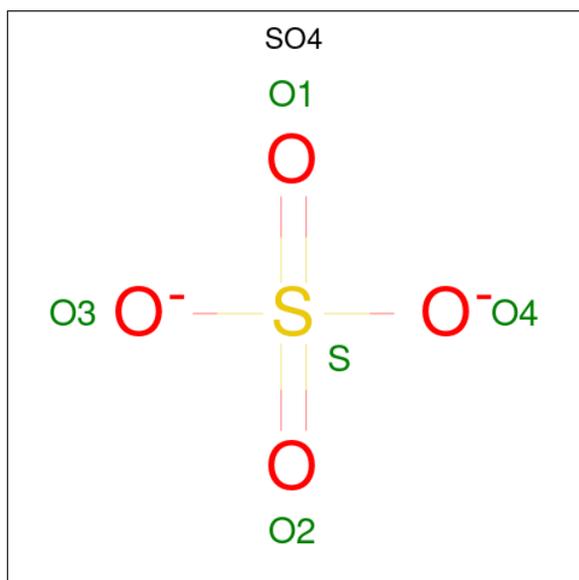
Chain	Residue	Modelled	Actual	Comment	Reference
Z	-2	GLY	-	expression tag	UNP Q5LI27
Z	-1	SER	-	expression tag	UNP Q5LI27
Z	0	HIS	-	expression tag	UNP Q5LI27
Z	242	LEU	THR	engineered mutation	UNP Q5LI27
C	-19	MET	-	expression tag	UNP Q5LI27
C	-18	GLY	-	expression tag	UNP Q5LI27
C	-17	SER	-	expression tag	UNP Q5LI27
C	-16	SER	-	expression tag	UNP Q5LI27
C	-15	HIS	-	expression tag	UNP Q5LI27
C	-14	HIS	-	expression tag	UNP Q5LI27
C	-13	HIS	-	expression tag	UNP Q5LI27
C	-12	HIS	-	expression tag	UNP Q5LI27
C	-11	HIS	-	expression tag	UNP Q5LI27
C	-10	HIS	-	expression tag	UNP Q5LI27
C	-9	SER	-	expression tag	UNP Q5LI27
C	-8	SER	-	expression tag	UNP Q5LI27
C	-7	GLY	-	expression tag	UNP Q5LI27
C	-6	LEU	-	expression tag	UNP Q5LI27
C	-5	VAL	-	expression tag	UNP Q5LI27
C	-4	PRO	-	expression tag	UNP Q5LI27
C	-3	ARG	-	expression tag	UNP Q5LI27
C	-2	GLY	-	expression tag	UNP Q5LI27
C	-1	SER	-	expression tag	UNP Q5LI27
C	0	HIS	-	expression tag	UNP Q5LI27
C	242	LEU	THR	engineered mutation	UNP Q5LI27
D	-19	MET	-	expression tag	UNP Q5LI27
D	-18	GLY	-	expression tag	UNP Q5LI27
D	-17	SER	-	expression tag	UNP Q5LI27
D	-16	SER	-	expression tag	UNP Q5LI27
D	-15	HIS	-	expression tag	UNP Q5LI27
D	-14	HIS	-	expression tag	UNP Q5LI27
D	-13	HIS	-	expression tag	UNP Q5LI27
D	-12	HIS	-	expression tag	UNP Q5LI27
D	-11	HIS	-	expression tag	UNP Q5LI27
D	-10	HIS	-	expression tag	UNP Q5LI27
D	-9	SER	-	expression tag	UNP Q5LI27
D	-8	SER	-	expression tag	UNP Q5LI27
D	-7	GLY	-	expression tag	UNP Q5LI27
D	-6	LEU	-	expression tag	UNP Q5LI27
D	-5	VAL	-	expression tag	UNP Q5LI27
D	-4	PRO	-	expression tag	UNP Q5LI27
D	-3	ARG	-	expression tag	UNP Q5LI27

*Continued on next page...*

Continued from previous page...

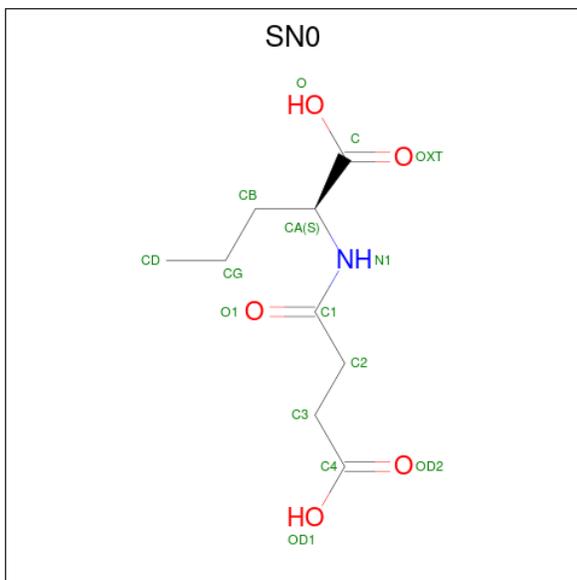
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP Q5LI27
D	-1	SER	-	expression tag	UNP Q5LI27
D	0	HIS	-	expression tag	UNP Q5LI27
D	242	LEU	THR	engineered mutation	UNP Q5LI27
E	-19	MET	-	expression tag	UNP Q5LI27
E	-18	GLY	-	expression tag	UNP Q5LI27
E	-17	SER	-	expression tag	UNP Q5LI27
E	-16	SER	-	expression tag	UNP Q5LI27
E	-15	HIS	-	expression tag	UNP Q5LI27
E	-14	HIS	-	expression tag	UNP Q5LI27
E	-13	HIS	-	expression tag	UNP Q5LI27
E	-12	HIS	-	expression tag	UNP Q5LI27
E	-11	HIS	-	expression tag	UNP Q5LI27
E	-10	HIS	-	expression tag	UNP Q5LI27
E	-9	SER	-	expression tag	UNP Q5LI27
E	-8	SER	-	expression tag	UNP Q5LI27
E	-7	GLY	-	expression tag	UNP Q5LI27
E	-6	LEU	-	expression tag	UNP Q5LI27
E	-5	VAL	-	expression tag	UNP Q5LI27
E	-4	PRO	-	expression tag	UNP Q5LI27
E	-3	ARG	-	expression tag	UNP Q5LI27
E	-2	GLY	-	expression tag	UNP Q5LI27
E	-1	SER	-	expression tag	UNP Q5LI27
E	0	HIS	-	expression tag	UNP Q5LI27
E	242	LEU	THR	engineered mutation	UNP Q5LI27

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



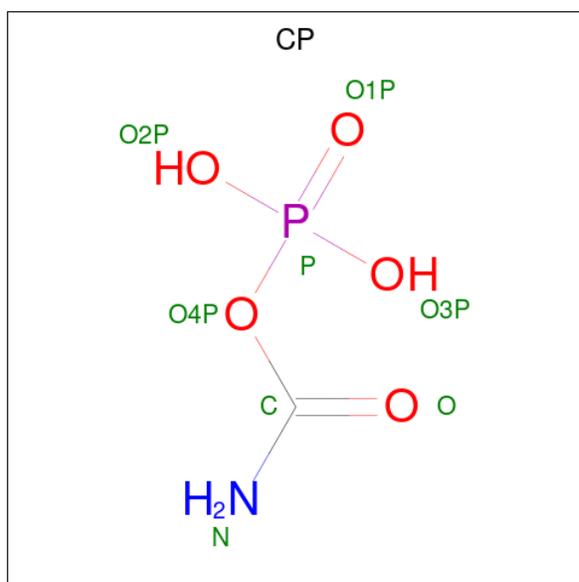
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	X	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is N-(3-CARBOXYPROPANOYL)-L-NORVALINE (three-letter code: SN0) (formula: C<sub>9</sub>H<sub>15</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	X	1	Total C N O 15 9 1 5	0	0
3	Y	1	Total C N O 15 9 1 5	0	0
3	Z	1	Total C N O 15 9 1 5	0	0
3	C	1	Total C N O 15 9 1 5	0	0
3	D	1	Total C N O 15 9 1 5	0	0
3	E	1	Total C N O 15 9 1 5	0	0

- Molecule 4 is PHOSPHORIC ACID MONO(FORMAMIDE)ESTER (three-letter code: CP) (formula: CH<sub>4</sub>NO<sub>5</sub>P).



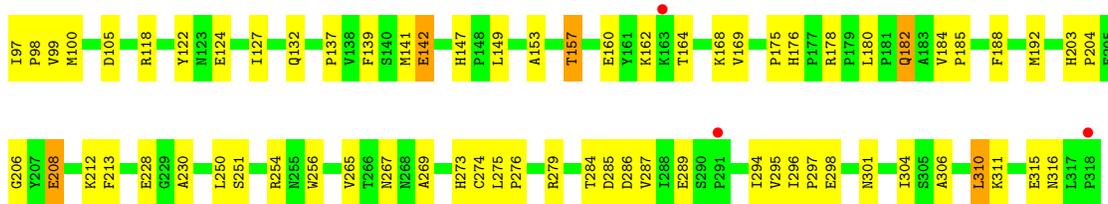
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	X	1	8	1	1	5	1	0	0
4	Y	1	8	1	1	5	1	0	0
4	Z	1	8	1	1	5	1	0	0
4	C	1	8	1	1	5	1	0	0
4	D	1	8	1	1	5	1	0	0
4	E	1	8	1	1	5	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	63	Total	O	0	0
			63	63		
5	Y	87	Total	O	0	0
			87	87		
5	Z	49	Total	O	0	0
			49	49		
5	C	12	Total	O	0	0
			12	12		
5	D	22	Total	O	0	0
			22	22		
5	E	32	Total	O	0	0
			32	32		







## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.42Å 156.42Å 120.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.90 19.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.94-2.90) 100.0 (19.94-2.90)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.88Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.204 , 0.229 0.197 , 0.223	Depositor DCC
$R_{free}$ test set	3253 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtrriage
Anisotropy	0.184	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: SN0, CP, 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	C	0.33	0/2638	0.61	0/3574
1	D	0.34	0/2638	0.62	0/3574
1	E	0.36	0/2638	0.62	0/3574
1	X	0.37	0/2642	0.63	0/3579
1	Y	0.39	0/2642	0.63	0/3579
1	Z	0.38	0/2638	0.63	0/3574
All	All	0.36	0/15836	0.62	0/21454

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	C	2578	0	2548	81	0
1	D	2578	0	2548	94	0
1	E	2578	0	2548	89	0
1	X	2582	0	2551	87	0
1	Y	2582	0	2551	85	0
1	Z	2578	0	2548	82	0
2	C	5	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	5	0	0	0	0
3	C	15	0	13	1	0
3	D	15	0	13	1	0
3	E	15	0	13	1	0
3	X	15	0	13	0	0
3	Y	15	0	13	0	0
3	Z	15	0	13	1	0
4	C	8	0	2	1	0
4	D	8	0	2	0	0
4	E	8	0	2	0	0
4	X	8	0	2	0	0
4	Y	8	0	2	0	0
4	Z	8	0	2	2	0
5	C	12	0	0	1	0
5	D	22	0	0	3	0
5	E	32	0	0	7	0
5	X	63	0	0	5	0
5	Y	87	0	0	8	0
5	Z	49	0	0	3	0
All	All	15889	0	15384	498	0

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 16.

The worst 5 of 498 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:D:254:ARG:HD3	5:D:366:HOH:O	1.62	0.96
1:X:254:ARG:HD3	5:X:439:HOH:O	1.68	0.92
1:Z:0:HIS:HA	1:Z:316:ASN:ND2	1.89	0.87
1:X:157:THR:HG21	1:X:298:GLU:HA	1.60	0.83
1:E:157:THR:HG21	1:E:298:GLU:HA	1.61	0.82

There are no symmetry-related clashes.

## 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	C	318/338 (94%)	292 (92%)	24 (8%)	2 (1%)	25 58
1	D	318/338 (94%)	292 (92%)	24 (8%)	2 (1%)	25 58
1	E	318/338 (94%)	293 (92%)	24 (8%)	1 (0%)	41 71
1	X	319/338 (94%)	291 (91%)	27 (8%)	1 (0%)	41 71
1	Y	319/338 (94%)	294 (92%)	24 (8%)	1 (0%)	41 71
1	Z	318/338 (94%)	293 (92%)	23 (7%)	2 (1%)	25 58
All	All	1910/2028 (94%)	1755 (92%)	146 (8%)	9 (0%)	29 61

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	142	GLU
1	Y	142	GLU
1	Z	142	GLU
1	C	142	GLU
1	E	142	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	C	279/294 (95%)	268 (96%)	11 (4%)	32 66
1	D	279/294 (95%)	267 (96%)	12 (4%)	29 62
1	E	279/294 (95%)	267 (96%)	12 (4%)	29 62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	279/294 (95%)	267 (96%)	12 (4%)	29	62
1	Y	279/294 (95%)	267 (96%)	12 (4%)	29	62
1	Z	279/294 (95%)	267 (96%)	12 (4%)	29	62
All	All	1674/1764 (95%)	1603 (96%)	71 (4%)	30	63

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	267	ASN
1	E	25	LYS
1	E	157	THR
1	Z	25	LYS
1	Y	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	316	ASN
1	E	316	ASN
1	C	301	ASN
1	E	301	ASN
1	E	182	GLN

### 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](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 ligands 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
4	CP	Z	350	-	6,7,7	1.71	2 (33%)	7,10,10	1.05	0
3	SN0	Y	347	-	14,14,14	0.73	0	17,17,17	1.34	3 (17%)
4	CP	E	356	-	6,7,7	1.87	1 (16%)	7,10,10	1.13	0
3	SN0	X	345	-	14,14,14	0.77	0	17,17,17	1.55	3 (17%)
3	SN0	Z	349	-	14,14,14	0.75	0	17,17,17	1.26	3 (17%)
4	CP	Y	348	-	6,7,7	1.85	2 (33%)	7,10,10	1.51	1 (14%)
4	CP	X	346	-	6,7,7	1.78	1 (16%)	7,10,10	1.10	0
2	SO4	C	401	-	4,4,4	0.26	0	6,6,6	0.08	0
4	CP	D	354	-	6,7,7	2.29	2 (33%)	7,10,10	1.53	1 (14%)
3	SN0	E	355	-	14,14,14	0.77	0	17,17,17	1.23	1 (5%)
3	SN0	D	353	-	14,14,14	0.79	0	17,17,17	1.22	1 (5%)
3	SN0	C	351	-	14,14,14	0.77	0	17,17,17	1.33	3 (17%)
2	SO4	X	400	-	4,4,4	0.29	0	6,6,6	0.08	0
4	CP	C	352	-	6,7,7	1.77	1 (16%)	7,10,10	1.31	1 (14%)

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
4	CP	Z	350	-	-	0/3/5/5	-
3	SN0	Y	347	-	-	1/16/16/16	-
4	CP	E	356	-	-	0/3/5/5	-
3	SN0	X	345	-	-	3/16/16/16	-
3	SN0	Z	349	-	-	0/16/16/16	-
4	CP	Y	348	-	-	0/3/5/5	-
4	CP	X	346	-	-	0/3/5/5	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CP	D	354	-	-	0/3/5/5	-
3	SN0	E	355	-	-	2/16/16/16	-
3	SN0	D	353	-	-	2/16/16/16	-
3	SN0	C	351	-	-	2/16/16/16	-
4	CP	C	352	-	-	0/3/5/5	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	354	CP	P-O1P	4.16	1.64	1.50
4	E	356	CP	P-O1P	3.61	1.62	1.50
4	C	352	CP	P-O1P	3.27	1.61	1.50
4	Y	348	CP	P-O1P	2.83	1.59	1.50
4	Z	350	CP	P-O1P	2.73	1.59	1.50

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	345	SN0	CB-CA-N1	-3.71	103.38	110.88
4	Y	348	CP	O2P-P-O4P	3.02	114.44	105.25
3	E	355	SN0	CB-CA-N1	-2.92	104.96	110.88
3	X	345	SN0	OD1-C4-C3	2.86	123.23	114.03
3	Z	349	SN0	OD1-C4-C3	2.74	122.85	114.03

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	345	SN0	O1-C1-N1-CA
3	D	353	SN0	O1-C1-N1-CA
3	X	345	SN0	C2-C1-N1-CA
3	C	351	SN0	C2-C3-C4-OD2
3	C	351	SN0	C2-C3-C4-OD1

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	350	CP	2	0
3	Z	349	SN0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	355	SN0	1	0
3	D	353	SN0	1	0
3	C	351	SN0	1	0
4	C	352	CP	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	C	320/338 (94%)	0.08	14 (4%) 34 30	56, 78, 96, 116	0
1	D	320/338 (94%)	-0.00	10 (3%) 49 44	52, 71, 94, 108	0
1	E	320/338 (94%)	-0.22	5 (1%) 72 71	38, 61, 79, 101	0
1	X	321/338 (94%)	-0.41	0 100 100	33, 51, 69, 79	0
1	Y	321/338 (94%)	-0.56	0 100 100	25, 40, 54, 74	0
1	Z	320/338 (94%)	-0.41	3 (0%) 84 84	33, 48, 67, 89	0
All	All	1922/2028 (94%)	-0.25	32 (1%) 70 69	25, 58, 90, 116	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	318	PRO	4.1
1	C	0	HIS	3.9
1	Z	0	HIS	3.8
1	C	318	PRO	3.8
1	D	318	PRO	3.8

### 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](#)

There are no monosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	SO4	C	401	5/5	0.89	0.29	125,125,125,126	0
2	SO4	X	400	5/5	0.92	0.19	92,93,93,93	0
3	SN0	Y	347	15/15	0.94	0.16	32,38,41,43	0
3	SN0	D	353	15/15	0.94	0.16	49,53,59,60	0
3	SN0	C	351	15/15	0.95	0.15	64,66,68,68	0
3	SN0	X	345	15/15	0.95	0.15	44,48,50,50	0
3	SN0	E	355	15/15	0.95	0.15	46,51,54,55	0
3	SN0	Z	349	15/15	0.97	0.15	33,37,41,41	0
4	CP	Z	350	8/8	0.98	0.14	36,39,40,40	0
4	CP	C	352	8/8	0.98	0.11	64,66,68,68	0
4	CP	D	354	8/8	0.98	0.09	51,55,57,57	0
4	CP	Y	348	8/8	0.99	0.12	30,30,31,31	0
4	CP	X	346	8/8	0.99	0.11	43,43,45,45	0
4	CP	E	356	8/8	0.99	0.11	44,45,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.