



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:43 PM GMT

PDB ID : 4A8P  
Title : Crystal structure of putrescine transcarbamylase from *Enterococcus faecalis* with N5-(phosphonoacetyl)-L-ornithine  
Authors : Polo, L.M.; Gil-Ortiz, F.; Rubio, V.  
Deposited on : 2011-11-21  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

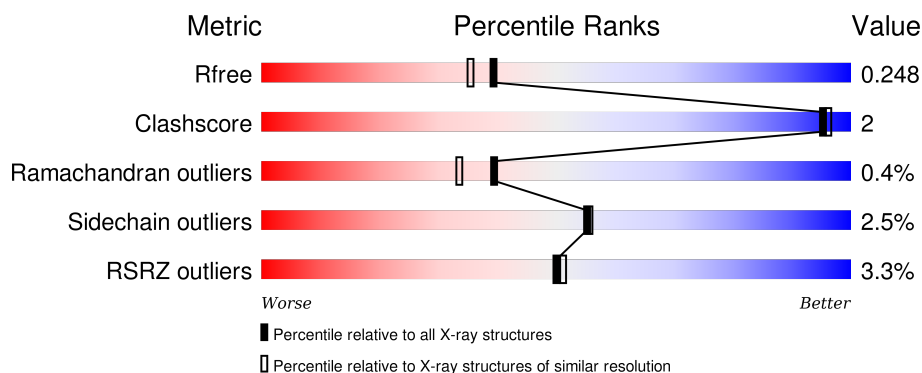
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	355	<div> <div>6%</div> <div>89% 6% • 5%</div> </div>
1	B	355	<div> <div>6%</div> <div>90% 5% 5%</div> </div>
1	C	355	<div> <div>6%</div> <div>88% 6% • 5%</div> </div>
1	D	355	<div> <div>6%</div> <div>89% 5% 6%</div> </div>
1	E	355	<div> <div>6%</div> <div>89% 5% 6%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	355	<div><div></div><div>4%</div><div>85%</div><div>6%</div><div>9%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16128 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 PUTRESCINE CARBAMOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2628	1656	440	510	22			
1	B	338	Total	C	N	O	S	0	0	0
			2627	1653	441	511	22			
1	C	339	Total	C	N	O	S	0	0	0
			2640	1661	441	517	21			
1	D	334	Total	C	N	O	S	0	0	0
			2553	1605	430	497	21			
1	E	333	Total	C	N	O	S	0	0	0
			2551	1608	428	494	21			
1	F	323	Total	C	N	O	S	0	0	0
			2480	1560	415	483	22			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	SER	-	EXPRESSION TAG	UNP Q837U7
A	341	ALA	-	EXPRESSION TAG	UNP Q837U7
A	342	ALA	-	EXPRESSION TAG	UNP Q837U7
A	343	LYS	-	EXPRESSION TAG	UNP Q837U7
A	344	LEU	-	EXPRESSION TAG	UNP Q837U7
A	345	ALA	-	EXPRESSION TAG	UNP Q837U7
A	346	ALA	-	EXPRESSION TAG	UNP Q837U7
A	347	ALA	-	EXPRESSION TAG	UNP Q837U7
A	348	LEU	-	EXPRESSION TAG	UNP Q837U7
A	349	GLU	-	EXPRESSION TAG	UNP Q837U7
A	350	HIS	-	EXPRESSION TAG	UNP Q837U7
A	351	HIS	-	EXPRESSION TAG	UNP Q837U7
A	352	HIS	-	EXPRESSION TAG	UNP Q837U7
A	353	HIS	-	EXPRESSION TAG	UNP Q837U7
A	354	HIS	-	EXPRESSION TAG	UNP Q837U7
A	355	HIS	-	EXPRESSION TAG	UNP Q837U7
B	340	SER	-	EXPRESSION TAG	UNP Q837U7

*Continued on next page...*

*Continued from previous page...*

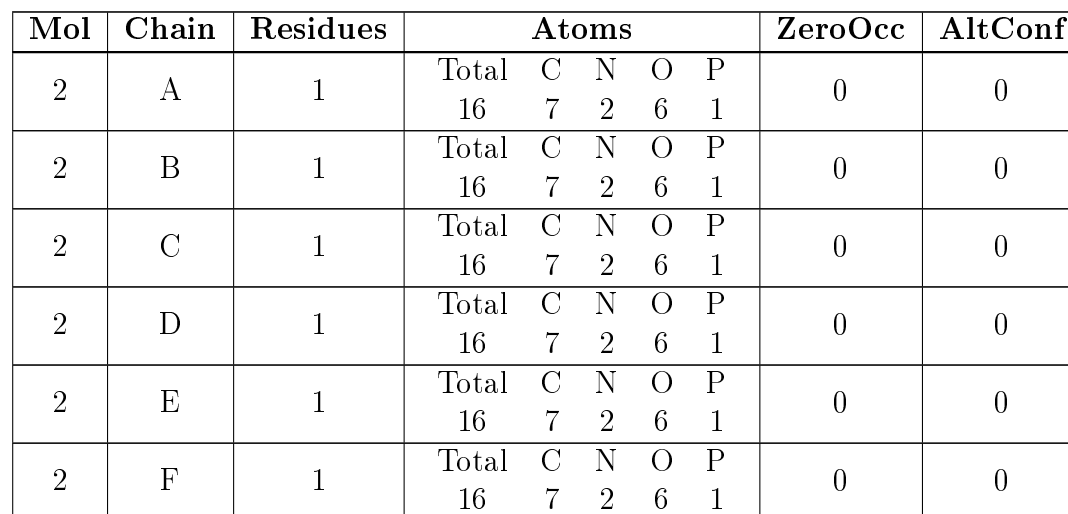
Chain	Residue	Modelled	Actual	Comment	Reference
B	341	ALA	-	EXPRESSION TAG	UNP Q837U7
B	342	ALA	-	EXPRESSION TAG	UNP Q837U7
B	343	LYS	-	EXPRESSION TAG	UNP Q837U7
B	344	LEU	-	EXPRESSION TAG	UNP Q837U7
B	345	ALA	-	EXPRESSION TAG	UNP Q837U7
B	346	ALA	-	EXPRESSION TAG	UNP Q837U7
B	347	ALA	-	EXPRESSION TAG	UNP Q837U7
B	348	LEU	-	EXPRESSION TAG	UNP Q837U7
B	349	GLU	-	EXPRESSION TAG	UNP Q837U7
B	350	HIS	-	EXPRESSION TAG	UNP Q837U7
B	351	HIS	-	EXPRESSION TAG	UNP Q837U7
B	352	HIS	-	EXPRESSION TAG	UNP Q837U7
B	353	HIS	-	EXPRESSION TAG	UNP Q837U7
B	354	HIS	-	EXPRESSION TAG	UNP Q837U7
B	355	HIS	-	EXPRESSION TAG	UNP Q837U7
C	340	SER	-	EXPRESSION TAG	UNP Q837U7
C	341	ALA	-	EXPRESSION TAG	UNP Q837U7
C	342	ALA	-	EXPRESSION TAG	UNP Q837U7
C	343	LYS	-	EXPRESSION TAG	UNP Q837U7
C	344	LEU	-	EXPRESSION TAG	UNP Q837U7
C	345	ALA	-	EXPRESSION TAG	UNP Q837U7
C	346	ALA	-	EXPRESSION TAG	UNP Q837U7
C	347	ALA	-	EXPRESSION TAG	UNP Q837U7
C	348	LEU	-	EXPRESSION TAG	UNP Q837U7
C	349	GLU	-	EXPRESSION TAG	UNP Q837U7
C	350	HIS	-	EXPRESSION TAG	UNP Q837U7
C	351	HIS	-	EXPRESSION TAG	UNP Q837U7
C	352	HIS	-	EXPRESSION TAG	UNP Q837U7
C	353	HIS	-	EXPRESSION TAG	UNP Q837U7
C	354	HIS	-	EXPRESSION TAG	UNP Q837U7
C	355	HIS	-	EXPRESSION TAG	UNP Q837U7
D	340	SER	-	EXPRESSION TAG	UNP Q837U7
D	341	ALA	-	EXPRESSION TAG	UNP Q837U7
D	342	ALA	-	EXPRESSION TAG	UNP Q837U7
D	343	LYS	-	EXPRESSION TAG	UNP Q837U7
D	344	LEU	-	EXPRESSION TAG	UNP Q837U7
D	345	ALA	-	EXPRESSION TAG	UNP Q837U7
D	346	ALA	-	EXPRESSION TAG	UNP Q837U7
D	347	ALA	-	EXPRESSION TAG	UNP Q837U7
D	348	LEU	-	EXPRESSION TAG	UNP Q837U7
D	349	GLU	-	EXPRESSION TAG	UNP Q837U7
D	350	HIS	-	EXPRESSION TAG	UNP Q837U7

*Continued on next page...*

*Continued from previous page...*

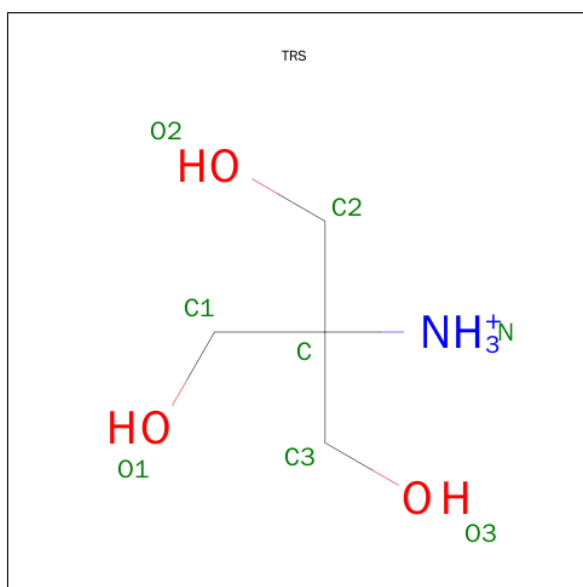
Chain	Residue	Modelled	Actual	Comment	Reference
D	351	HIS	-	EXPRESSION TAG	UNP Q837U7
D	352	HIS	-	EXPRESSION TAG	UNP Q837U7
D	353	HIS	-	EXPRESSION TAG	UNP Q837U7
D	354	HIS	-	EXPRESSION TAG	UNP Q837U7
D	355	HIS	-	EXPRESSION TAG	UNP Q837U7
E	340	SER	-	EXPRESSION TAG	UNP Q837U7
E	341	ALA	-	EXPRESSION TAG	UNP Q837U7
E	342	ALA	-	EXPRESSION TAG	UNP Q837U7
E	343	LYS	-	EXPRESSION TAG	UNP Q837U7
E	344	LEU	-	EXPRESSION TAG	UNP Q837U7
E	345	ALA	-	EXPRESSION TAG	UNP Q837U7
E	346	ALA	-	EXPRESSION TAG	UNP Q837U7
E	347	ALA	-	EXPRESSION TAG	UNP Q837U7
E	348	LEU	-	EXPRESSION TAG	UNP Q837U7
E	349	GLU	-	EXPRESSION TAG	UNP Q837U7
E	350	HIS	-	EXPRESSION TAG	UNP Q837U7
E	351	HIS	-	EXPRESSION TAG	UNP Q837U7
E	352	HIS	-	EXPRESSION TAG	UNP Q837U7
E	353	HIS	-	EXPRESSION TAG	UNP Q837U7
E	354	HIS	-	EXPRESSION TAG	UNP Q837U7
E	355	HIS	-	EXPRESSION TAG	UNP Q837U7
F	340	SER	-	EXPRESSION TAG	UNP Q837U7
F	341	ALA	-	EXPRESSION TAG	UNP Q837U7
F	342	ALA	-	EXPRESSION TAG	UNP Q837U7
F	343	LYS	-	EXPRESSION TAG	UNP Q837U7
F	344	LEU	-	EXPRESSION TAG	UNP Q837U7
F	345	ALA	-	EXPRESSION TAG	UNP Q837U7
F	346	ALA	-	EXPRESSION TAG	UNP Q837U7
F	347	ALA	-	EXPRESSION TAG	UNP Q837U7
F	348	LEU	-	EXPRESSION TAG	UNP Q837U7
F	349	GLU	-	EXPRESSION TAG	UNP Q837U7
F	350	HIS	-	EXPRESSION TAG	UNP Q837U7
F	351	HIS	-	EXPRESSION TAG	UNP Q837U7
F	352	HIS	-	EXPRESSION TAG	UNP Q837U7
F	353	HIS	-	EXPRESSION TAG	UNP Q837U7
F	354	HIS	-	EXPRESSION TAG	UNP Q837U7
F	355	HIS	-	EXPRESSION TAG	UNP Q837U7

- Molecule 2 is N-(PHOSPHONOACETYL)-L-ORNITHINE (three-letter code: PAO) (formula: C<sub>7</sub>H<sub>15</sub>N<sub>2</sub>O<sub>6</sub>P).



- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | A     | 1        | Total Ni<br>1 1 | 0       | 0       |
| 3   | D     | 1        | Total Ni<br>1 1 | 0       | 0       |

- 



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is water.

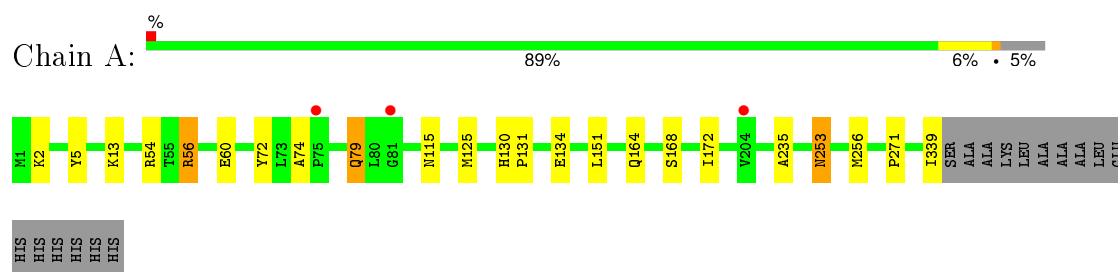
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total	O	0	0
			130	130		
5	B	113	Total	O	0	0
			113	113		
5	C	91	Total	O	0	0
			91	91		
5	D	102	Total	O	0	0
			102	102		
5	E	50	Total	O	0	0
			50	50		
5	F	49	Total	O	0	0
			49	49		



### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: PUTRESCINE CARBAMOYLTRANSFERASE



Chain E:

Position	Amino Acid	Information Content (bits)
1	Met	0.15
2	Val	0.05
3	Asp	0.15
4	Asp	0.15
5	Asp	0.15
6	Asp	0.15
7	Asp	0.15
8	Asp	0.15
9	Asp	0.15
10	Asp	0.15
11	Asp	0.15
12	Asp	0.15
13	Asp	0.15
14	Asp	0.15
15	Asp	0.15
16	Asp	0.15
17	Asp	0.15
18	Asp	0.15
19	Asp	0.15
20	Asp	0.15
21	Asp	0.15
22	Asp	0.15
23	Asp	0.15
24	Asp	0.15
25	Asp	0.15

Chain F:

85% 4% 6% 9%

TYR  
GLU  
ALA  
GLU  
LEU  
S238  
E239  
E240  
E241  
K244  
Y247  
P248  
N253  
A262  
N263  
E277  
I339  
SER  
ALA  
ALA  
LYS  
LEU  
ALA  
ALA  
ALA  
GLU  
GLU  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

M1  
K2  
Y5  
Q49  
R66  
A74  
PRO  
GLY  
GLN  
ILE  
GLN  
LEU  
GLY  
GLY  
HIS  
E84  
L93  
L100  
M101  
A102  
E105  
I110  
G124  
M125  
H130  
P131  
V157  
F158  
V159  
S168  
K175  
F180  
V181  
G187  
E192  
F209  
Y225  
W229  
Y230  
GLY  
LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.52Å 81.71Å 82.28Å 105.43° 102.80° 100.75°	Depositor
Resolution (Å)	25.00 – 2.00 24.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.6 (25.00-2.00) 75.5 (24.82-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.196 , 0.237 0.207 , 0.248	Depositor DCC
$R_{free}$ test set	5541 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.9	EDS
Estimated twinning fraction	0.019 for -h,-l,-k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 109164 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16128	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 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NI, TRS, PAO

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	0.41	0/2676	0.53	1/3619 (0.0%)
1	B	0.41	0/2673	0.52	0/3611
1	C	0.41	0/2688	0.51	0/3635
1	D	0.39	0/2598	0.50	0/3517
1	E	0.38	0/2597	0.49	0/3518
1	F	0.38	0/2523	0.48	0/3416
All	All	0.40	0/15755	0.51	1/21316 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	LEU	CA-CB-CG	5.01	126.82	115.30

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	2628	0	2536	11	0
1	B	2627	0	2545	9	0
1	C	2640	0	2545	14	0
1	D	2553	0	2417	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2551	0	2426	7	0
1	F	2480	0	2352	10	0
2	A	16	0	12	0	0
2	B	16	0	12	0	0
2	C	16	0	12	0	0
2	D	16	0	12	0	0
2	E	16	0	12	0	0
2	F	16	0	12	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	B	8	0	12	0	0
4	C	8	0	12	0	0
5	A	130	0	0	0	0
5	B	113	0	0	0	0
5	C	91	0	0	0	0
5	D	102	0	0	1	0
5	E	50	0	0	0	0
5	F	49	0	0	1	0
All	All	16128	0	14917	50	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 2.

The worst 5 of 50 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:79:GLN:HG3	1:C:271:PRO:HG3	1.65	0.77
1:A:72:TYR:CE2	1:A:74:ALA:HB2	2.28	0.68
1:D:339:ILE:HG12	1:E:15:GLU:HG2	1.81	0.62
1:A:79:GLN:NE2	1:C:53:THR:OG1	2.36	0.59
1:B:15:GLU:HG2	1:C:339:ILE:HG12	1.83	0.58

There are no symmetry-related clashes.

## 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	337/355 (95%)	329 (98%)	7 (2%)	1 (0%)	46	41
1	B	334/355 (94%)	325 (97%)	8 (2%)	1 (0%)	46	41
1	C	337/355 (95%)	329 (98%)	6 (2%)	2 (1%)	30	22
1	D	328/355 (92%)	323 (98%)	4 (1%)	1 (0%)	46	41
1	E	329/355 (93%)	321 (98%)	7 (2%)	1 (0%)	46	41
1	F	317/355 (89%)	311 (98%)	5 (2%)	1 (0%)	46	41
All	All	1982/2130 (93%)	1938 (98%)	37 (2%)	7 (0%)	39	33

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	MET
1	B	125	MET
1	C	125	MET
1	D	125	MET
1	E	125	MET

### 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	282/307 (92%)	272 (96%)	10 (4%)	43	40
1	B	284/307 (92%)	277 (98%)	7 (2%)	55	55
1	C	285/307 (93%)	278 (98%)	7 (2%)	55	55
1	D	268/307 (87%)	261 (97%)	7 (3%)	54	54
1	E	268/307 (87%)	262 (98%)	6 (2%)	60	62
1	F	263/307 (86%)	258 (98%)	5 (2%)	65	67
All	All	1650/1842 (90%)	1608 (98%)	42 (2%)	55	55

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	56	ARG
1	C	337	GLN
1	F	56	ARG
1	C	79	GLN
1	C	186	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	201	ASN
1	D	115	ASN
1	F	189	GLN
1	C	253	ASN
1	D	41	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PAO	A	1340	-	12,15,15	1.75	3 (25%)	14,20,20	1.40	2 (14%)
2	PAO	B	1340	-	12,15,15	1.93	3 (25%)	14,20,20	1.47	2 (14%)
4	TRS	B	1341	-	7,7,7	1.01	1 (14%)	9,9,9	0.83	0
2	PAO	C	1340	-	12,15,15	1.86	3 (25%)	14,20,20	1.47	4 (28%)
4	TRS	C	1341	-	7,7,7	1.06	1 (14%)	9,9,9	0.78	0
2	PAO	D	1340	-	12,15,15	1.84	3 (25%)	14,20,20	1.39	2 (14%)
2	PAO	E	1338	-	12,15,15	1.65	3 (25%)	14,20,20	1.38	1 (7%)
2	PAO	F	1340	-	12,15,15	1.94	3 (25%)	14,20,20	1.54	1 (7%)

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	PAO	A	1340	-	-	0/12/16/16	0/0/0/0
2	PAO	B	1340	-	-	0/12/16/16	0/0/0/0
4	TRS	B	1341	-	-	0/9/9/9	0/0/0/0
2	PAO	C	1340	-	-	0/12/16/16	0/0/0/0
4	TRS	C	1341	-	-	0/9/9/9	0/0/0/0
2	PAO	D	1340	-	-	0/12/16/16	0/0/0/0
2	PAO	E	1338	-	-	0/12/16/16	0/0/0/0
2	PAO	F	1340	-	-	0/12/16/16	0/0/0/0

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1340	PAO	P-O3P	-2.63	1.48	1.54
2	D	1340	PAO	P-O3P	-2.58	1.48	1.54
2	F	1340	PAO	P-O3P	-2.50	1.48	1.54
4	C	1341	TRS	C-N	-2.50	1.47	1.50
2	E	1338	PAO	P-O3P	-2.44	1.49	1.54

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1340	PAO	P-C1P-C1	-2.57	108.14	114.41
2	D	1340	PAO	O2P-P-O1P	-2.57	105.83	112.40
2	C	1340	PAO	P-C1P-C1	-2.32	108.74	114.41
2	A	1340	PAO	O2P-P-O1P	-2.28	106.57	112.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1340	PAO	O1P-P-C1P	-2.11	105.72	110.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	339/355 (95%)	-0.26	3 (0%) 85 86	17, 28, 45, 63	5 (1%)
1	B	338/355 (95%)	-0.22	5 (1%) 76 77	18, 27, 48, 62	4 (1%)
1	C	339/355 (95%)	-0.17	4 (1%) 81 81	17, 29, 49, 93	2 (0%)
1	D	334/355 (94%)	0.06	20 (5%) 25 27	19, 33, 57, 68	2 (0%)
1	E	333/355 (93%)	0.14	20 (6%) 25 27	19, 38, 61, 72	1 (0%)
1	F	323/355 (90%)	0.08	14 (4%) 39 40	19, 37, 58, 77	1 (0%)
All	All	2006/2130 (94%)	-0.07	66 (3%) 50 51	17, 31, 57, 93	15 (0%)

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	4.1
1	D	157	VAL	3.6
1	E	235	ALA	3.4
1	D	158	PHE	3.3
1	C	81	GLY	3.2

### 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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	TRS	C	1341	8/8	0.87	0.13	0.46	39,40,40,40	0
4	TRS	B	1341	8/8	0.91	0.12	0.43	37,37,37,38	0
2	PAO	A	1340	16/16	0.96	0.12	0.28	23,26,32,32	0
2	PAO	B	1340	16/16	0.97	0.12	-0.24	23,26,27,27	0
2	PAO	D	1340	16/16	0.96	0.10	-0.43	28,30,35,35	0
2	PAO	F	1340	16/16	0.94	0.10	-0.55	30,35,36,36	0
2	PAO	C	1340	16/16	0.98	0.11	-0.57	22,27,29,29	0
2	PAO	E	1338	16/16	0.97	0.09	-0.80	30,33,35,35	0
3	NI	A	1341	1/1	1.00	0.04	-1.69	34,34,34,34	0
3	NI	D	1341	1/1	0.98	0.06	-2.11	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.