



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:05 AM GMT

PDB ID : 2FG6  
Title : N-succinyl-L-ornithine transcarbamylase from *B. fragilis* complexed with sulfate and N-succinyl-L-norvaline  
Authors : Shi, D.; Yu, X.; Malamy, M.H.; Allewell, N.M.; Mendel, T.  
Deposited on : 2005-12-21  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
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

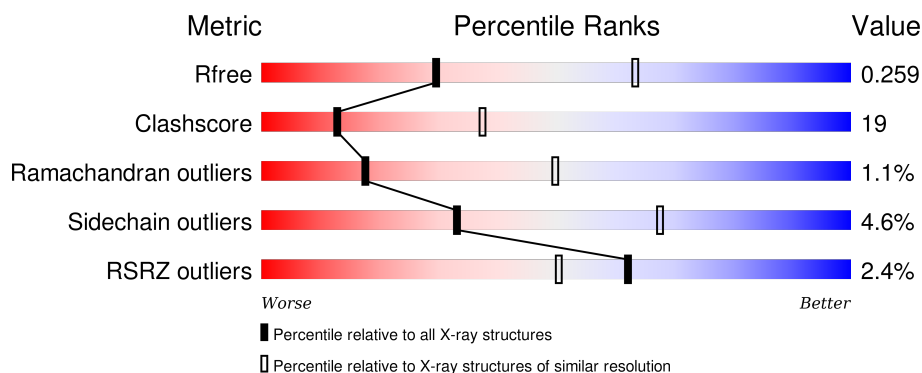
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	C	338	<div> <div>4%</div> <div>55%</div> <div>37%</div> <div>• 5%</div> </div>
1	D	338	<div> <div>4%</div> <div>54%</div> <div>38%</div> <div>• 5%</div> </div>
1	E	338	<div> <div>2%</div> <div>57%</div> <div>36%</div> <div>• 5%</div> </div>
1	X	338	<div> <div>%</div> <div>59%</div> <div>34%</div> <div>• 5%</div> </div>
1	Y	338	<div> <div>62%</div> <div>31%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	Z	338	<div><div><div>%</div><div><div></div><div>59%</div><div>35%</div><div>• 5%</div></div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15978 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
1	X	322	Total	C	N	O	S	0	0	0
			2593	1651	448	478	16			
1	Y	322	Total	C	N	O	S	0	0	0
			2593	1651	448	478	16			
1	Z	320	Total	C	N	O	S	0	0	0
			2578	1643	443	476	16			
1	C	321	Total	C	N	O	S	0	0	0
			2582	1645	444	477	16			
1	D	322	Total	C	N	O	S	0	0	0
			2593	1651	448	478	16			
1	E	322	Total	C	N	O	S	0	0	0
			2593	1651	448	478	16			

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

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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	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	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

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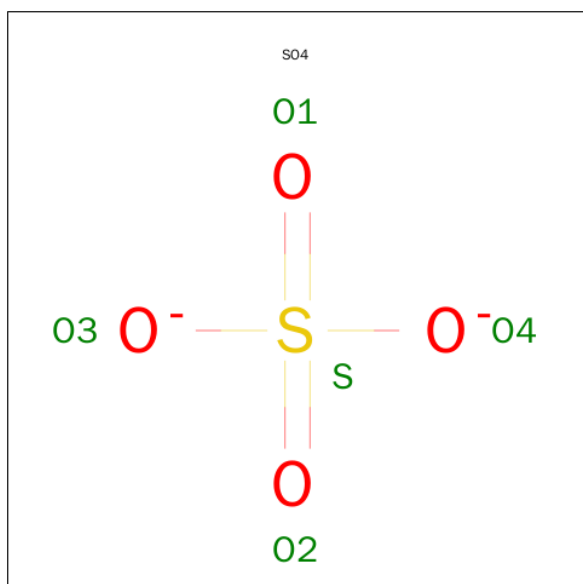
Chain	Residue	Modelled	Actual	Comment	Reference
Z	-2	GLY	-	EXPRESSION TAG	UNP Q5LI27
Z	-1	SER	-	EXPRESSION TAG	UNP Q5LI27
Z	0	HIS	-	EXPRESSION TAG	UNP Q5LI27
Z	242	LEU	THR	ENGINEERED	UNP Q5LI27
C	-19	MET	-	EXPRESSION TAG	UNP Q5LI27
C	-18	GLY	-	EXPRESSION TAG	UNP Q5LI27
C	-17	SER	-	EXPRESSION TAG	UNP 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	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

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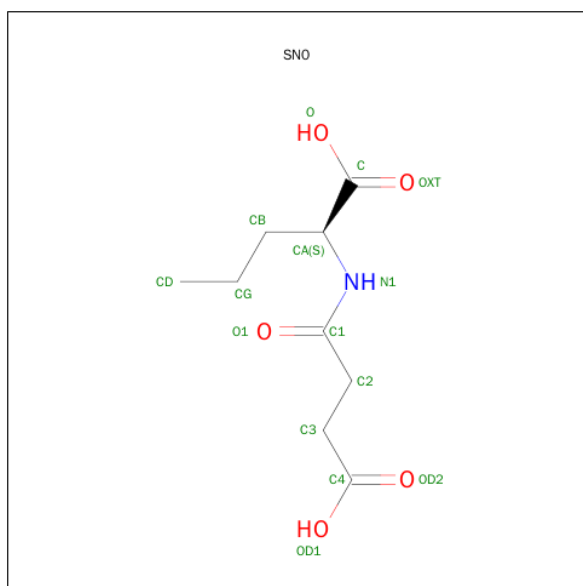
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	EXPRESSION TAG	UNP Q5LI27
D	-1	SER	-	EXPRESSION TAG	UNP Q5LI27
D	0	HIS	-	EXPRESSION TAG	UNP Q5LI27
D	242	LEU	THR	ENGINEERED	UNP Q5LI27
E	-19	MET	-	EXPRESSION TAG	UNP Q5LI27
E	-18	GLY	-	EXPRESSION TAG	UNP Q5LI27
E	-17	SER	-	EXPRESSION TAG	UNP 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	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	Y	1	Total O S 5 4 1	0	0
2	Z	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
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

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

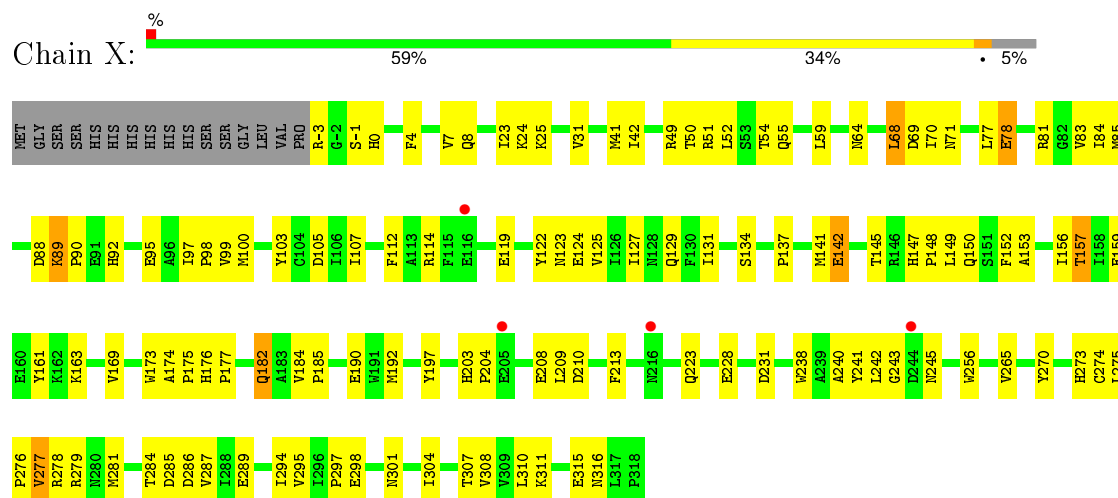
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	27	Total	O	0	0
			27	27		
4	D	25	Total	O	0	0
			25	25		
4	E	38	Total	O	0	0
			38	38		
4	X	62	Total	O	0	0
			62	62		
4	Y	109	Total	O	0	0
			109	109		
4	Z	55	Total	O	0	0
			55	55		

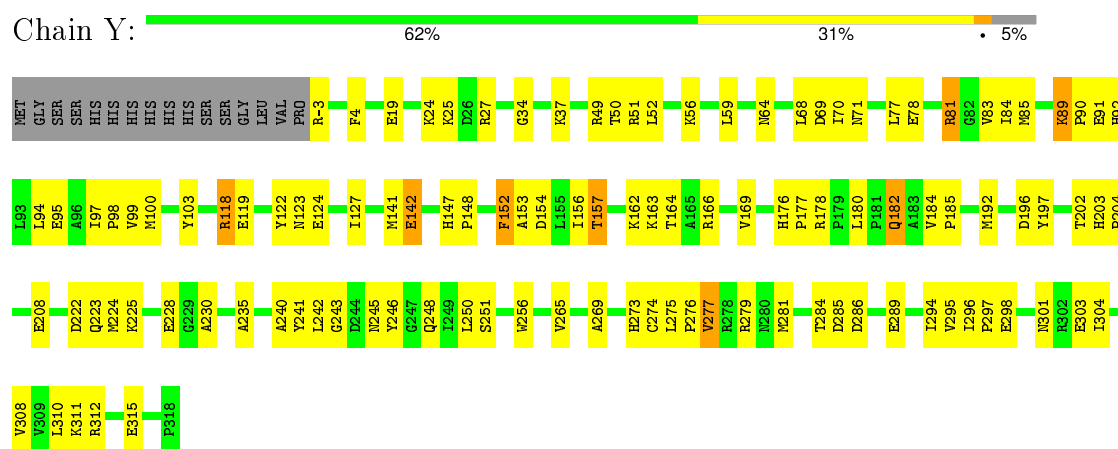
### 3 Residue-property plots

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.

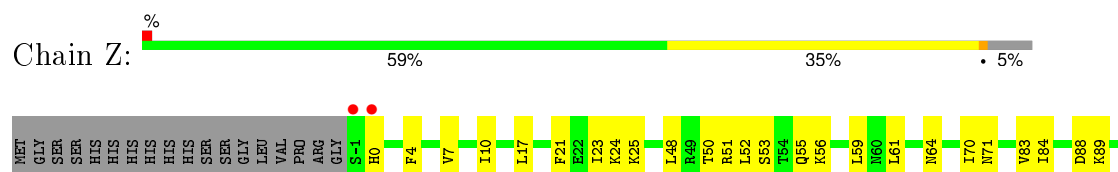
- Molecule 1: putative ornithine carbamoyltransferase



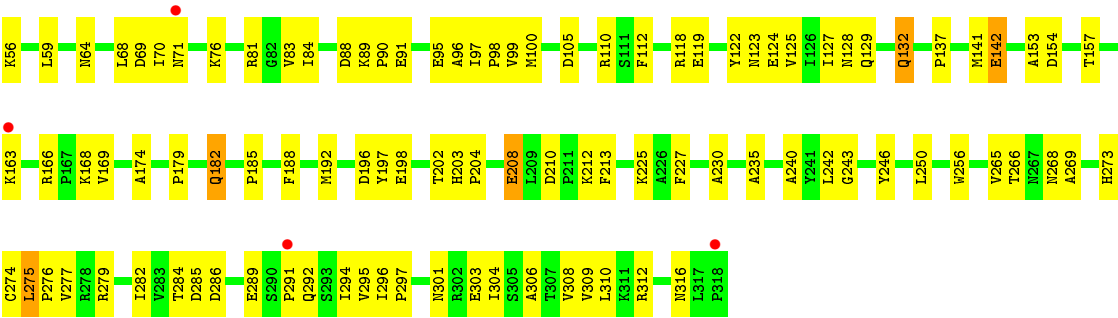
- Molecule 1: putative ornithine carbamoyltransferase



- Molecule 1: putative ornithine carbamoyltransferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.70Å 155.70Å 120.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.99-2.80) 99.6 (19.98-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.216 , 0.260 0.216 , 0.259	Depositor DCC
$R_{free}$ test set	3585 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.1	EDS
Estimated twinning fraction	0.012 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 70401 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: SO4, SN0

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	0.34	0/2642	0.60	0/3579
1	D	0.36	0/2653	0.61	0/3593
1	E	0.38	0/2653	0.63	0/3593
1	X	0.39	0/2653	0.65	0/3593
1	Y	0.42	0/2653	0.68	1/3593 (0.0%)
1	Z	0.40	0/2638	0.66	0/3574
All	All	0.38	0/15892	0.64	1/21525 (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	Y	68	LEU	CA-CB-CG	5.31	127.51	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	C	2582	0	2551	118	0
1	D	2593	0	2564	115	0
1	E	2593	0	2564	107	0
1	X	2593	0	2564	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	2593	0	2564	96	0
1	Z	2578	0	2548	93	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	X	10	0	0	0	0
2	Y	5	0	0	0	0
2	Z	5	0	0	0	0
3	C	15	0	13	2	0
3	D	15	0	13	1	0
3	E	15	0	13	2	0
3	X	15	0	13	0	0
3	Y	15	0	13	1	0
3	Z	15	0	13	0	0
4	C	27	0	0	4	0
4	D	25	0	0	8	0
4	E	38	0	0	4	0
4	X	62	0	0	5	0
4	Y	109	0	0	1	0
4	Z	55	0	0	4	0
All	All	15978	0	15433	597	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 19.

All (597) 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:Z:169:VAL:HG11	1:Z:192:MET:HE2	1.45	0.98
1:Y:153:ALA:O	1:Y:157:THR:HG22	1.67	0.94
1:X:24:LYS:HZ3	1:X:301:ASN:HD21	1.14	0.92
1:X:24:LYS:NZ	1:X:301:ASN:HD21	1.68	0.90
1:X:153:ALA:O	1:X:157:THR:HG22	1.72	0.89
1:D:153:ALA:O	1:D:157:THR:HG22	1.74	0.88
1:C:0:HIS:HA	1:C:316:ASN:ND2	1.90	0.86
1:C:97:ILE:HB	1:C:98:PRO:HD3	1.56	0.86
1:E:153:ALA:O	1:E:157:THR:HG22	1.77	0.84
1:Z:153:ALA:O	1:Z:157:THR:HG22	1.77	0.83
1:X:24:LYS:HG2	1:X:304:ILE:HG12	1.61	0.82
1:Y:24:LYS:NZ	1:Y:301:ASN:HD21	1.79	0.80
1:X:0:HIS:HA	1:X:316:ASN:ND2	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:MET:HE3	1:E:54:THR:HB	1.63	0.80
1:Y:24:LYS:HG2	1:Y:304:ILE:HG12	1.64	0.80
1:C:169:VAL:HG11	1:C:192:MET:HE2	1.64	0.80
1:C:119:GLU:HG2	1:C:123:ASN:HD21	1.47	0.79
1:Z:0:HIS:HA	1:Z:316:ASN:ND2	1.97	0.79
1:C:96:ALA:O	1:C:100:MET:HG3	1.83	0.78
1:D:169:VAL:HG11	1:D:192:MET:HE2	1.65	0.78
1:D:0:HIS:HA	1:D:316:ASN:ND2	1.98	0.78
1:C:119:GLU:HG2	1:C:123:ASN:ND2	1.98	0.78
1:X:311:LYS:O	1:X:315:GLU:HG3	1.84	0.78
1:Z:50:THR:HG21	1:Z:141:MET:HB3	1.64	0.78
1:D:124:GLU:HB3	1:D:127:ILE:CG2	2.15	0.77
1:D:24:LYS:HG2	1:D:304:ILE:HG12	1.66	0.77
1:Y:169:VAL:HG11	1:Y:192:MET:HE2	1.67	0.76
1:Z:24:LYS:NZ	1:Z:301:ASN:HD21	1.83	0.76
1:C:41:MET:HE3	1:C:54:THR:HB	1.68	0.75
1:X:284:THR:HG22	1:X:286:ASP:H	1.52	0.75
1:Y:24:LYS:HZ3	1:Y:301:ASN:HD21	1.30	0.75
1:C:284:THR:HG22	1:C:286:ASP:H	1.51	0.75
1:C:153:ALA:O	1:C:157:THR:HG22	1.87	0.75
1:E:0:HIS:HA	1:E:316:ASN:ND2	2.01	0.74
1:D:0:HIS:HA	1:D:316:ASN:HD22	1.52	0.74
1:D:97:ILE:HB	1:D:98:PRO:HD3	1.70	0.73
1:E:35:ARG:HG2	1:E:36:ASN:HD22	1.54	0.72
1:X:95:GLU:O	1:X:98:PRO:HD2	1.89	0.72
1:C:124:GLU:HB3	1:C:127:ILE:CG2	2.20	0.72
1:E:273:HIS:ND1	1:E:277:VAL:HG22	2.04	0.72
1:E:124:GLU:HB3	1:E:127:ILE:CG2	2.20	0.72
1:Y:284:THR:HG22	1:Y:286:ASP:H	1.53	0.72
1:E:294:ILE:C	1:E:297:PRO:HD2	2.11	0.70
1:E:169:VAL:HG11	1:E:192:MET:HE2	1.71	0.70
1:Y:124:GLU:HB3	1:Y:127:ILE:CG2	2.20	0.70
1:D:204:PRO:HG3	1:D:256:TRP:CE2	2.27	0.70
1:Y:284:THR:HG22	1:Y:286:ASP:N	2.07	0.69
1:X:122:TYR:OH	1:X:182:GLN:HG3	1.92	0.69
1:D:176:HIS:CD2	1:D:180:LEU:HD11	2.27	0.69
1:Z:169:VAL:HG11	1:Z:192:MET:CE	2.22	0.69
1:D:184:VAL:HB	1:D:185:PRO:HD3	1.76	0.68
1:X:-3:ARG:NH1	1:X:8:GLN:HB3	2.08	0.68
1:E:95:GLU:O	1:E:99:VAL:HG23	1.94	0.68
1:D:91:GLU:HG3	4:D:368:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:274:CYS:O	1:X:275:LEU:HB2	1.93	0.67
1:C:50:THR:HG21	1:C:141:MET:HB3	1.76	0.67
1:C:49:ARG:HH21	1:C:276:PRO:HG3	1.59	0.67
1:Z:311:LYS:O	1:Z:315:GLU:HG3	1.95	0.67
1:C:59:LEU:HD13	1:E:64:ASN:HB3	1.77	0.67
1:Y:192:MET:HE3	1:Y:197:TYR:HD1	1.60	0.66
1:C:24:LYS:HG2	1:C:304:ILE:HG12	1.76	0.66
1:Z:24:LYS:HG2	1:Z:304:ILE:HG12	1.76	0.66
1:X:124:GLU:HB3	1:X:127:ILE:CG2	2.26	0.66
1:X:285:ASP:O	1:X:289:GLU:HG3	1.95	0.66
1:E:-3:ARG:HH11	1:E:-3:ARG:HB3	1.60	0.65
1:C:61:LEU:HD13	1:C:314:LEU:HD12	1.79	0.65
1:Y:122:TYR:OH	1:Y:182:GLN:HG3	1.95	0.64
1:Z:24:LYS:HZ2	1:Z:301:ASN:HD21	1.44	0.64
1:Y:285:ASP:O	1:Y:289:GLU:HG3	1.96	0.64
1:Y:311:LYS:O	1:Y:315:GLU:HG3	1.97	0.64
1:Z:119:GLU:HG2	1:Z:123:ASN:ND2	2.13	0.64
1:D:208:GLU:CG	1:D:242:LEU:HD11	2.28	0.63
1:Z:70:ILE:O	1:Z:71:ASN:HB2	1.99	0.63
1:X:169:VAL:HG11	1:X:192:MET:HE2	1.80	0.63
1:X:24:LYS:NZ	1:X:301:ASN:ND2	2.45	0.63
1:Y:204:PRO:HG3	1:Y:256:TRP:CE2	2.34	0.63
1:E:24:LYS:HG2	1:E:304:ILE:HG12	1.81	0.63
1:E:279:ARG:HD3	1:E:285:ASP:OD2	1.97	0.62
1:Y:70:ILE:O	1:Y:71:ASN:HB2	1.99	0.62
1:Y:228:GLU:HA	1:Y:265:VAL:HG12	1.81	0.62
1:Y:208:GLU:HG2	1:Y:242:LEU:HD11	1.80	0.62
1:X:265:VAL:O	1:X:265:VAL:HG12	2.00	0.62
1:E:291:PRO:HG2	1:E:292:GLN:NE2	2.14	0.62
1:Z:274:CYS:O	1:Z:275:LEU:HB2	1.99	0.62
1:D:245:ASN:O	1:D:248:GLN:HB2	1.99	0.62
1:Z:89:LYS:HD2	1:Z:89:LYS:N	2.15	0.62
1:D:95:GLU:O	1:D:98:PRO:HD2	1.99	0.62
1:Z:97:ILE:HB	1:Z:98:PRO:HD3	1.82	0.62
1:E:88:ASP:HB3	1:E:89:LYS:HD2	1.82	0.62
1:Y:70:ILE:HD13	1:Y:77:LEU:HD11	1.82	0.62
1:Z:284:THR:HG21	4:Z:383:HOH:O	2.00	0.62
1:D:125:VAL:O	1:D:129:GLN:HG3	2.00	0.61
1:Z:95:GLU:O	1:Z:98:PRO:HD2	2.01	0.61
1:D:311:LYS:O	1:D:315:GLU:HG3	2.01	0.61
1:Y:97:ILE:HB	1:Y:98:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ILE:O	1:E:71:ASN:HB2	2.01	0.61
1:D:142:GLU:OE1	3:D:353:SN0:HD3	2.01	0.61
1:C:34:GLY:O	1:C:37:LYS:HB2	2.00	0.61
1:E:97:ILE:HB	1:E:98:PRO:HD3	1.83	0.60
1:D:208:GLU:HG2	1:D:242:LEU:HD11	1.81	0.60
1:X:284:THR:HG22	1:X:286:ASP:N	2.15	0.60
1:Z:279:ARG:HD3	1:Z:285:ASP:OD2	2.01	0.60
1:Y:279:ARG:HD3	1:Y:285:ASP:OD2	2.01	0.60
1:E:291:PRO:HG2	1:E:292:GLN:HE22	1.66	0.60
1:E:89:LYS:N	1:E:89:LYS:HD2	2.17	0.60
1:E:56:LYS:NZ	1:E:303:GLU:OE2	2.33	0.60
1:C:95:GLU:O	1:C:99:VAL:HG23	2.02	0.60
1:D:70:ILE:O	1:D:71:ASN:HB2	2.02	0.59
1:E:35:ARG:HG2	1:E:36:ASN:ND2	2.17	0.59
1:Z:204:PRO:HG3	1:Z:256:TRP:CE2	2.36	0.59
1:D:51:ARG:NH2	1:D:69:ASP:OD2	2.35	0.59
1:D:61:LEU:HD13	1:D:314:LEU:HD12	1.83	0.59
1:D:279:ARG:HD3	1:D:285:ASP:OD2	2.02	0.59
1:C:176:HIS:CD2	1:C:180:LEU:HD11	2.37	0.59
1:D:51:ARG:O	1:D:55:GLN:HG3	2.02	0.59
1:D:304:ILE:O	1:D:308:VAL:HG23	2.04	0.58
1:X:192:MET:HE3	1:X:197:TYR:HD1	1.67	0.58
1:Y:49:ARG:NH2	1:Y:276:PRO:HG3	2.17	0.58
1:D:96:ALA:O	1:D:100:MET:HG3	2.03	0.58
1:E:124:GLU:HB3	1:E:127:ILE:HG22	1.86	0.58
1:Y:124:GLU:HB3	1:Y:127:ILE:HG22	1.85	0.58
1:X:41:MET:HE3	1:X:54:THR:HB	1.85	0.58
1:X:0:HIS:HA	1:X:316:ASN:HD21	1.68	0.58
1:Z:275:LEU:HD12	1:Z:277:VAL:CG2	2.34	0.58
1:C:279:ARG:HD3	1:C:285:ASP:OD2	2.04	0.58
1:Y:95:GLU:O	1:Y:98:PRO:HD2	2.03	0.58
1:E:294:ILE:O	1:E:297:PRO:HD2	2.03	0.58
1:C:284:THR:HG21	4:C:359:HOH:O	2.03	0.58
1:C:296:ILE:HB	1:C:297:PRO:HD3	1.86	0.57
1:X:284:THR:HB	1:X:287:VAL:HG23	1.85	0.57
1:C:70:ILE:O	1:C:71:ASN:HB2	2.05	0.57
1:E:19:GLU:O	1:E:23:ILE:HG13	2.04	0.57
1:Z:124:GLU:HB3	1:Z:127:ILE:CG2	2.34	0.57
1:D:169:VAL:HG11	1:D:192:MET:CE	2.33	0.57
1:E:284:THR:HG22	1:E:286:ASP:H	1.70	0.57
1:Y:176:HIS:CD2	1:Y:180:LEU:HD11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:208:GLU:CG	1:Y:242:LEU:HD11	2.34	0.57
1:C:7:VAL:O	1:C:10:ILE:HG22	2.04	0.57
1:E:96:ALA:O	1:E:100:MET:HG3	2.05	0.57
1:X:157:THR:HG21	1:X:298:GLU:HG3	1.86	0.57
1:D:64:ASN:HB3	1:E:59:LEU:HD13	1.86	0.57
1:Y:184:VAL:HB	1:Y:185:PRO:HD3	1.86	0.57
1:C:0:HIS:HA	1:C:316:ASN:HD22	1.64	0.56
1:Y:203:HIS:HD2	1:Y:204:PRO:O	1.88	0.56
1:Z:182:GLN:C	1:Z:185:PRO:HD2	2.25	0.56
1:X:70:ILE:HD11	1:X:100:MET:HE1	1.87	0.56
1:X:114:ARG:HD3	4:X:396:HOH:O	2.05	0.56
1:C:70:ILE:HD13	1:C:77:LEU:HD11	1.86	0.56
1:Z:305:SER:O	1:Z:309:VAL:HG23	2.06	0.56
1:Y:192:MET:CE	1:Y:197:TYR:HD1	2.19	0.56
1:E:203:HIS:HD2	1:E:204:PRO:O	1.88	0.56
1:X:4:PHE:CE2	1:X:148:PRO:HB2	2.39	0.56
1:C:241:TYR:CD2	1:C:242:LEU:HD23	2.41	0.55
1:X:192:MET:CE	1:X:197:TYR:HD1	2.19	0.55
1:D:50:THR:HG22	1:D:141:MET:HE2	1.87	0.55
1:C:184:VAL:HB	1:C:185:PRO:HD3	1.88	0.55
1:X:24:LYS:HZ3	1:X:301:ASN:ND2	1.94	0.55
1:C:47:SER:HB2	1:C:110:ARG:NH1	2.22	0.55
1:Z:285:ASP:O	1:Z:289:GLU:HG3	2.06	0.55
1:Z:267:ASN:O	4:Z:372:HOH:O	2.18	0.55
1:Y:24:LYS:NZ	1:Y:301:ASN:ND2	2.54	0.55
1:C:285:ASP:O	1:C:289:GLU:HG3	2.06	0.55
1:E:230:ALA:O	1:E:269:ALA:HB2	2.06	0.55
1:D:166:ARG:HG2	1:D:196:ASP:OD2	2.06	0.55
1:E:70:ILE:HG22	1:E:71:ASN:N	2.22	0.55
1:Z:161:TYR:HB3	1:Z:270:TYR:CE1	2.42	0.55
1:X:88:ASP:HB3	1:X:89:LYS:HD2	1.88	0.55
1:Z:176:HIS:CD2	1:Z:180:LEU:HD11	2.42	0.55
1:D:45:ASN:ND2	1:D:112:PHE:HB2	2.22	0.55
1:Y:274:CYS:O	1:Y:275:LEU:HB2	2.06	0.54
1:D:0:HIS:CA	1:D:316:ASN:ND2	2.69	0.54
1:D:50:THR:HG21	1:D:141:MET:HB3	1.88	0.54
1:X:182:GLN:C	1:X:185:PRO:HD2	2.28	0.54
1:Z:4:PHE:CE2	1:Z:148:PRO:HB2	2.42	0.54
1:E:182:GLN:C	1:E:185:PRO:HD2	2.28	0.54
1:Z:184:VAL:HB	1:Z:185:PRO:HD3	1.88	0.54
1:E:49:ARG:HH21	1:E:276:PRO:HG3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:ASP:O	1:E:137:PRO:HD2	2.07	0.54
1:D:305:SER:O	1:D:309:VAL:HG23	2.08	0.54
1:X:210:ASP:HA	1:X:241:TYR:CE2	2.43	0.54
1:Y:49:ARG:HH21	1:Y:276:PRO:HG3	1.71	0.54
1:E:-3:ARG:HH11	1:E:-3:ARG:CB	2.19	0.54
1:X:7:VAL:HG12	1:X:190:GLU:OE2	2.07	0.54
1:E:306:ALA:O	1:E:310:LEU:HB2	2.08	0.54
1:Y:119:GLU:HG2	1:Y:123:ASN:ND2	2.22	0.54
1:C:56:LYS:HE2	4:E:378:HOH:O	2.07	0.54
1:X:294:ILE:C	1:X:297:PRO:HD2	2.28	0.54
1:C:245:ASN:HB3	1:C:250:LEU:HD21	1.90	0.53
1:C:119:GLU:HB2	4:C:371:HOH:O	2.09	0.53
1:C:305:SER:O	1:C:309:VAL:HG23	2.08	0.53
1:X:97:ILE:HB	1:X:98:PRO:HD3	1.91	0.53
1:D:122:TYR:OH	1:D:182:GLN:HG3	2.08	0.53
1:C:230:ALA:O	1:C:269:ALA:HB2	2.09	0.53
1:D:189:ALA:HA	1:D:199:PHE:CE2	2.43	0.53
1:Y:154:ASP:O	1:Y:157:THR:HG23	2.09	0.53
1:X:51:ARG:O	1:X:55:GLN:HG3	2.08	0.53
1:D:161:TYR:HB3	1:D:270:TYR:CE1	2.44	0.53
1:D:242:LEU:HG	4:D:363:HOH:O	2.07	0.53
1:D:265:VAL:HG12	1:D:265:VAL:O	2.09	0.53
1:Y:50:THR:HG21	1:Y:141:MET:HB3	1.89	0.53
1:Z:0:HIS:HA	1:Z:316:ASN:HD22	1.74	0.53
1:D:24:LYS:CG	1:D:304:ILE:HG12	2.39	0.53
1:D:284:THR:HG21	4:D:355:HOH:O	2.09	0.53
1:C:120:TYR:O	1:C:125:VAL:HG23	2.08	0.53
1:D:93:LEU:HG	1:D:97:ILE:HD11	1.91	0.52
1:Y:27:ARG:HD2	1:Y:303:GLU:OE2	2.09	0.52
1:X:70:ILE:O	1:X:71:ASN:HB2	2.09	0.52
1:Y:275:LEU:HD11	1:Y:295:VAL:HG13	1.91	0.52
1:D:4:PHE:CE2	1:D:148:PRO:HB2	2.44	0.52
1:E:235:ALA:O	1:E:273:HIS:CD2	2.63	0.52
1:C:4:PHE:CD2	1:C:309:VAL:HG11	2.45	0.52
1:C:203:HIS:HD2	1:C:204:PRO:O	1.93	0.52
1:C:24:LYS:NZ	1:C:301:ASN:HD21	2.08	0.52
1:C:83:VAL:HG12	1:C:84:ILE:N	2.24	0.52
1:C:45:ASN:ND2	1:C:112:PHE:HB2	2.25	0.52
1:Y:24:LYS:HG2	1:Y:304:ILE:CG1	2.39	0.52
1:E:273:HIS:CE1	1:E:277:VAL:HG22	2.45	0.52
1:D:68:LEU:HD22	1:D:69:ASP:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:89:LYS:N	1:X:89:LYS:HD2	2.25	0.52
1:Y:273:HIS:O	1:Y:275:LEU:HD13	2.09	0.52
1:D:230:ALA:O	1:D:269:ALA:HB2	2.09	0.52
1:C:240:ALA:HB2	1:C:250:LEU:HG	1.92	0.52
1:E:188:PHE:O	1:E:192:MET:HG2	2.10	0.52
1:C:77:LEU:O	1:C:89:LYS:HG2	2.10	0.52
1:Z:83:VAL:HG12	1:Z:84:ILE:N	2.25	0.52
1:Z:228:GLU:HG2	4:Z:401:HOH:O	2.10	0.52
1:D:273:HIS:CD2	1:D:277:VAL:HG13	2.45	0.52
1:D:291:PRO:HG2	1:D:292:GLN:HE22	1.75	0.52
1:D:291:PRO:HG2	1:D:292:GLN:NE2	2.25	0.51
1:C:122:TYR:OH	1:C:182:GLN:HG3	2.10	0.51
1:C:189:ALA:HA	1:C:199:PHE:CE2	2.45	0.51
1:X:294:ILE:O	1:X:297:PRO:HD2	2.11	0.51
1:X:175:PRO:HG2	1:X:281:MET:O	2.10	0.51
1:E:210:ASP:HB3	1:E:213:PHE:HD1	1.74	0.51
1:C:51:ARG:O	1:C:55:GLN:HG3	2.11	0.51
1:D:90:PRO:HB3	3:E:355:SN0:C4	2.40	0.51
1:X:24:LYS:CG	1:X:304:ILE:HG12	2.37	0.51
1:C:284:THR:HG22	1:C:286:ASP:N	2.23	0.51
1:C:24:LYS:CG	1:C:304:ILE:HG12	2.40	0.51
1:D:41:MET:HE3	1:D:54:THR:HB	1.93	0.51
1:D:170:VAL:HG22	1:D:200:VAL:HB	1.91	0.51
1:E:208:GLU:HG2	1:E:242:LEU:HD11	1.93	0.51
1:D:98:PRO:HB3	1:E:296:ILE:HD13	1.93	0.51
1:C:274:CYS:O	1:C:275:LEU:HB2	2.11	0.51
1:Y:157:THR:HG21	1:Y:298:GLU:HG3	1.92	0.51
1:D:98:PRO:CB	1:E:296:ILE:HD13	2.41	0.51
1:Y:70:ILE:HD11	1:Y:100:MET:HE1	1.92	0.51
1:Z:124:GLU:OE1	1:Z:144:ALA:HB3	2.11	0.51
1:E:125:VAL:O	1:E:129:GLN:HG3	2.10	0.51
1:X:49:ARG:HH21	1:X:276:PRO:HG3	1.76	0.51
1:C:285:ASP:HB3	1:E:81:ARG:HH12	1.75	0.50
1:X:83:VAL:HG12	1:X:84:ILE:N	2.25	0.50
1:X:240:ALA:HB3	1:X:245:ASN:O	2.10	0.50
1:Y:308:VAL:O	1:Y:312:ARG:HG2	2.11	0.50
1:X:23:ILE:HD13	1:X:307:THR:HG22	1.91	0.50
1:X:122:TYR:HA	1:X:145:THR:HG21	1.93	0.50
1:Z:118:ARG:NH2	1:Z:243:GLY:N	2.60	0.50
1:C:210:ASP:HB3	1:C:213:PHE:HD1	1.75	0.50
1:C:105:ASP:O	1:C:137:PRO:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:112:PHE:HA	4:X:369:HOH:O	2.10	0.50
1:C:124:GLU:HB3	1:C:127:ILE:HG21	1.92	0.50
1:C:59:LEU:HD13	1:E:64:ASN:CB	2.41	0.50
1:Y:208:GLU:CD	1:Y:208:GLU:H	2.14	0.50
1:X:70:ILE:HD13	1:X:77:LEU:HD11	1.92	0.50
1:C:168:LYS:HA	1:C:198:GLU:HB3	1.94	0.50
1:C:49:ARG:HH22	1:E:91:GLU:CD	2.15	0.50
1:D:208:GLU:HG3	1:D:242:LEU:HD11	1.94	0.50
1:E:212:LYS:HE3	1:E:213:PHE:CE1	2.47	0.50
1:E:118:ARG:HG3	1:E:246:TYR:CD1	2.47	0.50
1:X:184:VAL:HB	1:X:185:PRO:HD3	1.92	0.50
1:X:68:LEU:HD22	1:X:69:ASP:N	2.27	0.50
1:C:51:ARG:HD3	1:E:68:LEU:HD23	1.94	0.50
1:C:169:VAL:HG11	1:C:192:MET:CE	2.38	0.50
1:C:284:THR:HG22	1:C:285:ASP:N	2.27	0.50
1:X:127:ILE:O	1:X:131:ILE:HG13	2.12	0.50
1:Y:70:ILE:O	1:Y:71:ASN:CB	2.60	0.50
1:D:208:GLU:HG2	1:D:242:LEU:CD1	2.41	0.49
1:X:209:LEU:HD21	1:X:238:TRP:CE2	2.47	0.49
1:Y:162:LYS:HD2	1:Y:164:THR:O	2.11	0.49
1:X:95:GLU:O	1:X:99:VAL:HG23	2.12	0.49
1:D:89:LYS:N	1:D:89:LYS:HD2	2.26	0.49
1:C:228:GLU:HG3	1:C:265:VAL:CG1	2.41	0.49
1:Y:81:ARG:HH12	1:Z:285:ASP:HB3	1.78	0.49
1:Z:153:ALA:O	1:Z:157:THR:CG2	2.56	0.49
1:X:279:ARG:HD3	1:X:285:ASP:OD2	2.13	0.49
1:C:70:ILE:O	1:C:71:ASN:CB	2.60	0.49
1:Y:240:ALA:HB3	1:Y:245:ASN:O	2.11	0.49
1:Z:284:THR:HG22	1:Z:285:ASP:N	2.28	0.49
1:E:308:VAL:O	1:E:312:ARG:HG2	2.13	0.49
1:Y:95:GLU:O	1:Y:99:VAL:HG23	2.12	0.49
1:D:314:LEU:HD23	1:D:317:LEU:HD12	1.94	0.49
1:X:210:ASP:HB3	1:X:213:PHE:HD1	1.77	0.49
1:E:0:HIS:HA	1:E:316:ASN:HD21	1.75	0.49
1:E:0:HIS:HA	1:E:316:ASN:HD22	1.77	0.49
1:E:285:ASP:O	1:E:289:GLU:HG3	2.12	0.49
1:E:39:LEU:HD22	1:E:310:LEU:HD21	1.95	0.48
1:D:228:GLU:HA	1:D:265:VAL:HG12	1.95	0.48
1:X:203:HIS:HD2	1:X:204:PRO:O	1.96	0.48
1:D:4:PHE:CZ	1:D:148:PRO:HB2	2.48	0.48
1:C:97:ILE:CB	1:C:98:PRO:HD3	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:TYR:OH	1:E:182:GLN:HG3	2.13	0.48
1:E:132:GLN:HG2	4:E:362:HOH:O	2.13	0.48
1:Z:125:VAL:O	1:Z:129:GLN:HG3	2.13	0.48
1:Z:24:LYS:HZ3	1:Z:301:ASN:HD21	1.56	0.48
1:E:168:LYS:HA	1:E:198:GLU:HB3	1.95	0.48
1:E:1:MET:HE1	1:E:10:ILE:HD12	1.96	0.48
1:Z:24:LYS:HZ2	1:Z:301:ASN:ND2	2.10	0.48
1:X:273:HIS:O	1:X:275:LEU:HD13	2.12	0.48
1:D:70:ILE:HG22	1:D:71:ASN:N	2.29	0.48
1:E:51:ARG:O	1:E:55:GLN:HG3	2.14	0.48
1:D:35:ARG:HG2	1:D:36:ASN:ND2	2.29	0.48
1:Z:286:ASP:O	1:Z:290:SER:HB3	2.13	0.48
1:C:204:PRO:HG3	1:C:256:TRP:CE2	2.49	0.48
1:D:188:PHE:O	1:D:192:MET:HG2	2.13	0.48
1:E:70:ILE:O	1:E:71:ASN:CB	2.62	0.48
1:C:294:ILE:C	1:C:297:PRO:HD2	2.34	0.48
1:Z:228:GLU:HA	1:Z:265:VAL:HG12	1.95	0.48
1:E:208:GLU:CG	1:E:242:LEU:HD11	2.43	0.48
1:E:4:PHE:CE2	1:E:309:VAL:HG21	2.49	0.48
1:E:43:PHE:CZ	1:E:141:MET:HE1	2.49	0.48
1:D:82:GLY:HA2	1:E:285:ASP:OD1	2.14	0.48
1:D:202:THR:HG23	1:D:202:THR:O	2.13	0.48
1:X:103:TYR:O	1:Y:56:LYS:HD3	2.14	0.48
1:Z:209:LEU:HD21	1:Z:238:TRP:CE2	2.49	0.47
1:X:161:TYR:HB3	1:X:270:TYR:CZ	2.49	0.47
1:C:118:ARG:HA	1:C:246:TYR:CE2	2.50	0.47
1:D:216:ASN:ND2	4:D:372:HOH:O	2.46	0.47
1:D:83:VAL:HG12	1:D:84:ILE:N	2.28	0.47
1:X:51:ARG:NH2	1:X:69:ASP:OD1	2.47	0.47
1:Z:17:LEU:HD13	1:Z:159:GLU:HG3	1.96	0.47
1:Z:168:LYS:HA	1:Z:198:GLU:HB3	1.95	0.47
1:Z:23:ILE:HD13	1:Z:307:THR:HG22	1.97	0.47
1:X:95:GLU:C	1:X:98:PRO:HD2	2.34	0.47
1:Z:203:HIS:HD2	1:Z:204:PRO:O	1.97	0.47
1:X:70:ILE:HD11	1:X:100:MET:CE	2.45	0.47
1:C:4:PHE:CE2	1:C:309:VAL:HG21	2.49	0.47
1:Z:61:LEU:CD1	1:Z:310:LEU:HB3	2.44	0.47
1:D:24:LYS:NZ	1:D:301:ASN:HD21	2.12	0.47
1:C:59:LEU:CD1	1:E:64:ASN:HB3	2.45	0.47
1:X:127:ILE:HG22	4:X:397:HOH:O	2.15	0.47
1:X:204:PRO:HG3	1:X:256:TRP:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:230:ALA:O	1:Z:269:ALA:HB2	2.15	0.47
1:E:50:THR:HG21	1:E:141:MET:HB3	1.97	0.47
1:Z:294:ILE:C	1:Z:297:PRO:HD2	2.34	0.47
1:C:49:ARG:NH2	1:C:276:PRO:HG3	2.26	0.47
1:E:7:VAL:O	1:E:10:ILE:HG22	2.15	0.47
1:Y:294:ILE:C	1:Y:297:PRO:HD2	2.36	0.47
1:D:296:ILE:HB	1:D:297:PRO:HD3	1.97	0.47
1:X:98:PRO:CB	1:Y:296:ILE:HD13	2.45	0.46
1:X:150:GLN:O	1:X:153:ALA:HB3	2.15	0.46
1:C:64:ASN:HB3	1:D:59:LEU:HD13	1.97	0.46
1:X:208:GLU:CG	1:X:242:LEU:HD11	2.46	0.46
1:E:154:ASP:HA	1:E:157:THR:CG2	2.45	0.46
1:E:192:MET:CE	1:E:197:TYR:HD1	2.28	0.46
1:Z:70:ILE:O	1:Z:71:ASN:CB	2.61	0.46
1:E:265:VAL:HG12	1:E:265:VAL:O	2.16	0.46
1:C:127:ILE:HG22	4:C:376:HOH:O	2.16	0.46
1:Y:177:PRO:HD3	1:Y:281:MET:CE	2.46	0.46
1:D:152:PHE:CE1	1:D:156:ILE:HD11	2.50	0.46
1:C:306:ALA:O	1:C:310:LEU:HB2	2.15	0.46
1:Y:70:ILE:HD11	1:Y:100:MET:CE	2.45	0.46
1:C:80:GLU:O	1:C:92:HIS:NE2	2.45	0.46
1:X:105:ASP:O	1:X:137:PRO:HD2	2.14	0.46
1:D:282:ILE:HG13	4:D:366:HOH:O	2.15	0.46
1:D:70:ILE:O	1:D:71:ASN:CB	2.64	0.46
1:D:26:ASP:CG	1:D:29:LYS:HB2	2.35	0.46
1:C:27:ARG:HB2	4:C:366:HOH:O	2.16	0.46
1:X:152:PHE:O	1:X:156:ILE:HG13	2.16	0.46
1:E:127:ILE:HG23	1:E:128:ASN:N	2.31	0.46
1:D:203:HIS:HD2	1:D:204:PRO:O	1.98	0.46
1:C:275:LEU:HD23	1:E:99:VAL:HG21	1.97	0.46
1:Z:273:HIS:O	1:Z:275:LEU:HD13	2.16	0.46
1:Z:4:PHE:CZ	1:Z:148:PRO:HB2	2.50	0.46
1:E:45:ASN:ND2	1:E:112:PHE:HB2	2.31	0.46
3:C:351:SN0:C4	1:E:90:PRO:HB3	2.46	0.46
1:E:240:ALA:HB2	1:E:250:LEU:HG	1.98	0.46
1:Z:227:PHE:CD2	1:Z:262:GLN:HB3	2.50	0.46
1:X:107:ILE:HD12	1:X:134:SER:HB2	1.98	0.46
1:Y:202:THR:HG23	1:Y:202:THR:O	2.15	0.46
1:X:149:LEU:HB2	4:X:364:HOH:O	2.16	0.46
1:D:116:GLU:HB2	4:D:357:HOH:O	2.15	0.45
1:Y:265:VAL:HG12	1:Y:265:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:64:ASN:HB3	1:Y:59:LEU:HD13	1.97	0.45
1:D:7:VAL:O	1:D:10:ILE:HG22	2.16	0.45
1:X:50:THR:HG21	1:X:141:MET:HB3	1.97	0.45
1:E:0:HIS:CE1	4:E:377:HOH:O	2.70	0.45
1:X:159:GLU:HG2	1:X:197:TYR:OH	2.16	0.45
1:D:162:LYS:HD2	1:D:164:THR:O	2.15	0.45
1:Y:89:LYS:HA	1:Y:90:PRO:HD3	1.84	0.45
1:D:43:PHE:CZ	1:D:141:MET:HE1	2.52	0.45
1:D:274:CYS:O	1:D:275:LEU:HB2	2.16	0.45
1:Z:88:ASP:HB3	1:Z:89:LYS:HD2	1.99	0.45
1:Y:166:ARG:HG2	1:Y:196:ASP:OD2	2.16	0.45
1:C:44:PHE:CZ	1:C:70:ILE:HD12	2.51	0.45
1:X:141:MET:O	1:X:142:GLU:CB	2.65	0.45
1:C:175:PRO:HG2	1:C:281:MET:O	2.16	0.45
1:Y:223:GLN:HB2	1:Y:256:TRP:CZ3	2.52	0.45
1:Z:118:ARG:HG3	1:Z:246:TYR:CD1	2.52	0.45
1:X:98:PRO:HB2	1:Y:296:ILE:HD13	1.99	0.45
1:E:95:GLU:O	1:E:98:PRO:HD2	2.17	0.45
1:Y:122:TYR:OH	1:Y:182:GLN:CG	2.64	0.45
1:X:208:GLU:HG2	1:X:242:LEU:HD11	1.98	0.45
1:Y:222:ASP:HB3	1:Y:225:LYS:HB2	1.98	0.45
1:C:311:LYS:O	1:C:315:GLU:HG3	2.17	0.45
1:Z:187:SER:O	1:Z:191:TRP:HD1	2.00	0.45
1:D:284:THR:HG22	1:D:286:ASP:H	1.82	0.44
1:C:294:ILE:O	1:C:297:PRO:HD2	2.18	0.44
1:Y:91:GLU:HG3	4:Y:366:HOH:O	2.17	0.44
1:Z:119:GLU:HG2	1:Z:123:ASN:HD21	1.82	0.44
1:X:23:ILE:HD12	1:X:308:VAL:HG22	1.97	0.44
1:D:294:ILE:C	1:D:297:PRO:HD2	2.38	0.44
1:Z:189:ALA:HA	1:Z:199:PHE:CE2	2.51	0.44
1:X:125:VAL:O	1:X:129:GLN:HG3	2.18	0.44
1:Y:24:LYS:HZ2	1:Y:301:ASN:ND2	2.15	0.44
1:D:184:VAL:CG1	1:D:236:LYS:HG2	2.47	0.44
1:C:49:ARG:HB2	2:C:352:SO4:O4	2.18	0.44
1:C:176:HIS:NE2	1:C:278:ARG:HD2	2.33	0.44
1:Z:124:GLU:O	1:Z:128:ASN:HB2	2.17	0.44
1:C:241:TYR:HD2	1:C:242:LEU:HD23	1.80	0.44
1:C:228:GLU:HA	1:C:265:VAL:HG12	2.00	0.44
1:C:228:GLU:HG3	1:C:265:VAL:HG11	1.98	0.44
1:Y:230:ALA:O	1:Y:269:ALA:HB2	2.17	0.44
1:Y:118:ARG:HA	1:Y:246:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:MET:HE3	1:E:197:TYR:HD1	1.81	0.44
1:Y:78:GLU:HG3	1:Y:85:MET:HG2	1.99	0.44
1:E:41:MET:HE3	1:E:54:THR:CB	2.42	0.44
1:Y:192:MET:CE	1:Y:197:TYR:CD1	3.00	0.44
1:C:276:PRO:HB3	1:E:91:GLU:HB2	1.99	0.44
1:X:275:LEU:HD12	1:X:277:VAL:HG22	2.00	0.44
1:Z:225:LYS:HB3	1:Z:225:LYS:HE2	1.86	0.44
1:D:267:ASN:O	1:D:268:ASN:C	2.55	0.44
1:Z:122:TYR:HA	1:Z:145:THR:HG21	1.98	0.44
1:C:49:ARG:CZ	1:C:275:LEU:HB3	2.47	0.44
1:C:68:LEU:HD23	1:D:51:ARG:HD3	1.99	0.44
1:Y:34:GLY:O	1:Y:37:LYS:HB2	2.16	0.44
1:Z:212:LYS:HE3	1:Z:213:PHE:CZ	2.52	0.44
1:Z:105:ASP:O	1:Z:137:PRO:HD2	2.17	0.44
1:X:-3:ARG:O	1:X:-1:SER:N	2.43	0.44
1:X:70:ILE:HG22	1:X:71:ASN:N	2.32	0.44
1:Y:275:LEU:HD12	1:Y:277:VAL:CG2	2.47	0.44
1:C:4:PHE:CE2	1:C:148:PRO:HB2	2.53	0.44
1:C:88:ASP:HB3	1:C:89:LYS:HD2	1.98	0.44
1:E:-2:GLY:O	1:E:312:ARG:HD2	2.18	0.44
1:E:51:ARG:NH2	1:E:69:ASP:OD2	2.51	0.44
1:Z:51:ARG:O	1:Z:55:GLN:HG3	2.17	0.44
1:D:175:PRO:HG3	1:D:254:ARG:HA	2.00	0.44
1:Z:95:GLU:C	1:Z:98:PRO:HD2	2.38	0.44
1:D:170:VAL:HG21	1:D:226:ALA:O	2.18	0.44
1:X:176:HIS:CG	1:X:177:PRO:HD2	2.53	0.44
1:Y:154:ASP:HA	1:Y:157:THR:CG2	2.47	0.43
1:Y:182:GLN:HE21	1:Y:182:GLN:HB3	1.54	0.43
1:Z:89:LYS:CD	1:Z:89:LYS:N	2.81	0.43
1:Z:7:VAL:O	1:Z:10:ILE:HG22	2.18	0.43
1:E:179:PRO:HA	4:E:381:HOH:O	2.18	0.43
1:X:-3:ARG:HH12	1:X:8:GLN:HB3	1.79	0.43
1:Y:51:ARG:NH2	1:Y:69:ASP:OD2	2.51	0.43
1:C:162:LYS:HD2	1:C:164:THR:O	2.18	0.43
1:E:83:VAL:HG12	1:E:84:ILE:N	2.33	0.43
1:D:284:THR:HG22	1:D:285:ASP:N	2.33	0.43
1:C:89:LYS:HA	1:C:90:PRO:HD3	1.70	0.43
1:Y:245:ASN:HA	1:Y:248:GLN:HG3	1.99	0.43
1:D:45:ASN:HD21	1:D:112:PHE:HB2	1.82	0.43
1:E:44:PHE:HB2	1:E:110:ARG:O	2.18	0.43
1:D:124:GLU:HB3	1:D:127:ILE:HG23	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:MET:HG2	1:C:141:MET:HE3	2.00	0.43
1:X:279:ARG:NE	1:Z:95:GLU:OE2	2.43	0.43
1:D:310:LEU:HD12	1:D:310:LEU:HA	1.82	0.43
1:D:272:MET:O	1:D:273:HIS:HB2	2.17	0.43
1:Y:83:VAL:HG12	1:Y:84:ILE:N	2.34	0.43
1:D:61:LEU:HD12	1:D:310:LEU:HB3	2.01	0.43
1:Z:17:LEU:O	1:Z:21:PHE:HD1	2.02	0.43
1:D:227:PHE:CD2	1:D:262:GLN:HB3	2.53	0.43
1:E:119:GLU:HG2	1:E:123:ASN:ND2	2.34	0.43
1:Y:152:PHE:O	1:Y:156:ILE:HG13	2.19	0.43
1:C:310:LEU:HA	1:C:310:LEU:HD12	1.89	0.43
1:Z:70:ILE:HG22	1:Z:71:ASN:N	2.32	0.43
1:Z:284:THR:HG22	1:Z:286:ASP:H	1.82	0.43
1:Y:89:LYS:HD2	1:Y:89:LYS:N	2.34	0.43
1:Y:103:TYR:CE2	1:Z:53:SER:HB3	2.53	0.43
1:Y:240:ALA:HB2	1:Y:250:LEU:HG	2.00	0.43
1:Z:250:LEU:O	1:D:252:THR:HG23	2.18	0.43
1:C:43:PHE:CZ	1:C:141:MET:HE1	2.53	0.43
1:D:93:LEU:O	1:D:97:ILE:HG13	2.19	0.43
1:D:61:LEU:CD1	1:D:310:LEU:HB3	2.49	0.43
1:C:212:LYS:HE3	1:C:213:PHE:CE1	2.54	0.43
1:Y:294:ILE:O	1:Y:297:PRO:HD2	2.19	0.43
1:E:174:ALA:HB1	1:E:282:ILE:HA	1.99	0.43
1:Z:245:ASN:O	1:Z:248:GLN:HB2	2.19	0.43
1:C:154:ASP:O	1:C:157:THR:HG23	2.19	0.42
1:Z:185:PRO:HG2	1:Z:238:TRP:HB3	2.01	0.42
1:E:310:LEU:HD12	1:E:310:LEU:HA	1.81	0.42
1:C:186:ASN:HB3	1:C:213:PHE:CG	2.54	0.42
1:E:202:THR:HG23	1:E:202:THR:O	2.19	0.42
1:E:227:PHE:O	1:E:266:THR:HG22	2.19	0.42
1:C:70:ILE:HG22	1:C:71:ASN:N	2.34	0.42
1:C:89:LYS:HD2	1:C:89:LYS:N	2.34	0.42
1:X:70:ILE:O	1:X:71:ASN:CB	2.67	0.42
1:E:182:GLN:HB3	1:E:182:GLN:HE21	1.66	0.42
1:D:206:GLY:N	1:D:208:GLU:OE2	2.52	0.42
1:C:176:HIS:ND1	1:C:177:PRO:HD2	2.34	0.42
1:X:41:MET:HB3	1:X:41:MET:HE2	1.92	0.42
1:E:141:MET:O	1:E:142:GLU:CB	2.67	0.42
1:D:93:LEU:HG	1:D:97:ILE:CD1	2.50	0.42
1:X:228:GLU:HA	1:X:265:VAL:HG12	2.01	0.42
1:Y:98:PRO:CB	1:Z:296:ILE:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:98:PRO:HB3	1:Z:296:ILE:HD13	2.01	0.42
1:Y:176:HIS:CG	1:Y:177:PRO:HD2	2.55	0.42
1:E:204:PRO:HG3	1:E:256:TRP:CE2	2.55	0.42
1:C:97:ILE:HB	1:C:98:PRO:CD	2.39	0.42
1:X:122:TYR:OH	1:X:182:GLN:CG	2.66	0.42
1:C:95:GLU:CD	1:D:279:ARG:HH21	2.22	0.42
1:Z:150:GLN:OE1	1:Z:302:ARG:NH1	2.53	0.42
1:C:156:ILE:O	1:C:160:GLU:HB2	2.19	0.42
1:X:83:VAL:CG1	1:X:84:ILE:N	2.83	0.42
1:C:265:VAL:HG12	1:C:265:VAL:O	2.18	0.42
1:Z:170:VAL:HG22	1:Z:200:VAL:HB	2.01	0.42
1:D:176:HIS:ND1	1:D:177:PRO:HD2	2.35	0.42
1:Z:285:ASP:O	1:Z:288:ILE:HG22	2.20	0.42
1:C:182:GLN:HE21	1:C:182:GLN:HB3	1.60	0.42
1:D:21:PHE:O	1:D:25:LYS:HE2	2.19	0.42
1:E:166:ARG:HG2	1:E:196:ASP:OD2	2.20	0.42
1:E:17:LEU:O	1:E:20:SER:HB2	2.20	0.42
1:Z:296:ILE:HB	1:Z:297:PRO:HD3	2.02	0.42
1:X:223:GLN:HB2	1:X:256:TRP:CZ3	2.55	0.42
1:C:118:ARG:NH2	1:C:243:GLY:N	2.68	0.42
1:X:119:GLU:HG2	1:X:123:ASN:ND2	2.35	0.42
1:Y:64:ASN:HB3	1:Z:59:LEU:HD13	2.02	0.42
1:X:173:TRP:CG	1:X:174:ALA:N	2.88	0.42
1:C:78:GLU:HG3	1:C:85:MET:HG2	2.02	0.41
1:D:254:ARG:HD3	4:D:379:HOH:O	2.20	0.41
1:E:-3:ARG:HH12	1:E:9:ASP:HA	1.86	0.41
1:Z:184:VAL:N	1:Z:185:PRO:CD	2.83	0.41
1:X:59:LEU:HD13	1:Z:64:ASN:HB3	2.01	0.41
1:X:157:THR:HB	1:X:301:ASN:OD1	2.19	0.41
1:C:61:LEU:HD12	1:C:310:LEU:HB3	2.03	0.41
1:Y:228:GLU:HG3	1:Y:265:VAL:CG1	2.49	0.41
1:X:78:GLU:HB3	1:X:92:HIS:CD2	2.56	0.41
1:C:31:VAL:O	1:C:62:GLY:HA3	2.19	0.41
1:D:151:SER:O	1:D:154:ASP:HB2	2.21	0.41
1:C:141:MET:O	1:C:142:GLU:CB	2.67	0.41
1:X:98:PRO:HB2	1:Y:296:ILE:CD1	2.51	0.41
1:C:24:LYS:HZ2	1:C:301:ASN:HD21	1.68	0.41
1:Y:224:MET:HE3	1:Y:265:VAL:HG21	2.03	0.41
1:E:89:LYS:CD	1:E:89:LYS:N	2.84	0.41
1:Y:95:GLU:HG2	4:Z:384:HOH:O	2.19	0.41
1:C:122:TYR:CD2	1:C:145:THR:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:306:ALA:O	1:Z:310:LEU:HB2	2.19	0.41
1:Z:191:TRP:O	1:Z:195:THR:HG23	2.20	0.41
1:E:30:TYR:C	1:E:32:GLU:H	2.23	0.41
1:Y:208:GLU:HG2	1:Y:242:LEU:CD1	2.48	0.41
1:D:49:ARG:CZ	1:D:275:LEU:HB3	2.51	0.41
1:X:90:PRO:HB3	3:Y:347:SN0:C4	2.50	0.41
1:Y:4:PHE:CE2	1:Y:148:PRO:HB2	2.56	0.41
1:D:154:ASP:HA	1:D:157:THR:CG2	2.50	0.41
1:E:296:ILE:N	1:E:297:PRO:CD	2.83	0.41
1:Y:241:TYR:CD2	1:Y:242:LEU:HD23	2.55	0.41
1:Y:19:GLU:OE2	1:Y:312:ARG:NE	2.44	0.41
1:E:225:LYS:HB3	1:E:225:LYS:HE2	1.82	0.41
1:X:-3:ARG:C	1:X:-1:SER:H	2.22	0.41
1:Z:70:ILE:HD11	1:Z:100:MET:HE1	2.02	0.41
1:Z:162:LYS:HD2	1:Z:164:THR:O	2.20	0.41
1:E:274:CYS:O	1:E:275:LEU:O	2.38	0.41
1:D:171:MET:HG3	1:D:188:PHE:CD2	2.56	0.41
1:C:50:THR:HG22	1:C:141:MET:HE2	2.03	0.41
1:Z:294:ILE:O	1:Z:297:PRO:HD2	2.21	0.41
1:C:176:HIS:CG	1:C:177:PRO:HD2	2.56	0.41
1:Y:103:TYR:O	1:Z:56:LYS:HD3	2.21	0.41
1:X:231:ASP:HB3	4:X:403:HOH:O	2.21	0.41
1:Z:304:ILE:HD12	1:Z:304:ILE:N	2.36	0.41
1:D:89:LYS:HA	1:D:90:PRO:HD3	1.90	0.41
1:D:17:LEU:O	1:D:21:PHE:HD1	2.03	0.41
1:E:31:VAL:HG22	1:E:31:VAL:O	2.21	0.41
1:Y:70:ILE:HG22	1:Y:71:ASN:N	2.36	0.40
1:Y:235:ALA:O	1:Y:273:HIS:CD2	2.75	0.40
1:D:114:ARG:HB2	4:D:357:HOH:O	2.21	0.40
1:E:41:MET:CE	1:E:141:MET:HE3	2.50	0.40
1:D:41:MET:CE	1:D:141:MET:HE1	2.51	0.40
1:D:174:ALA:HB1	1:D:282:ILE:HA	2.03	0.40
1:E:76:LYS:O	1:E:90:PRO:HD2	2.21	0.40
1:C:227:PHE:O	1:C:266:THR:HG22	2.22	0.40
1:C:73:GLY:O	1:D:51:ARG:NH1	2.53	0.40
1:D:90:PRO:HB3	3:E:355:SN0:H32	2.03	0.40
1:X:176:HIS:NE2	1:X:278:ARG:HD2	2.36	0.40
1:Y:103:TYR:CZ	1:Z:53:SER:HB3	2.56	0.40
1:Y:92:HIS:CE1	1:Y:94:LEU:HG	2.56	0.40
1:Z:317:LEU:O	1:Z:318:PRO:O	2.39	0.40
1:C:259:GLY:HA2	1:C:284:THR:OG1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLU:OE1	1:C:144:ALA:HB3	2.22	0.40
1:X:42:ILE:HD13	1:X:100:MET:SD	2.61	0.40
1:Y:141:MET:O	1:Y:142:GLU:CB	2.69	0.40
1:C:45:ASN:HD21	1:C:112:PHE:HB2	1.86	0.40
1:E:24:LYS:NZ	1:E:301:ASN:HD21	2.20	0.40
1:D:42:ILE:HD13	1:D:100:MET:HE1	2.03	0.40
1:D:168:LYS:HD3	1:D:230:ALA:HA	2.02	0.40
1:C:118:ARG:NH2	1:C:243:GLY:H	2.19	0.40
3:C:351:SN0:OD2	1:E:90:PRO:HB3	2.21	0.40
1:D:103:TYR:CZ	1:E:53:SER:HB3	2.57	0.40

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	319/338 (94%)	290 (91%)	26 (8%)	3 (1%)	21	55
1	D	320/338 (95%)	289 (90%)	25 (8%)	6 (2%)	10	32
1	E	320/338 (95%)	292 (91%)	24 (8%)	4 (1%)	15	44
1	X	320/338 (95%)	290 (91%)	27 (8%)	3 (1%)	21	55
1	Y	320/338 (95%)	298 (93%)	20 (6%)	2 (1%)	30	65
1	Z	318/338 (94%)	287 (90%)	28 (9%)	3 (1%)	21	55
All	All	1917/2028 (94%)	1746 (91%)	150 (8%)	21 (1%)	17	50

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	142	GLU
1	Y	142	GLU

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Mol	Chain	Res	Type
1	Z	142	GLU
1	C	142	GLU
1	D	142	GLU
1	E	142	GLU
1	X	243	GLY
1	Z	240	ALA
1	Z	243	GLY
1	C	243	GLY
1	E	243	GLY
1	D	243	GLY
1	C	71	ASN
1	D	240	ALA
1	D	273	HIS
1	X	85	MET
1	D	31	VAL
1	Y	243	GLY
1	E	275	LEU
1	D	258	VAL
1	E	31	VAL

### 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	C	279/294 (95%)	265 (95%)	14 (5%)	30	64
1	D	280/294 (95%)	266 (95%)	14 (5%)	30	64
1	E	280/294 (95%)	270 (96%)	10 (4%)	42	76
1	X	280/294 (95%)	266 (95%)	14 (5%)	30	64
1	Y	280/294 (95%)	265 (95%)	15 (5%)	27	60
1	Z	279/294 (95%)	269 (96%)	10 (4%)	42	76
All	All	1678/1764 (95%)	1601 (95%)	77 (5%)	33	67

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	25	LYS
1	X	31	VAL
1	X	52	LEU
1	X	68	LEU
1	X	78	GLU
1	X	81	ARG
1	X	89	LYS
1	X	147	HIS
1	X	157	THR
1	X	163	LYS
1	X	182	GLN
1	X	277	VAL
1	X	295	VAL
1	X	310	LEU
1	Y	-3	ARG
1	Y	25	LYS
1	Y	52	LEU
1	Y	81	ARG
1	Y	89	LYS
1	Y	118	ARG
1	Y	147	HIS
1	Y	152	PHE
1	Y	157	THR
1	Y	163	LYS
1	Y	178	ARG
1	Y	182	GLN
1	Y	251	SER
1	Y	277	VAL
1	Y	310	LEU
1	Z	25	LYS
1	Z	48	LEU
1	Z	52	LEU
1	Z	132	GLN
1	Z	147	HIS
1	Z	152	PHE
1	Z	157	THR
1	Z	163	LYS
1	Z	182	GLN
1	Z	310	LEU
1	C	0	HIS
1	C	25	LYS
1	C	48	LEU
1	C	52	LEU

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Mol	Chain	Res	Type
1	C	81	ARG
1	C	89	LYS
1	C	95	GLU
1	C	147	HIS
1	C	157	THR
1	C	166	ARG
1	C	178	ARG
1	C	182	GLN
1	C	208	GLU
1	C	295	VAL
1	D	-3	ARG
1	D	25	LYS
1	D	48	LEU
1	D	52	LEU
1	D	68	LEU
1	D	81	ARG
1	D	95	GLU
1	D	152	PHE
1	D	157	THR
1	D	178	ARG
1	D	182	GLN
1	D	208	GLU
1	D	267	ASN
1	D	310	LEU
1	E	-3	ARG
1	E	25	LYS
1	E	51	ARG
1	E	52	LEU
1	E	132	GLN
1	E	163	LYS
1	E	182	GLN
1	E	208	GLU
1	E	268	ASN
1	E	295	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	0	HIS
1	X	64	ASN
1	X	182	GLN
1	X	203	HIS

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Mol	Chain	Res	Type
1	X	267	ASN
1	X	268	ASN
1	X	301	ASN
1	X	316	ASN
1	Y	64	ASN
1	Y	182	GLN
1	Y	203	HIS
1	Y	248	GLN
1	Y	267	ASN
1	Y	268	ASN
1	Y	301	ASN
1	Z	64	ASN
1	Z	123	ASN
1	Z	182	GLN
1	Z	203	HIS
1	Z	255	ASN
1	Z	267	ASN
1	Z	268	ASN
1	Z	301	ASN
1	Z	316	ASN
1	C	64	ASN
1	C	123	ASN
1	C	182	GLN
1	C	203	HIS
1	C	267	ASN
1	C	268	ASN
1	C	301	ASN
1	C	316	ASN
1	D	8	GLN
1	D	64	ASN
1	D	182	GLN
1	D	203	HIS
1	D	267	ASN
1	D	268	ASN
1	D	292	GLN
1	D	301	ASN
1	D	316	ASN
1	E	0	HIS
1	E	182	GLN
1	E	203	HIS
1	E	267	ASN
1	E	268	ASN

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Mol	Chain	Res	Type
1	E	292	GLN
1	E	301	ASN
1	E	316	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
3	SN0	C	351	-	8,14,14	0.29	0	7,17,17	0.64	0
2	SO4	C	352	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	C	358	-	4,4,4	0.28	0	6,6,6	0.17	0
3	SN0	D	353	-	8,14,14	0.44	0	7,17,17	0.68	0
2	SO4	D	354	-	4,4,4	0.33	0	6,6,6	0.29	0
3	SN0	E	355	-	8,14,14	0.26	0	7,17,17	0.86	0
2	SO4	E	356	-	4,4,4	0.17	0	6,6,6	0.20	0
3	SN0	X	345	-	8,14,14	0.32	0	7,17,17	0.99	0
2	SO4	X	346	-	4,4,4	0.18	0	6,6,6	0.20	0
2	SO4	X	357	-	4,4,4	0.07	0	6,6,6	0.08	0
3	SN0	Y	347	-	8,14,14	0.46	0	7,17,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	Y	348	-	4,4,4	0.20	0	6,6,6	0.27	0
3	SN0	Z	349	-	8,14,14	0.57	0	7,17,17	0.98	0
2	SO4	Z	350	-	4,4,4	0.28	0	6,6,6	0.14	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
3	SN0	C	351	-	-	0/10/16/16	0/0/0/0
2	SO4	C	352	-	-	0/0/0/0	0/0/0/0
2	SO4	C	358	-	-	0/0/0/0	0/0/0/0
3	SN0	D	353	-	-	0/10/16/16	0/0/0/0
2	SO4	D	354	-	-	0/0/0/0	0/0/0/0
3	SN0	E	355	-	-	0/10/16/16	0/0/0/0
2	SO4	E	356	-	-	0/0/0/0	0/0/0/0
3	SN0	X	345	-	-	0/10/16/16	0/0/0/0
2	SO4	X	346	-	-	0/0/0/0	0/0/0/0
2	SO4	X	357	-	-	0/0/0/0	0/0/0/0
3	SN0	Y	347	-	-	0/10/16/16	0/0/0/0
2	SO4	Y	348	-	-	0/0/0/0	0/0/0/0
3	SN0	Z	349	-	-	0/10/16/16	0/0/0/0
2	SO4	Z	350	-	-	0/0/0/0	0/0/0/0

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.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	351	SN0	2	0
2	C	352	SO4	1	0
3	D	353	SN0	1	0
3	E	355	SN0	2	0
3	Y	347	SN0	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	C	321/338 (94%)	0.08	15 (4%) 35 24	54, 72, 92, 108	0
1	D	322/338 (95%)	0.18	15 (4%) 35 24	46, 71, 96, 117	0
1	E	322/338 (95%)	-0.17	8 (2%) 61 48	38, 58, 78, 101	0
1	X	322/338 (95%)	-0.41	4 (1%) 81 73	28, 48, 71, 84	0
1	Y	322/338 (95%)	-0.62	0 100 100	22, 35, 51, 78	0
1	Z	320/338 (94%)	-0.43	5 (1%) 74 66	27, 44, 62, 82	0
All	All	1929/2028 (95%)	-0.23	47 (2%) 62 50	22, 55, 86, 117	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-3	ARG	5.0
1	D	-2	GLY	4.9
1	C	318	PRO	4.3
1	C	-1	SER	4.1
1	C	254	ARG	3.9
1	E	-2	GLY	3.9
1	D	25	LYS	3.8
1	Z	-1	SER	3.4
1	D	318	PRO	3.3
1	C	116	GLU	3.3
1	D	0	HIS	3.3
1	C	-2	GLY	3.1
1	E	-3	ARG	3.1
1	D	267	ASN	3.1
1	D	166	ARG	2.9
1	Z	318	PRO	2.9
1	C	26	ASP	2.8
1	X	205	GLU	2.8
1	E	318	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	254	ARG	2.8
1	D	-1	SER	2.7
1	D	14	LYS	2.7
1	C	166	ARG	2.6
1	E	0	HIS	2.6
1	C	0	HIS	2.6
1	C	172	THR	2.6
1	E	291	PRO	2.5
1	C	242	LEU	2.5
1	Z	117	ASN	2.5
1	E	71	ASN	2.5
1	Z	0	HIS	2.4
1	C	14	LYS	2.4
1	X	244	ASP	2.4
1	D	2	LYS	2.3
1	C	309	VAL	2.3
1	Z	116	GLU	2.2
1	D	196	ASP	2.2
1	C	25	LYS	2.2
1	D	132	GLN	2.2
1	D	216	ASN	2.2
1	C	253	ASP	2.1
1	E	163	LYS	2.1
1	E	-1	SER	2.1
1	C	205	GLU	2.1
1	X	116	GLU	2.0
1	X	216	ASN	2.0
1	D	163	LYS	2.0

## 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
3	SN0	X	345	15/15	0.95	0.19	0.77	46,51,54,56	0
3	SN0	D	353	15/15	0.93	0.20	0.57	41,52,57,57	0
2	SO4	Y	348	5/5	0.99	0.14	0.42	32,35,35,36	0
3	SN0	E	355	15/15	0.94	0.15	0.05	46,51,54,56	0
3	SN0	Y	347	15/15	0.97	0.13	-0.12	30,35,41,41	0
3	SN0	C	351	15/15	0.95	0.17	-0.16	68,69,71,71	0
2	SO4	Z	350	5/5	0.99	0.13	-0.27	32,36,38,38	0
2	SO4	D	354	5/5	0.94	0.18	-0.34	57,60,62,63	0
2	SO4	E	356	5/5	0.96	0.14	-0.36	49,50,53,55	0
3	SN0	Z	349	15/15	0.97	0.12	-0.88	37,39,41,41	0
2	SO4	X	346	5/5	0.99	0.10	-1.78	42,44,44,44	0
2	SO4	C	352	5/5	0.99	0.11	-2.00	59,60,60,62	0
2	SO4	X	357	5/5	0.98	0.10	-	53,55,56,58	0
2	SO4	C	358	5/5	0.97	0.17	-	83,83,85,85	0

## 6.5 Other polymers

There are no such residues in this entry.