



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:29 PM UTC

PDB ID : 2FG6 / pdb_00002fg6
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

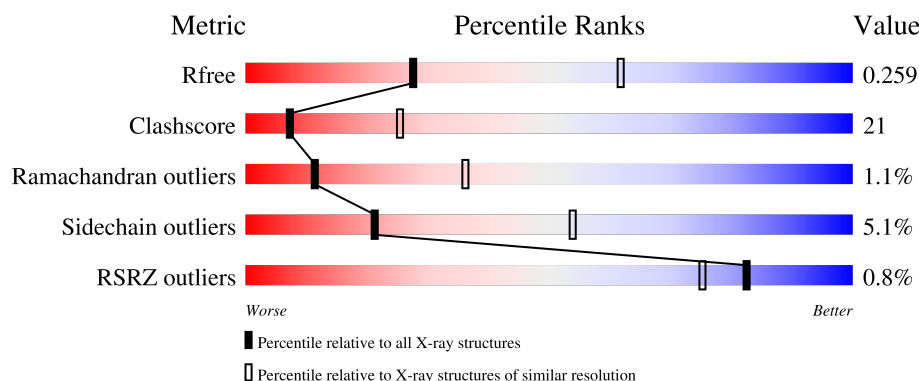
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	338	% 54% 37% • 5%
1	D	338	2% 50% 41% • 5%
1	E	338	% 53% 37% 5% 5%
1	X	338	57% 34% • 5%
1	Y	338	60% 31% • 5%

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Mol	Chain	Length	Quality of chain
1	Z	338	55% 36% • 5%

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 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

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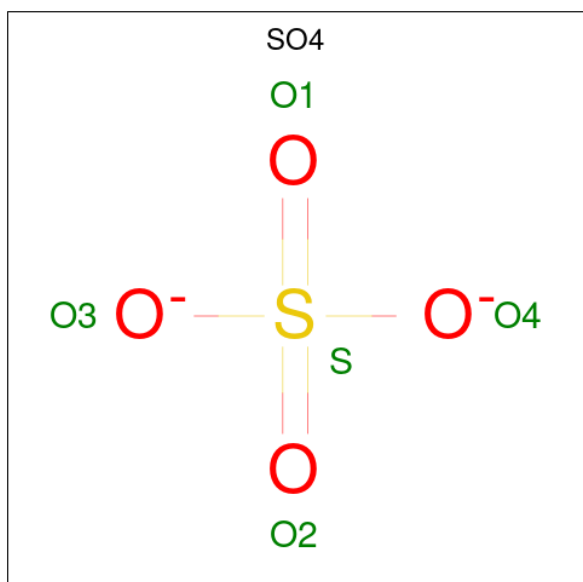
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Z	-1	SER	-	expression tag	UNP Q5LI27
Z	0	HIS	-	expression tag	UNP Q5LI27
Z	242	LEU	THR	engineered mutation	UNP Q5LI27
C	-19	MET	-	expression tag	UNP Q5LI27
C	-18	GLY	-	expression tag	UNP Q5LI27
C	-17	SER	-	expression tag	UNP Q5LI27
C	-16	SER	-	expression 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

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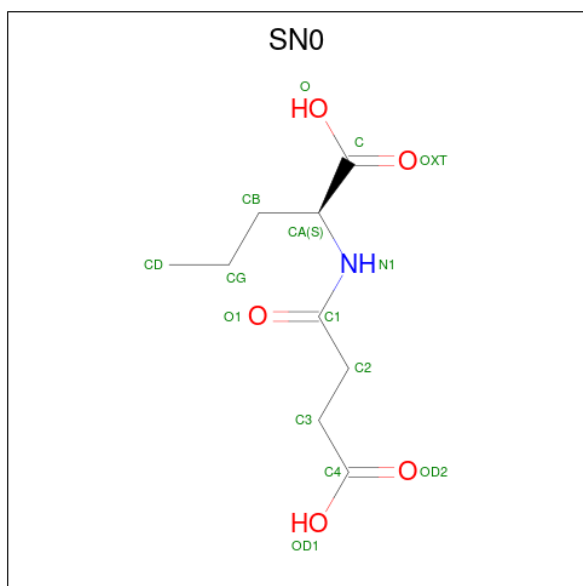
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D	-1	SER	-	expression tag	UNP Q5LI27
D	0	HIS	-	expression tag	UNP Q5LI27
D	242	LEU	THR	engineered mutation	UNP Q5LI27
E	-19	MET	-	expression tag	UNP Q5LI27
E	-18	GLY	-	expression tag	UNP Q5LI27
E	-17	SER	-	expression tag	UNP Q5LI27
E	-16	SER	-	expression 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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is N-(3-CARBOXYPROPANOYL)-L-NORVALINE (CCD ID: SN0) (formula: $C_9H_{15}NO_5$).



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		

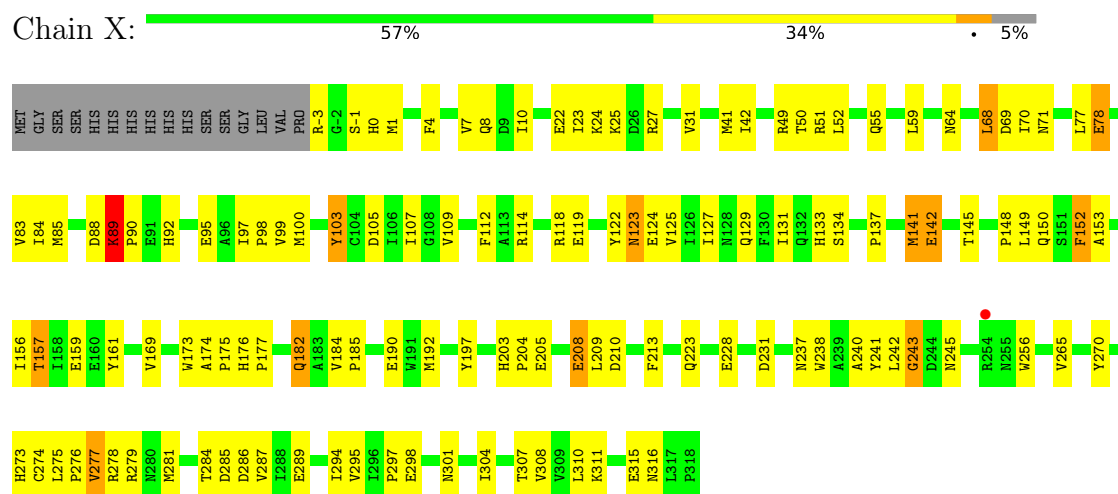
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	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		
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		

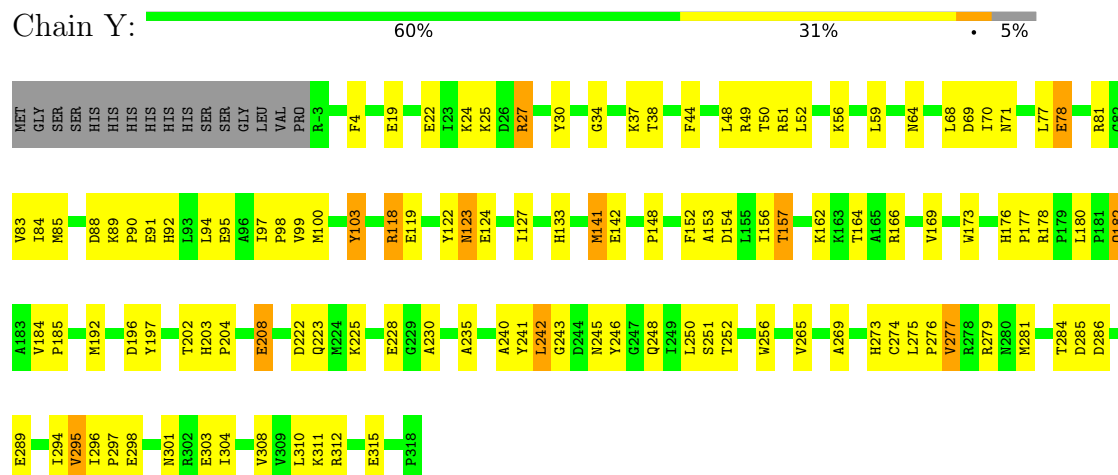
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: putative ornithine carbamoyltransferase

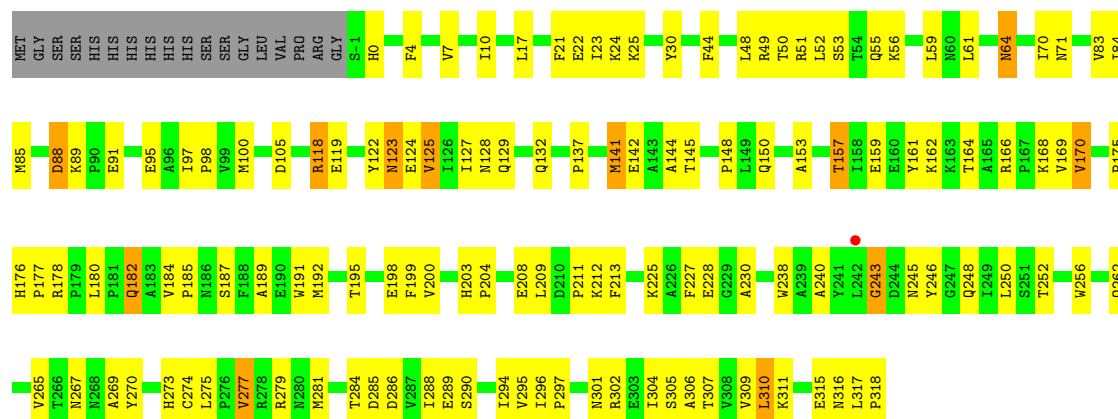


- Molecule 1: putative ornithine carbamoyltransferase

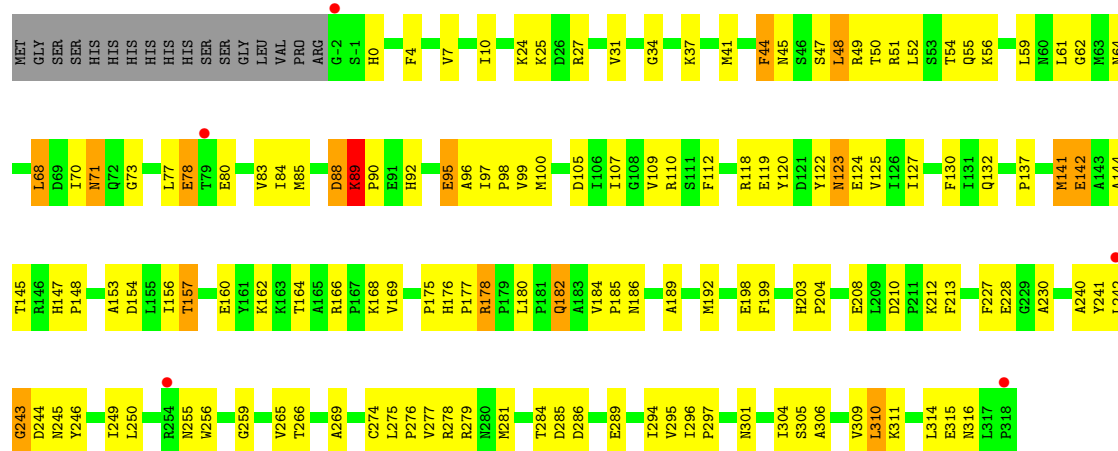


- Molecule 1: putative ornithine carbamoyltransferase

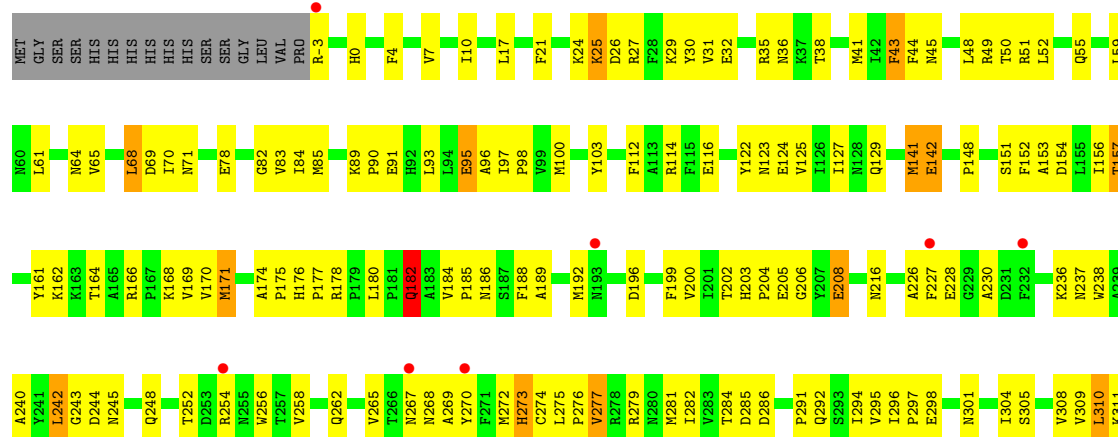




• Molecule 1: putative ornithine carbamoyltransferase

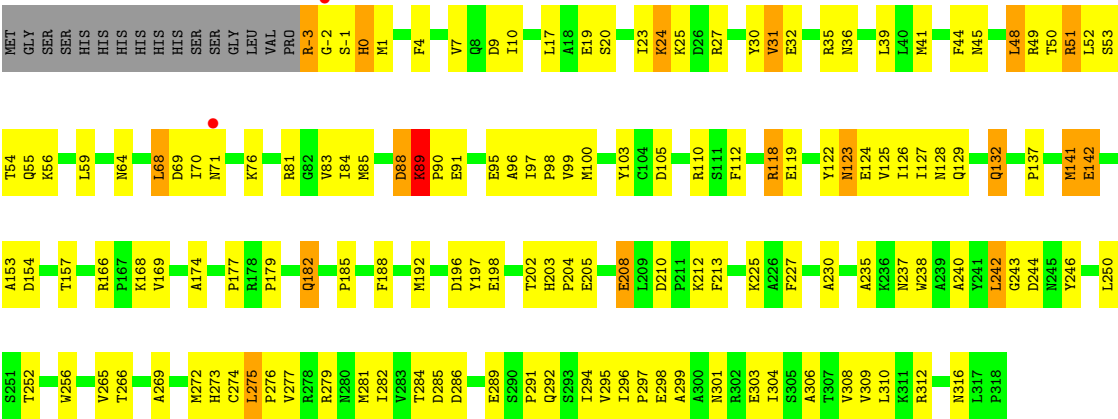


• Molecule 1: putative ornithine carbamoyltransferase



L314
E315
N316
L317
E318

- Molecule 1: putative ornithine carbamoyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	155.70Å 155.70Å 120.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.99-2.80) 99.3 (19.99-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15978	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SN0, 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	0.39	0/2642	0.98	14/3579 (0.4%)
1	D	0.41	0/2653	0.95	10/3593 (0.3%)
1	E	0.44	0/2653	0.99	13/3593 (0.4%)
1	X	0.49	1/2653 (0.0%)	1.00	8/3593 (0.2%)
1	Y	0.52	0/2653	1.02	11/3593 (0.3%)
1	Z	0.49	0/2638	0.99	9/3574 (0.3%)
All	All	0.46	1/15892 (0.0%)	0.99	65/21525 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	141	MET	SD-CE	-5.43	1.66	1.79

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	44	PHE	N-CA-C	-7.69	103.92	113.38
1	Y	88	ASP	N-CA-C	7.31	120.11	111.71
1	X	133	HIS	N-CA-C	6.95	121.93	113.38
1	Y	141	MET	N-CA-C	-6.87	104.21	112.59
1	Y	27	ARG	N-CA-C	6.75	119.50	111.33
1	C	123	ASN	N-CA-C	-6.63	104.94	113.16
1	D	242	LEU	N-CA-C	6.53	119.75	109.96
1	Z	141	MET	N-CA-C	-6.47	104.69	112.59
1	X	103	TYR	N-CA-C	6.39	120.79	112.92
1	Y	103	TYR	N-CA-C	6.32	120.69	112.92
1	D	141	MET	N-CA-C	-6.30	105.17	112.92
1	Y	44	PHE	N-CA-C	-6.24	105.70	113.38
1	Z	88	ASP	N-CA-C	6.23	118.87	111.33
1	X	141	MET	N-CA-C	-6.18	105.05	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	HIS	CA-C-N	6.18	125.67	119.24
1	C	147	HIS	C-N-CA	6.18	125.67	119.24
1	C	141	MET	N-CA-C	-6.12	104.99	112.88
1	C	132	GLN	N-CA-C	6.09	117.99	111.36
1	E	141	MET	N-CA-C	-6.06	105.81	112.72
1	C	255	ASN	N-CA-C	-6.02	105.93	113.28
1	Y	242	LEU	N-CA-C	5.93	118.41	110.35
1	Z	170	VAL	N-CA-C	5.87	116.26	107.51
1	Y	133	HIS	N-CA-C	5.85	121.32	113.72
1	Y	123	ASN	N-CA-C	-5.77	106.00	113.16
1	E	89	LYS	N-CA-C	5.77	116.93	109.72
1	E	0	HIS	N-CA-C	-5.76	103.40	110.61
1	D	65	VAL	N-CA-C	5.74	116.12	107.75
1	E	27	ARG	N-CA-C	5.66	117.14	110.97
1	X	27	ARG	N-CA-C	5.64	118.16	111.33
1	Y	38	THR	N-CA-C	5.64	118.10	108.90
1	Z	64	ASN	N-CA-C	-5.59	101.44	110.32
1	X	123	ASN	N-CA-C	-5.58	106.42	113.18
1	C	130	PHE	N-CA-C	-5.58	105.27	111.36
1	X	89	LYS	N-CA-C	5.58	116.99	109.24
1	Y	173	TRP	N-CA-C	-5.52	103.41	110.53
1	C	107	ILE	N-CA-C	5.50	115.80	108.11
1	C	244	ASP	N-CA-C	5.49	119.46	112.87
1	C	88	ASP	N-CA-C	5.48	117.68	111.11
1	D	244	ASP	N-CA-C	5.47	119.05	112.38
1	E	88	ASP	N-CA-C	5.40	117.59	111.11
1	E	252	THR	N-CA-C	-5.38	104.98	112.30
1	C	109	VAL	N-CA-C	5.38	115.86	108.12
1	C	89	LYS	CA-C-N	5.36	126.54	119.84
1	C	89	LYS	C-N-CA	5.36	126.54	119.84
1	X	152	PHE	N-CA-C	-5.33	105.64	111.82
1	D	27	ARG	N-CA-C	5.32	117.49	111.11
1	Y	252	THR	N-CA-C	-5.28	104.01	110.61
1	E	242	LEU	N-CA-C	5.24	117.05	110.24
1	Z	252	THR	N-CA-C	-5.24	104.69	111.71
1	D	44	PHE	N-CA-C	-5.23	106.74	113.23
1	C	44	PHE	N-CA-C	-5.22	106.96	113.38
1	D	43	PHE	N-CA-C	5.16	116.82	108.41
1	E	244	ASP	N-CA-C	5.14	119.04	112.87
1	D	182	GLN	N-CA-C	-5.11	106.35	112.59
1	X	22	GLU	N-CA-C	-5.07	105.67	111.14
1	E	126	ILE	N-CA-C	5.06	115.18	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	ASN	N-CA-C	-5.05	106.89	113.16
1	D	123	ASN	N-CA-C	-5.05	106.90	113.16
1	Z	49	ARG	N-CA-C	5.04	116.46	110.97
1	E	-1	SER	N-CA-C	-5.04	106.73	112.92
1	Z	125	VAL	N-CA-C	5.03	115.25	110.42
1	E	24	LYS	N-CA-C	-5.03	105.88	111.36
1	E	103	TYR	N-CA-C	5.03	119.36	112.88
1	D	38	THR	N-CA-C	5.02	116.70	108.52
1	Z	123	ASN	N-CA-C	-5.01	106.95	113.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2582	0	2551	125	0
1	D	2593	0	2564	129	0
1	E	2593	0	2564	120	0
1	X	2593	0	2564	106	0
1	Y	2593	0	2564	98	0
1	Z	2578	0	2548	97	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	640	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 21.

All (640) 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:X:41:MET:HE3	1:X:141:MET:HE1	1.42	1.00
1:Z:169:VAL:HG11	1:Z:192:MET:HE2	1.45	0.97
1:Y:153:ALA:O	1:Y:157:THR:HG22	1.67	0.94
1:X:70:ILE:HD11	1:X:100:MET:HE1	1.50	0.93
1:Y:177:PRO:HD3	1:Y:281:MET:HE2	1.52	0.91
1:X:24:LYS:NZ	1:X:301:ASN:HD21	1.68	0.90
1:X:24:LYS:HZ3	1:X:301:ASN:HD21	1.15	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:D:169:VAL:HG11	1:D:192:MET:HE2	1.60	0.83
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:C:169:VAL:HG11	1:C:192:MET:HE2	1.62	0.81
1:X:0:HIS:HA	1:X:316:ASN:ND2	1.95	0.80
1:Y:24:LYS:NZ	1:Y:301:ASN:HD21	1.79	0.80
1:Y:24:LYS:HG2	1:Y:304:ILE:HG12	1.64	0.80
1:C:119:GLU:HG2	1:C:123:ASN:HD21	1.47	0.79
1:Y:70:ILE:HD11	1:Y:100:MET:HE1	1.65	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:Y:169:VAL:HG11	1:Y:192:MET:HE2	1.64	0.78
1:D:0:HIS:HA	1:D:316:ASN:ND2	1.98	0.78
1:X:311:LYS:O	1:X:315:GLU:HG3	1.84	0.78
1:C:119:GLU:HG2	1:C:123:ASN:ND2	1.98	0.78
1:Z:50:THR:HG21	1:Z:141:MET:HB3	1.64	0.78
1:E:169:VAL:HG11	1:E:192:MET:HE2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Z:24:LYS:NZ	1:Z:301:ASN:HD21	1.83	0.76
1:Z:24:LYS:HZ3	1:Z:301:ASN:HD21	1.34	0.75
1:X:284:THR:HG22	1:X:286:ASP:H	1.52	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:E:294:ILE:C	1:E:297:PRO:HD2	2.11	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:X:50:THR:HG22	1:X:141:MET:HE2	1.69	0.72
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:50:THR:HG22	1:E:141:MET:HE2	1.72	0.71
1:Y:124:GLU:HB3	1:Y:127:ILE:CG2	2.20	0.70
1:Y:24:LYS:HZ3	1:Y:301:ASN:HD21	1.37	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:E:41:MET:HE3	1:E:141:MET:HE1	1.75	0.69
1:Z:169:VAL:HG11	1:Z:192:MET:CE	2.22	0.69
1:C:50:THR:HG22	1:C:141:MET:HE2	1.73	0.68
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:C:70:ILE:HD11	1:C:100:MET:HE1	1.74	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
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:Z:311:LYS:O	1:Z:315:GLU:HG3	1.95	0.67
1:C:49:ARG:HH21	1:C:276:PRO:HG3	1.59	0.67
1:C:59:LEU:HD13	1:E:64:ASN:HB3	1.77	0.67
1:D:177:PRO:HD3	1:D:281:MET:HE2	1.75	0.66
1:C:24:LYS:HG2	1:C:304:ILE:HG12	1.76	0.66
1:C:177:PRO:HD3	1:C:281:MET:HE2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Z:24:LYS:HG2	1:Z:304:ILE:HG12	1.76	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:Y:285:ASP:O	1:Y:289:GLU:HG3	1.96	0.64
1:Z:175:PRO:O	1:Z:281:MET:HE3	1.97	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:X:169:VAL:HG11	1:X:192:MET:HE2	1.79	0.63
1:D:208:GLU:CG	1:D:242:LEU:HD11	2.28	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:Z:70:ILE:O	1:Z:71:ASN:HB2	1.99	0.62
1:X:265:VAL:HG12	1:X:265:VAL:O	2.00	0.62
1:Y:208:GLU:HG2	1:Y:242:LEU:HD11	1.80	0.62
1:Y:228:GLU:HA	1:Y:265:VAL:HG12	1.81	0.62
1:Z:89:LYS:N	1:Z:89:LYS:HD2	2.15	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:E:291:PRO:HG2	1:E:292:GLN:NE2	2.14	0.62
1:Z:97:ILE:HB	1:Z:98:PRO:HD3	1.82	0.62
1:D:95:GLU:O	1:D:98:PRO:HD2	1.99	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:Z:182:GLN:C	1:Z:185:PRO:HD2	2.25	0.61
1:D:125:VAL:O	1:D:129:GLN:HG3	2.00	0.61
1:Y:97:ILE:HB	1:Y:98:PRO:HD3	1.81	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:C:34:GLY:O	1:C:37:LYS:HB2	2.00	0.61
1:D:142:GLU:OE1	3:D:353:SN0:HD3	2.01	0.61
1:E:70:ILE:O	1:E:71:ASN:HB2	2.01	0.61
1:D:208:GLU:HG2	1:D:242:LEU:HD11	1.81	0.60
1:E:97:ILE:HB	1:E:98:PRO:HD3	1.83	0.60
1:X:284:THR:HG22	1:X:286:ASP:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:279:ARG:HD3	1:Z:285:ASP:OD2	2.01	0.60
1:X:41:MET:CE	1:X:141:MET:HE1	2.23	0.60
1:Y:279:ARG:HD3	1:Y:285:ASP:OD2	2.01	0.60
1:E:56:LYS:NZ	1:E:303:GLU:OE2	2.33	0.60
1:E:89:LYS:HD2	1:E:89:LYS:N	2.17	0.60
1:E:291:PRO:HG2	1:E:292:GLN:HE22	1.66	0.60
1:C:41:MET:HE3	1:C:141:MET:HE1	1.83	0.60
1:D:41:MET:HE3	1:D:141:MET:HE1	1.83	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:D:175:PRO:O	1:D:281:MET:HE3	2.02	0.59
1:Z:204:PRO:HG3	1:Z:256:TRP:CE2	2.36	0.59
1:E:35:ARG:HG2	1:E:36:ASN:ND2	2.17	0.59
1:E:41:MET:CE	1:E:141:MET:HE1	2.32	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:X:41:MET:HE3	1:X:141:MET:CE	2.24	0.59
1:X:182:GLN:C	1:X:185:PRO:HD2	2.28	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:E:182:GLN:C	1:E:185:PRO:HD2	2.28	0.59
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:D:304:ILE:O	1:D:308:VAL:HG23	2.04	0.58
1:Y:124:GLU:HB3	1:Y:127:ILE:HG22	1.85	0.58
1:E:124:GLU:HB3	1:E:127:ILE:HG22	1.86	0.58
1:X:0:HIS:HA	1:X:316:ASN:HD21	1.68	0.58
1:X:294:ILE:C	1:X:297:PRO:HD2	2.28	0.58
1:Z:275:LEU:HD12	1:Z:277:VAL:CG2	2.34	0.58
1:Y:95:GLU:O	1:Y:98:PRO:HD2	2.03	0.58
1:C:279:ARG:HD3	1:C:285:ASP:OD2	2.04	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:Z:124:GLU:HB3	1:Z:127:ILE:CG2	2.34	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:Y:176:HIS:CD2	1:Y:180:LEU:HD11	2.39	0.57
1:E:284:THR:HG22	1:E:286:ASP:H	1.70	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:Y:184:VAL:HB	1:Y:185:PRO:HD3	1.86	0.57
1:D:64:ASN:HB3	1:E:59:LEU:HD13	1.86	0.57
1:Y:203:HIS:HD2	1:Y:204:PRO:O	1.88	0.56
1:C:0:HIS:HA	1:C:316:ASN:HD22	1.64	0.56
1:D:50:THR:HG22	1:D:141:MET:HE2	1.86	0.56
1:X:114:ARG:HD3	4:X:396:HOH:O	2.05	0.56
1:Y:208:GLU:CD	1:Y:208:GLU:H	2.14	0.56
1:Z:177:PRO:HD3	1:Z:281:MET:HE2	1.86	0.56
1:Z:305:SER:O	1:Z:309:VAL:HG23	2.06	0.56
1:C:41:MET:CE	1:C:141:MET:HE1	2.35	0.56
1:C:70:ILE:HD13	1:C:77:LEU:HD11	1.86	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:C:184:VAL:HB	1:C:185:PRO:HD3	1.88	0.55
1:C:47:SER:HB2	1:C:110:ARG:NH1	2.22	0.55
1:C:49:ARG:HH22	1:E:91:GLU:CD	2.15	0.55
1:Z:267:ASN:O	4:Z:372:HOH:O	2.18	0.55
1:Z:285:ASP:O	1:Z:289:GLU:HG3	2.06	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:D:166:ARG:HG2	1:D:196:ASP:OD2	2.06	0.55
1:E:230:ALA:O	1:E:269:ALA:HB2	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:X:24:LYS:HZ3	1:X:301:ASN:ND2	1.96	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:D:169:VAL:HG11	1:D:192:MET:CE	2.33	0.54
1:Z:4:PHE:CE2	1:Z:148:PRO:HB2	2.42	0.54
1:X:210:ASP:HA	1:X:241:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:184:VAL:HB	1:Z:185:PRO:HD3	1.88	0.54
1:D:305:SER:O	1:D:309:VAL:HG23	2.08	0.54
1:E:49:ARG:HH21	1:E:276:PRO:HG3	1.73	0.54
1:E:105:ASP:O	1:E:137:PRO:HD2	2.07	0.54
1:Y:49:ARG:HH21	1:Y:276:PRO:HG3	1.71	0.54
1:X:7:VAL:HG12	1:X:190:GLU:OE2	2.07	0.54
1:Y:192:MET:HE3	1:Y:197:TYR:HD1	1.73	0.54
1:E:-3:ARG:HH11	1:E:-3:ARG:CB	2.19	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: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:C:230:ALA:O	1:C:269:ALA:HB2	2.09	0.53
1:D:122:TYR:OH	1:D:182:GLN:HG3	2.08	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:C:41:MET:HE3	1:C:54:THR:HB	1.89	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:Y:50:THR:HG21	1:Y:141:MET:HB3	1.89	0.53
1:C:41:MET:HE3	1:C:141:MET:CE	2.39	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: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:C:294:ILE:C	1:C:297:PRO:HD2	2.34	0.53
1:D:41:MET:HE3	1:D:141:MET:CE	2.39	0.52
1:D:93:LEU:HG	1:D:97:ILE:HD11	1.91	0.52
1:E:41:MET:HE3	1:E:54:THR:HB	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:C:4:PHE:CD2	1:C:309:VAL:HG11	2.45	0.52
1:E:235:ALA:O	1:E:273:HIS:CD2	2.63	0.52
1:C:203:HIS:HD2	1:C:204:PRO:O	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LYS:NZ	1:C:301:ASN:HD21	2.08	0.52
1:C:45:ASN:ND2	1:C:112:PHE:HB2	2.25	0.52
1:X:89:LYS:HD2	1:X:89:LYS:N	2.25	0.52
1:Y:24:LYS:HG2	1:Y:304:ILE:CG1	2.39	0.52
1:Y:273:HIS:O	1:Y:275:LEU:HD13	2.09	0.52
1:D:68:LEU:HD22	1:D:69:ASP:N	2.24	0.52
1:D:230:ALA:O	1:D:269:ALA:HB2	2.09	0.52
1:E:273:HIS:CE1	1:E:277:VAL:HG22	2.45	0.52
1:C:240:ALA:HB2	1:C:250:LEU:HG	1.92	0.52
1:X:95:GLU:C	1:X:98:PRO:HD2	2.34	0.52
1:Z:228:GLU:HG2	4:Z:401:HOH:O	2.10	0.52
1:Z:294:ILE:C	1:Z:297:PRO:HD2	2.34	0.52
1:C:77:LEU:O	1:C:89:LYS:HG2	2.10	0.52
1:E:188:PHE:O	1:E:192:MET:HG2	2.10	0.52
1:C:83:VAL:HG12	1:C:84:ILE:N	2.24	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: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:D:291:PRO:HG2	1:D:292:GLN:NE2	2.25	0.51
1:E:177:PRO:HD3	1:E:281:MET:HE2	1.92	0.51
1:X:175:PRO:HG2	1:X:281:MET:O	2.10	0.51
1:X:294:ILE:O	1:X:297:PRO:HD2	2.11	0.51
1:Y:294:ILE:C	1:Y:297:PRO:HD2	2.36	0.51
1:X:192:MET:HE3	1:X:197:TYR:HD1	1.75	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:E:210:ASP:HB3	1:E:213:PHE:HD1	1.74	0.51
1:X:24:LYS:CG	1:X:304:ILE:HG12	2.37	0.51
1:Y:24:LYS:HZ2	1:Y:301:ASN:ND2	2.09	0.51
1:C:24:LYS:CG	1:C:304:ILE:HG12	2.40	0.51
1:C:284:THR:HG22	1:C:286:ASP:N	2.23	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:Z:124:GLU:OE1	1:Z:144:ALA:HB3	2.11	0.51
1:D:26:ASP:CG	1:D:29:LYS:HB2	2.35	0.51
1:D:98:PRO:CB	1:E:296:ILE:HD13	2.41	0.51
1:E:41:MET:HE3	1:E:141:MET:CE	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:285:ASP:HB3	1:E:81:ARG:HH12	1.75	0.50
1:X:23:ILE:HD13	1:X:307:THR:HG22	1.91	0.50
1:Y:308:VAL:O	1:Y:312:ARG:HG2	2.11	0.50
1:X:112:PHE:HA	4:X:369:HOH:O	2.10	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:105:ASP:O	1:C:137:PRO:HD2	2.12	0.50
1:C:210:ASP:HB3	1:C:213:PHE:HD1	1.75	0.50
1:X:70:ILE:HD13	1:X:77:LEU:HD11	1.92	0.50
1:C:59:LEU:HD13	1:E:64:ASN:CB	2.41	0.50
1:C:124:GLU:HB3	1:C:127:ILE:HG21	1.92	0.50
1:C:168:LYS:HA	1:C:198:GLU:HB3	1.94	0.50
1:Z:83:VAL:HG12	1:Z:84:ILE:N	2.25	0.50
1:D:208:GLU:HG3	1:D:242:LEU:HD11	1.94	0.50
1:E:118:ARG:HG3	1:E:246:TYR:CD1	2.47	0.50
1:E:212:LYS:HE3	1:E:213:PHE:CE1	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: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:C:169:VAL:HG11	1:C:192:MET:CE	2.38	0.50
1:E:50:THR:CG2	1:E:141:MET:HE2	2.41	0.50
1:X:209:LEU:HD21	1:X:238:TRP:CE2	2.47	0.49
1:D:208:GLU:HG2	1:D:242:LEU:CD1	2.41	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:C:228:GLU:HG3	1:C:265:VAL:CG1	2.41	0.49
1:D:89:LYS:HD2	1:D:89:LYS:N	2.26	0.49
1:Y:81:ARG:HH12	1:Z:285:ASP:HB3	1.78	0.49
1:X:279:ARG:HD3	1:X:285:ASP:OD2	2.13	0.49
1:Y:240:ALA:HB3	1:Y:245:ASN:O	2.11	0.49
1:Z:153:ALA:O	1:Z:157:THR:CG2	2.56	0.49
1:C:70:ILE:O	1:C:71:ASN:CB	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:210:ASP:HB3	1:X:213:PHE:HD1	1.77	0.49
1:D:314:LEU:HD23	1:D:317:LEU:HD12	1.94	0.49
1:D:267:ASN:O	1:D:268:ASN:C	2.55	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:X:203:HIS:HD2	1:X:204:PRO:O	1.96	0.48
1:C:284:THR:HG22	1:C:285:ASP:N	2.27	0.48
1:D:228:GLU:HA	1:D:265:VAL:HG12	1.95	0.48
1:E:39:LEU:HD22	1:E:310:LEU:HD21	1.95	0.48
1:Z:95:GLU:C	1:Z:98:PRO:HD2	2.38	0.48
1:D:4:PHE:CZ	1:D:148:PRO:HB2	2.48	0.48
1:Z:125:VAL:O	1:Z:129:GLN:HG3	2.13	0.48
1:C:97:ILE:CB	1:C:98:PRO:HD3	2.37	0.48
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:Y:24:LYS:HZ2	1:Y:301:ASN:HD21	1.56	0.48
1:D:294:ILE:C	1:D:297:PRO:HD2	2.38	0.48
1:E:168:LYS:HA	1:E:198:GLU:HB3	1.95	0.48
1:X:273:HIS:O	1:X:275:LEU:HD13	2.12	0.48
1:D:35:ARG:HG2	1:D:36:ASN:ND2	2.29	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: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:Z:228:GLU:HA	1:Z:265:VAL:HG12	1.95	0.48
1:D:188:PHE:O	1:D:192:MET:HG2	2.13	0.48
1:E:4:PHE:CE2	1:E:309:VAL:HG21	2.49	0.48
1:E:70:ILE:O	1:E:71:ASN:CB	2.62	0.48
1:E:208:GLU:CG	1:E:242:LEU:HD11	2.43	0.48
1:D:43:PHE:CZ	1:D: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:22:GLU:OE2	1:Z:30:TYR:OH	2.28	0.47
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:83:VAL:HG12	1:D:84:ILE:N	2.28	0.47
1:D:216:ASN:ND2	4:D:372:HOH:O	2.46	0.47
1:E:1:MET:HE1	1:E:10:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:TYR:C	1:E:32:GLU:H	2.23	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:23:ILE:HD13	1:Z:307:THR:HG22	1.97	0.47
1:Z:168:LYS:HA	1:Z:198:GLU:HB3	1.95	0.47
1:D:85:MET:HE1	1:D:91:GLU:C	2.39	0.47
1:D:100:MET:HE3	1:E:48:LEU:HD21	1.97	0.47
1:Z:61:LEU:CD1	1:Z:310:LEU:HB3	2.44	0.47
1:Z:203:HIS:HD2	1:Z:204:PRO:O	1.97	0.47
1:C:4:PHE:CE2	1:C:309:VAL:HG21	2.49	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
1:Z:230:ALA:O	1:Z:269:ALA:HB2	2.15	0.47
1:C:59:LEU:CD1	1:E:64:ASN:HB3	2.45	0.47
1:D:24:LYS:NZ	1:D:301:ASN:HD21	2.12	0.47
1:E:85:MET:HE1	1:E:91:GLU:C	2.40	0.47
1:C:95:GLU:CD	1:D:279:ARG:HH21	2.22	0.47
1:E:50:THR:HG21	1:E:141:MET:HB3	1.97	0.47
1:Z:70:ILE:HD11	1:Z:100:MET:HE1	1.97	0.47
1:C:49:ARG:NH2	1:C:276:PRO:HG3	2.26	0.47
1:D:296:ILE:HB	1:D:297:PRO:HD3	1.97	0.47
1:E:7:VAL:O	1:E:10:ILE:HG22	2.15	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:X:208:GLU:CG	1:X:242:LEU:HD11	2.46	0.46
1:C:64:ASN:HB3	1:D:59:LEU:HD13	1.97	0.46
1:Z:70:ILE:O	1:Z:71:ASN:CB	2.61	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: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:D:152:PHE:CE1	1:D:156:ILE:HD11	2.50	0.46
1:X:105:ASP:O	1:X:137:PRO:HD2	2.14	0.46
1:C:80:GLU:O	1:C:92:HIS:NE2	2.45	0.46
1:C:306:ALA:O	1:C:310:LEU:HB2	2.15	0.46
1:D:282:ILE:HG13	4:D:366:HOH:O	2.15	0.46
1:X:1:MET:HE1	1:X:10:ILE:HD12	1.98	0.46
1:X:152:PHE:O	1:X:156:ILE:HG13	2.16	0.46
1:C:27:ARG:HB2	4:C:366:HOH:O	2.16	0.46
1:D:70:ILE:O	1:D:71:ASN:CB	2.64	0.46
1:Z:4:PHE:CZ	1:Z:148:PRO:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:273:HIS:O	1:Z:275:LEU:HD13	2.16	0.46
1:C:275:LEU:HD23	1:E:99:VAL:HG21	1.97	0.46
1:D:203:HIS:HD2	1:D:204:PRO:O	1.98	0.46
3:C:351:SN0:C4	1:E:90:PRO:HB3	2.46	0.46
1:E:45:ASN:ND2	1:E:112:PHE:HB2	2.31	0.46
1:E:240:ALA:HB2	1:E:250:LEU:HG	1.98	0.46
1:X:-3:ARG:C	1:X:-1:SER:H	2.22	0.46
1:X:107:ILE:HD12	1:X:134:SER:HB2	1.98	0.46
1:Y:202:THR:O	1:Y:202:THR:HG23	2.15	0.46
1:Z:227:PHE:CD2	1:Z:262:GLN:HB3	2.50	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:E:127:ILE:HG23	1:E:128:ASN:N	2.31	0.45
1:X:50:THR:HG21	1:X:141:MET:HB3	1.97	0.45
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:159:GLU:HG2	1:X:197:TYR:OH	2.16	0.45
1:Y:89:LYS:HA	1:Y:90:PRO:HD3	1.84	0.45
1:Y:265:VAL:HG12	1:Y:265:VAL:O	2.16	0.45
1:Z:85:MET:HE1	1:Z:91:GLU:C	2.42	0.45
1:D:162:LYS:HD2	1:D:164:THR:O	2.15	0.45
1:E:0:HIS:CE1	4:E:377:HOH:O	2.70	0.45
1:D:274:CYS:O	1:D:275:LEU:HB2	2.16	0.45
1:Y:166:ARG:HG2	1:Y:196:ASP:OD2	2.16	0.45
1:Z:88:ASP:HB3	1:Z:89:LYS:HD2	1.99	0.45
1:D:78:GLU:HB2	1:D:85:MET:HE3	1.99	0.45
1:X:141:MET:O	1:X:142:GLU:CB	2.65	0.45
1:Y:182:GLN:C	1:Y:185:PRO:HD2	2.42	0.45
1:C:44:PHE:CZ	1:C:70:ILE:HD12	2.51	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:C:182:GLN:C	1:C:185:PRO:HD2	2.42	0.45
1:X:98:PRO:HB2	1:Y:296:ILE:HD13	1.99	0.45
1:X:208:GLU:HG2	1:X:242:LEU:HD11	1.98	0.45
1:Y:122:TYR:OH	1:Y:182:GLN:CG	2.64	0.45
1:Y:222:ASP:HB3	1:Y:225:LYS:HB2	1.98	0.45
1:E:95:GLU:O	1:E:98:PRO:HD2	2.17	0.45
1:Z:187:SER:O	1:Z:191:TRP:HD1	2.00	0.45
1:C:311:LYS:O	1:C:315:GLU:HG3	2.17	0.45
1:Y:91:GLU:HG3	4:Y:366:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ILE:O	1:C:297:PRO:HD2	2.18	0.44
1:D:284:THR:HG22	1:D:286:ASP:H	1.82	0.44
1:X:23:ILE:HD12	1:X:308:VAL:HG22	1.97	0.44
1:X:125:VAL:O	1:X:129:GLN:HG3	2.18	0.44
1:Z:119:GLU:HG2	1:Z:123:ASN:HD21	1.82	0.44
1:Z:189:ALA:HA	1:Z:199:PHE:CE2	2.51	0.44
1:D:78:GLU:CB	1:D:85:MET:HE3	2.48	0.44
1:D:237:ASN:CG	1:D:238:TRP:N	2.76	0.44
1:Y:118:ARG:HA	1:Y:246:TYR:CE2	2.53	0.44
1:Y:230:ALA:O	1:Y:269:ALA:HB2	2.17	0.44
1:Z:124:GLU:O	1:Z:128:ASN:HB2	2.17	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:C:228:GLU:HG3	1:C:265:VAL:HG11	1.98	0.44
1:C:228:GLU:HA	1:C:265:VAL:HG12	2.00	0.44
1:C:241:TYR:HD2	1:C:242:LEU:HD23	1.80	0.44
1:D:184:VAL:CG1	1:D:236:LYS:HG2	2.47	0.44
1:Y:78:GLU:HG3	1:Y:85:MET:HG2	1.99	0.44
1:D:182:GLN:C	1:D:185:PRO:HD2	2.42	0.44
1:X:275:LEU:HD12	1:X:277:VAL:HG22	2.00	0.44
1:Y:192:MET:CE	1:Y:197:TYR:CD1	3.00	0.44
1:Y:192:MET:HE1	1:Y:197:TYR:CD1	2.53	0.44
1:Z:122:TYR:HA	1:Z:145:THR:HG21	1.98	0.44
1:Z:225:LYS:HE2	1:Z:225:LYS:HB3	1.86	0.44
1:C:276:PRO:HB3	1:E:91:GLU:HB2	1.99	0.44
1:Y:34:GLY:O	1:Y:37:LYS:HB2	2.16	0.44
1:Z:105:ASP:O	1:Z:137:PRO:HD2	2.17	0.44
1:Z:212:LYS:HE3	1:Z:213:PHE:CZ	2.52	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: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:Z:51:ARG:O	1:Z:55:GLN:HG3	2.17	0.44
1:C:88:ASP:HB3	1:C:89:LYS:HD2	1.98	0.44
1:D:175:PRO:HG3	1:D:254:ARG:HA	2.00	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:X:176:HIS:CG	1:X:177:PRO:HD2	2.53	0.44
1:X:192:MET:HE1	1:X:197:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:VAL:HG21	1:D:226:ALA:O	2.18	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:7:VAL:O	1:Z:10:ILE:HG22	2.18	0.43
1:Z:89:LYS:N	1:Z:89:LYS:CD	2.81	0.43
1:D:208:GLU:CD	1:D:208:GLU:H	2.26	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:E:192:MET:HE1	1:E:197:TYR:HD1	1.82	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:Y:245:ASN:HA	1:Y:248:GLN:HG3	1.99	0.43
1:C:89:LYS:HA	1:C:90:PRO:HD3	1.70	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:X:279:ARG:NE	1:Z:95:GLU:OE2	2.43	0.43
1:Y:83:VAL:HG12	1:Y:84:ILE:N	2.34	0.43
1:D:124:GLU:HB3	1:D:127:ILE:HG23	1.96	0.43
1:D:272:MET:O	1:D:273:HIS:HB2	2.17	0.43
1:D:310:LEU:HD12	1:D:310:LEU:HA	1.82	0.43
1:Y:152:PHE:O	1:Y:156:ILE:HG13	2.19	0.43
1:Z:17:LEU:O	1:Z:21:PHE:HD1	2.02	0.43
1:D:61:LEU:HD12	1:D:310:LEU:HB3	2.01	0.43
1:D:227:PHE:CD2	1:D:262:GLN:HB3	2.53	0.43
1:D:284:THR:HG22	1:D:285:ASP:N	2.33	0.43
1:E:119:GLU:HG2	1:E:123:ASN:ND2	2.34	0.43
1:E:275:LEU:HA	1:E:276:PRO:C	2.43	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: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:C:178:ARG:C	1:C:249:ILE:HD11	2.43	0.43
1:C:310:LEU:HD12	1:C:310:LEU:HA	1.89	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:Y:294:ILE:O	1:Y:297:PRO:HD2	2.19	0.43
1:Z:245:ASN:O	1:Z:246:TYR:C	2.61	0.43
1:Z:245:ASN:O	1:Z:248:GLN:HB2	2.19	0.43
1:C:212:LYS:HE3	1:C:213:PHE:CE1	2.54	0.43
1:D:61:LEU:CD1	1:D:310:LEU:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:LEU:O	1:D:97:ILE:HG13	2.19	0.43
1:D:275:LEU:HA	1:D:276:PRO:C	2.44	0.43
1:E:174:ALA:HB1	1:E:282:ILE:HA	1.99	0.43
1:Z:185:PRO:HG2	1:Z:238:TRP:HB3	2.01	0.42
1:C:154:ASP:O	1:C:157:THR:HG23	2.19	0.42
1:C:186:ASN:HB3	1:C:213:PHE:CG	2.54	0.42
1:E:202:THR:O	1:E:202:THR:HG23	2.19	0.42
1:E:227:PHE:O	1:E:266:THR:HG22	2.19	0.42
1:E:310:LEU:HD12	1:E:310:LEU:HA	1.81	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:X:242:LEU:O	1:X:243:GLY:C	2.62	0.42
1:E:182:GLN:HE21	1:E:182:GLN:HB3	1.66	0.42
1:C:176:HIS:ND1	1:C:177:PRO:HD2	2.34	0.42
1:D:206:GLY:N	1:D:208:GLU:OE2	2.52	0.42
1:D:93:LEU:HG	1:D:97:ILE:CD1	2.50	0.42
1:E:141:MET:O	1:E:142:GLU:CB	2.67	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
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:X:122:TYR:OH	1:X:182:GLN:CG	2.66	0.42
1:Z:150:GLN:OE1	1:Z:302:ARG:NH1	2.53	0.42
1:C:97:ILE:HB	1:C:98:PRO:CD	2.39	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:Z:170:VAL:HG22	1:Z:200:VAL:HB	2.01	0.42
1:C:265:VAL:HG12	1:C:265:VAL:O	2.18	0.42
1:Z:285:ASP:O	1:Z:288:ILE:HG22	2.20	0.42
1:C:70:ILE:HG22	1:C:71:ASN:N	2.34	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:D:176:HIS:ND1	1:D:177:PRO:HD2	2.35	0.42
1:E:17:LEU:O	1:E:20:SER:HB2	2.20	0.42
1:E:166:ARG:HG2	1:E:196:ASP:OD2	2.20	0.42
1:X:119:GLU:HG2	1:X:123:ASN:ND2	2.35	0.42
1:X:223:GLN:HB2	1:X:256:TRP:CZ3	2.55	0.42
1:Y:64:ASN:HB3	1:Z:59:LEU:HD13	2.02	0.42
1:Z:296:ILE:HB	1:Z:297:PRO:HD3	2.02	0.42
1:C:118:ARG:NH2	1:C:243:GLY:N	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:MET:HE2	1:E:298:GLU:OE2	2.19	0.42
1:C:78:GLU:HG3	1:C:85:MET:HG2	2.02	0.41
1:C:48:LEU:HD21	1:E:100:MET:HE3	2.01	0.41
1:D:254:ARG:HD3	4:D:379:HOH:O	2.20	0.41
1:X:59:LEU:HD13	1:Z:64:ASN:HB3	2.01	0.41
1:Z:184:VAL:N	1:Z:185:PRO:CD	2.83	0.41
1:E:-3:ARG:HH12	1:E:9:ASP:HA	1.86	0.41
1:X:50:THR:CG2	1:X:141:MET:HE2	2.43	0.41
1:X:78:GLU:HB3	1:X:92:HIS:CD2	2.56	0.41
1:X:157:THR:HB	1:X:301:ASN:OD1	2.19	0.41
1:X:173:TRP:CG	1:X:174:ALA:N	2.88	0.41
1:Y:228:GLU:HG3	1:Y:265:VAL:CG1	2.49	0.41
1:C:31:VAL:O	1:C:62:GLY:HA3	2.19	0.41
1:C:61:LEU:HD12	1:C:310:LEU:HB3	2.03	0.41
1:X:98:PRO:HB2	1:Y:296:ILE:CD1	2.51	0.41
1:Y:95:GLU:HG2	4:Z:384:HOH:O	2.19	0.41
1:Z:191:TRP:O	1:Z:195:THR:HG23	2.20	0.41
1:Z:306:ALA:O	1:Z:310:LEU:HB2	2.19	0.41
1:C:24:LYS:HZ2	1:C:301:ASN:HD21	1.68	0.41
1:C:122:TYR:CD2	1:C:145:THR:HG21	2.56	0.41
1:C:141:MET:O	1:C:142:GLU:CB	2.67	0.41
1:D:151:SER:O	1:D:154:ASP:HB2	2.21	0.41
1:E:89:LYS:N	1:E:89:LYS:CD	2.84	0.41
1:E:192:MET:HE1	1:E:197:TYR:CD1	2.56	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: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:D:182:GLN:O	1:D:186:ASN:CG	2.64	0.41
1:Y:19:GLU:OE2	1:Y:312:ARG:NE	2.44	0.41
1:Y:241:TYR:CD2	1:Y:242:LEU:HD23	2.55	0.41
1:D:154:ASP:HA	1:D:157:THR:CG2	2.50	0.41
1:D:272:MET:HE2	1:D:298:GLU:OE2	2.20	0.41
1:E:225:LYS:HE2	1:E:225:LYS:HB3	1.82	0.41
1:E:296:ILE:N	1:E:297:PRO:CD	2.83	0.41
1:Y:95:GLU:C	1:Y:98:PRO:HD2	2.46	0.41
1:Z:162:LYS:HD2	1:Z:164:THR:O	2.20	0.41
1:D:30:TYR:C	1:D:32:GLU:H	2.28	0.41
1:E:237:ASN:CG	1:E:238:TRP:N	2.78	0.41
1:E:274:CYS:O	1:E:275:LEU:O	2.38	0.41
1:X:231:ASP:HB3	4:X:403:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:103:TYR:O	1:Z:56:LYS:HD3	2.21	0.41
1:Z:211:PRO:C	1:Z:213:PHE:N	2.78	0.41
1:C:176:HIS:CG	1:C:177:PRO:HD2	2.56	0.41
1:D:171:MET:HG3	1:D:188:PHE:CD2	2.56	0.41
1:Z:304:ILE:N	1:Z:304:ILE:HD12	2.36	0.41
1:C:242:LEU:O	1:C:243:GLY:C	2.64	0.41
1:D:17:LEU:O	1:D:21:PHE:HD1	2.03	0.41
1:D:89:LYS:HA	1:D:90:PRO:HD3	1.90	0.41
1:E:31:VAL:O	1:E:31:VAL:HG22	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:103:TYR:OH	1:E:299:ALA:O	2.36	0.40
1:D:114:ARG:HB2	4:D:357:HOH:O	2.21	0.40
1:Y:22:GLU:OE2	1:Y:30:TYR:OH	2.36	0.40
1:C:227:PHE:O	1:C:266:THR:HG22	2.22	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:X:176:HIS:NE2	1:X:278:ARG:HD2	2.36	0.40
1:Y:92:HIS:CE1	1:Y:94:LEU:HG	2.56	0.40
1:Y:103:TYR:CZ	1:Z:53:SER:HB3	2.56	0.40
1:Z:317:LEU:O	1:Z:318:PRO:O	2.39	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:D:152:PHE:C	1:D:152:PHE:CD1	2.98	0.40
1:X:42:ILE:HD13	1:X:100:MET:SD	2.61	0.40
1:X:237:ASN:CG	1:X:238:TRP:N	2.79	0.40
1:C:45:ASN:HD21	1:C:112:PHE:HB2	1.86	0.40
1:C:124:GLU:OE1	1:C:144:ALA:HB3	2.22	0.40
1:C:259:GLY:HA2	1:C:284:THR:OG1	2.22	0.40
1:E:1:MET:HE2	1:E:9:ASP:O	2.22	0.40
1:Z:294:ILE:O	1:Z:297:PRO:HD2	2.21	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
1:D:168:LYS:HD3	1:D:230:ALA:HA	2.02	0.40
1:E:24:LYS:NZ	1:E:301:ASN:HD21	2.20	0.40
1:E:30:TYR:C	1:E:32:GLU:N	2.79	0.40

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	C	319/338 (94%)	290 (91%)	26 (8%)	3 (1%)	14	41
1	D	320/338 (95%)	289 (90%)	25 (8%)	6 (2%)	6	22
1	E	320/338 (95%)	292 (91%)	24 (8%)	4 (1%)	9	31
1	X	320/338 (95%)	290 (91%)	27 (8%)	3 (1%)	14	41
1	Y	320/338 (95%)	298 (93%)	20 (6%)	2 (1%)	21	51
1	Z	318/338 (94%)	287 (90%)	28 (9%)	3 (1%)	14	41
All	All	1917/2028 (94%)	1746 (91%)	150 (8%)	21 (1%)	11	36

All (21) 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	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

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Mol	Chain	Res	Type
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%)	264 (95%)	15 (5%)	20	51
1	D	280/294 (95%)	265 (95%)	15 (5%)	20	51
1	E	280/294 (95%)	267 (95%)	13 (5%)	24	58
1	X	280/294 (95%)	265 (95%)	15 (5%)	20	51
1	Y	280/294 (95%)	266 (95%)	14 (5%)	22	54
1	Z	279/294 (95%)	266 (95%)	13 (5%)	23	57
All	All	1678/1764 (95%)	1593 (95%)	85 (5%)	21	54

All (85) 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	89	LYS
1	X	109	VAL
1	X	118	ARG
1	X	157	THR
1	X	182	GLN
1	X	205	GLU
1	X	208	GLU
1	X	277	VAL
1	X	295	VAL
1	X	310	LEU
1	Y	25	LYS
1	Y	48	LEU

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Mol	Chain	Res	Type
1	Y	52	LEU
1	Y	68	LEU
1	Y	78	GLU
1	Y	118	ARG
1	Y	157	THR
1	Y	178	ARG
1	Y	182	GLN
1	Y	208	GLU
1	Y	251	SER
1	Y	277	VAL
1	Y	295	VAL
1	Y	310	LEU
1	Z	25	LYS
1	Z	48	LEU
1	Z	52	LEU
1	Z	118	ARG
1	Z	132	GLN
1	Z	157	THR
1	Z	166	ARG
1	Z	178	ARG
1	Z	182	GLN
1	Z	208	GLU
1	Z	277	VAL
1	Z	295	VAL
1	Z	310	LEU
1	C	25	LYS
1	C	48	LEU
1	C	52	LEU
1	C	68	LEU
1	C	78	GLU
1	C	89	LYS
1	C	95	GLU
1	C	157	THR
1	C	166	ARG
1	C	178	ARG
1	C	182	GLN
1	C	208	GLU
1	C	277	VAL
1	C	295	VAL
1	C	310	LEU
1	D	-3	ARG
1	D	25	LYS

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Mol	Chain	Res	Type
1	D	48	LEU
1	D	52	LEU
1	D	68	LEU
1	D	95	GLU
1	D	157	THR
1	D	171	MET
1	D	178	ARG
1	D	182	GLN
1	D	205	GLU
1	D	208	GLU
1	D	277	VAL
1	D	295	VAL
1	D	310	LEU
1	E	-3	ARG
1	E	25	LYS
1	E	48	LEU
1	E	51	ARG
1	E	52	LEU
1	E	68	LEU
1	E	89	LYS
1	E	118	ARG
1	E	132	GLN
1	E	182	GLN
1	E	205	GLU
1	E	208	GLU
1	E	295	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	0	HIS
1	X	64	ASN
1	X	71	ASN
1	X	132	GLN
1	X	133	HIS
1	X	182	GLN
1	X	203	HIS
1	X	267	ASN
1	X	268	ASN
1	X	301	ASN
1	X	316	ASN
1	Y	64	ASN

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Mol	Chain	Res	Type
1	Y	72	GLN
1	Y	129	GLN
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	280	ASN
1	Z	301	ASN
1	Z	316	ASN
1	C	64	ASN
1	C	123	ASN
1	C	182	GLN
1	C	186	ASN
1	C	203	HIS
1	C	267	ASN
1	C	268	ASN
1	C	301	ASN
1	C	316	ASN
1	D	64	ASN
1	D	132	GLN
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	72	GLN
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 [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 oligosaccharides 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	$\# Z > 2$
3	SN0	X	345	-	14,14,14	0.76	0	17,17,17	1.27	2 (11%)
3	SN0	C	351	-	14,14,14	0.80	0	17,17,17	1.21	2 (11%)
3	SN0	Y	347	-	14,14,14	0.79	0	17,17,17	1.25	3 (17%)
3	SN0	Z	349	-	14,14,14	0.95	0	17,17,17	1.41	1 (5%)
3	SN0	D	353	-	14,14,14	0.89	0	17,17,17	1.21	2 (11%)
2	SO4	X	357	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	C	352	-	4,4,4	0.31	0	6,6,6	0.10	0
2	SO4	X	346	-	4,4,4	0.35	0	6,6,6	0.18	0
2	SO4	Z	350	-	4,4,4	0.41	0	6,6,6	0.14	0
2	SO4	C	358	-	4,4,4	0.41	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	E	356	-	4,4,4	0.36	0	6,6,6	0.21	0
2	SO4	D	354	-	4,4,4	0.38	0	6,6,6	0.26	0
3	SN0	E	355	-	14,14,14	0.78	0	17,17,17	0.95	0
2	SO4	Y	348	-	4,4,4	0.38	0	6,6,6	0.19	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	X	345	-	-	3/16/16/16	-
3	SN0	C	351	-	-	1/16/16/16	-
3	SN0	Z	349	-	-	0/16/16/16	-
3	SN0	D	353	-	-	1/16/16/16	-
3	SN0	Y	347	-	-	0/16/16/16	-
3	SN0	E	355	-	-	3/16/16/16	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	349	SN0	C-CA-N1	4.42	120.82	110.57
3	D	353	SN0	CB-CA-N1	3.05	116.95	110.91
3	Y	347	SN0	OD2-C4-C3	-2.76	114.35	123.09
3	Y	347	SN0	OD1-C4-C3	2.64	122.34	114.00
3	C	351	SN0	CB-CA-N1	2.50	115.86	110.91
3	D	353	SN0	C-CA-N1	2.48	116.32	110.57
3	C	351	SN0	C-CA-N1	2.36	116.05	110.57
3	X	345	SN0	CB-CA-N1	2.34	115.53	110.91
3	Y	347	SN0	C-CA-N1	2.29	115.88	110.57
3	X	345	SN0	C-CA-N1	2.13	115.51	110.57

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	355	SN0	C1-C2-C3-C4
3	E	355	SN0	C2-C3-C4-OD2
3	E	355	SN0	C2-C3-C4-OD1
3	X	345	SN0	C1-C2-C3-C4

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

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
3	Y	347	SN0	1	0
3	D	353	SN0	1	0
2	C	352	SO4	1	0
3	E	355	SN0	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	321/338 (94%)	0.34	5 (1%) 70 61	54, 72, 92, 108	0
1	D	322/338 (95%)	0.55	7 (2%) 62 52	46, 71, 96, 117	0
1	E	322/338 (95%)	0.04	2 (0%) 85 80	38, 58, 78, 101	0
1	X	322/338 (95%)	-0.27	1 (0%) 90 86	28, 48, 71, 84	0
1	Y	322/338 (95%)	-0.61	0 100 100	22, 35, 51, 78	0
1	Z	320/338 (94%)	-0.34	1 (0%) 90 86	27, 44, 62, 82	0
All	All	1929/2028 (95%)	-0.05	16 (0%) 82 75	22, 55, 86, 117	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	-2	GLY	3.3
1	C	254	ARG	3.1
1	D	227	PHE	2.7
1	D	254	ARG	2.6
1	D	232	PHE	2.5
1	C	-2	GLY	2.4
1	D	270	TYR	2.4
1	C	318	PRO	2.3
1	C	242	LEU	2.3
1	D	267	ASN	2.2
1	D	-3	ARG	2.2
1	D	193	ASN	2.2
1	Z	242	LEU	2.1
1	C	79	THR	2.1
1	E	71	ASN	2.1
1	X	254	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	354	5/5	0.85	0.12	57,60,62,63	0
2	SO4	C	358	5/5	0.86	0.12	83,83,85,85	0
3	SN0	D	353	15/15	0.89	0.12	41,52,57,57	0
3	SN0	C	351	15/15	0.92	0.11	68,69,71,71	0
3	SN0	X	345	15/15	0.94	0.09	46,51,54,56	0
2	SO4	E	356	5/5	0.95	0.09	49,50,53,55	0
3	SN0	E	355	15/15	0.95	0.09	46,51,54,56	0
2	SO4	X	357	5/5	0.96	0.06	53,55,56,58	0
3	SN0	Y	347	15/15	0.96	0.07	30,35,41,41	0
3	SN0	Z	349	15/15	0.96	0.08	37,39,41,41	0
2	SO4	X	346	5/5	0.98	0.04	42,44,44,44	0
2	SO4	Z	350	5/5	0.98	0.05	32,36,38,38	0
2	SO4	C	352	5/5	0.98	0.05	59,60,60,62	0
2	SO4	Y	348	5/5	0.99	0.06	32,35,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.