



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 11:44 PM EDT

PDB ID : 2NV2  
Title : Structure of the PLP synthase complex Pdx1/2 (YaaD/E) from *Bacillus subtilis*  
Authors : Strohmeier, M.; Tews, I.; Sinning, I.  
Deposited on : unknown  
Resolution : 2.12 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

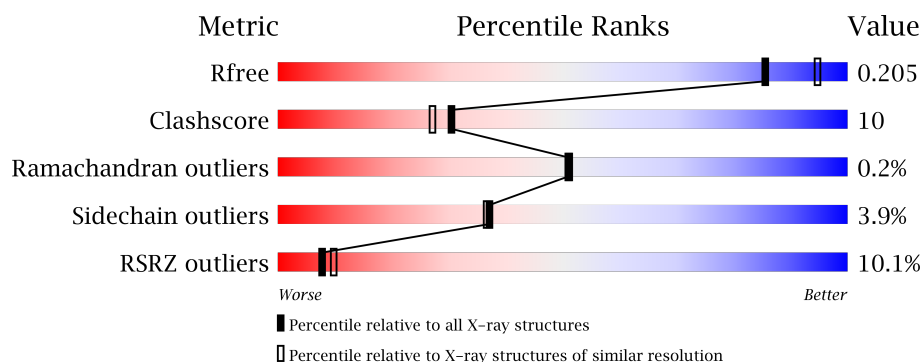
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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))
$R_{free}$	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	294	<div> <div>4%</div> <div>78% 13% • 9%</div> </div>
1	C	294	<div> <div>4%</div> <div>80% 11% • 9%</div> </div>
1	E	294	<div> <div>4%</div> <div>76% 14% • 9%</div> </div>
1	G	294	<div> <div>4%</div> <div>78% 13% • 9%</div> </div>
1	I	294	<div> <div>4%</div> <div>77% 14% • 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	294	
1	M	294	
1	O	294	
1	Q	294	
1	S	294	
1	U	294	
1	W	294	
2	B	204	
2	D	204	
2	F	204	
2	H	204	
2	J	204	
2	L	204	
2	N	204	
2	P	204	
2	R	204	
2	T	204	
2	V	204	
2	X	204	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	6001	-	-	X	-
3	CL	C	6005	-	-	X	-
3	CL	E	6009	-	-	X	-
3	CL	I	6017	-	-	X	-
3	CL	Q	6033	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	S	6037	-	-	X	-
3	CL	U	6041	-	-	X	-
3	CL	W	6045	-	-	X	-
4	EDO	A	6030	-	-	-	X
4	EDO	A	6031	-	-	X	-
4	EDO	E	6047	-	-	X	-
4	EDO	G	6043	-	-	X	X
4	EDO	I	6039	-	-	X	X
4	EDO	M	6007	-	-	X	X
4	EDO	Q	6035	-	-	X	-
5	GLN	R	6036	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 48293 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 Pyridoxal biosynthesis lyase pdxS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	6	0
			2028	1270	354	388	16			
1	C	269	Total	C	N	O	S	0	5	0
			2037	1273	355	393	16			
1	E	269	Total	C	N	O	S	0	5	0
			2037	1273	356	392	16			
1	G	268	Total	C	N	O	S	0	3	0
			2007	1255	348	388	16			
1	I	271	Total	C	N	O	S	0	4	0
			2042	1276	357	393	16			
1	K	270	Total	C	N	O	S	0	4	0
			2032	1272	356	388	16			
1	M	269	Total	C	N	O	S	0	5	0
			2036	1273	356	391	16			
1	O	268	Total	C	N	O	S	0	4	0
			2024	1265	357	386	16			
1	Q	270	Total	C	N	O	S	0	3	0
			2028	1268	356	388	16			
1	S	270	Total	C	N	O	S	0	3	0
			2028	1267	355	390	16			
1	U	271	Total	C	N	O	S	0	4	0
			2034	1271	356	391	16			
1	W	270	Total	C	N	O	S	0	6	0
			2044	1280	357	391	16			

- Molecule 2 is a protein called Glutamine amidotransferase subunit pdxT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	2	0
			1500	948	264	280	8			
2	D	194	Total	C	N	O	S	0	1	0
			1497	946	262	281	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	191	Total	C	N	O	S	0	1	0
			1474	932	257	277	8			
2	H	193	Total	C	N	O	S	0	2	0
			1494	944	260	282	8			
2	J	196	Total	C	N	O	S	0	1	0
			1512	957	264	283	8			
2	L	192	Total	C	N	O	S	0	1	0
			1483	937	259	279	8			
2	N	193	Total	C	N	O	S	0	1	0
			1488	940	260	280	8			
2	P	193	Total	C	N	O	S	0	2	0
			1496	947	261	280	8			
2	R	193	Total	C	N	O	S	0	2	0
			1500	948	264	280	8			
2	T	194	Total	C	N	O	S	0	1	0
			1493	944	262	279	8			
2	V	194	Total	C	N	O	S	0	1	0
			1497	946	262	281	8			
2	X	195	Total	C	N	O	S	0	1	0
			1505	952	263	282	8			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	170	ASN	HIS	ENGINEERED	UNP P37528
B	197	LEU	-	EXPRESSION TAG	UNP P37528
B	198	GLU	-	EXPRESSION TAG	UNP P37528
B	199	HIS	-	EXPRESSION TAG	UNP P37528
B	200	HIS	-	EXPRESSION TAG	UNP P37528
B	201	HIS	-	EXPRESSION TAG	UNP P37528
B	202	HIS	-	EXPRESSION TAG	UNP P37528
B	203	HIS	-	EXPRESSION TAG	UNP P37528
B	204	HIS	-	EXPRESSION TAG	UNP P37528
D	170	ASN	HIS	ENGINEERED	UNP P37528
D	197	LEU	-	EXPRESSION TAG	UNP P37528
D	198	GLU	-	EXPRESSION TAG	UNP P37528
D	199	HIS	-	EXPRESSION TAG	UNP P37528
D	200	HIS	-	EXPRESSION TAG	UNP P37528
D	201	HIS	-	EXPRESSION TAG	UNP P37528
D	202	HIS	-	EXPRESSION TAG	UNP P37528
D	203	HIS	-	EXPRESSION TAG	UNP P37528
D	204	HIS	-	EXPRESSION TAG	UNP P37528
F	170	ASN	HIS	ENGINEERED	UNP P37528

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Chain	Residue	Modelled	Actual	Comment	Reference
F	197	LEU	-	EXPRESSION TAG	UNP P37528
F	198	GLU	-	EXPRESSION TAG	UNP P37528
F	199	HIS	-	EXPRESSION TAG	UNP P37528
F	200	HIS	-	EXPRESSION TAG	UNP P37528
F	201	HIS	-	EXPRESSION TAG	UNP P37528
F	202	HIS	-	EXPRESSION TAG	UNP P37528
F	203	HIS	-	EXPRESSION TAG	UNP P37528
F	204	HIS	-	EXPRESSION TAG	UNP P37528
H	170	ASN	HIS	ENGINEERED	UNP P37528
H	197	LEU	-	EXPRESSION TAG	UNP P37528
H	198	GLU	-	EXPRESSION TAG	UNP P37528
H	199	HIS	-	EXPRESSION TAG	UNP P37528
H	200	HIS	-	EXPRESSION TAG	UNP P37528
H	201	HIS	-	EXPRESSION TAG	UNP P37528
H	202	HIS	-	EXPRESSION TAG	UNP P37528
H	203	HIS	-	EXPRESSION TAG	UNP P37528
H	204	HIS	-	EXPRESSION TAG	UNP P37528
J	170	ASN	HIS	ENGINEERED	UNP P37528
J	197	LEU	-	EXPRESSION TAG	UNP P37528
J	198	GLU	-	EXPRESSION TAG	UNP P37528
J	199	HIS	-	EXPRESSION TAG	UNP P37528
J	200	HIS	-	EXPRESSION TAG	UNP P37528
J	201	HIS	-	EXPRESSION TAG	UNP P37528
J	202	HIS	-	EXPRESSION TAG	UNP P37528
J	203	HIS	-	EXPRESSION TAG	UNP P37528
J	204	HIS	-	EXPRESSION TAG	UNP P37528
L	170	ASN	HIS	ENGINEERED	UNP P37528
L	197	LEU	-	EXPRESSION TAG	UNP P37528
L	198	GLU	-	EXPRESSION TAG	UNP P37528
L	199	HIS	-	EXPRESSION TAG	UNP P37528
L	200	HIS	-	EXPRESSION TAG	UNP P37528
L	201	HIS	-	EXPRESSION TAG	UNP P37528
L	202	HIS	-	EXPRESSION TAG	UNP P37528
L	203	HIS	-	EXPRESSION TAG	UNP P37528
L	204	HIS	-	EXPRESSION TAG	UNP P37528
N	170	ASN	HIS	ENGINEERED	UNP P37528
N	197	LEU	-	EXPRESSION TAG	UNP P37528
N	198	GLU	-	EXPRESSION TAG	UNP P37528
N	199	HIS	-	EXPRESSION TAG	UNP P37528
N	200	HIS	-	EXPRESSION TAG	UNP P37528
N	201	HIS	-	EXPRESSION TAG	UNP P37528
N	202	HIS	-	EXPRESSION TAG	UNP P37528

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Chain	Residue	Modelled	Actual	Comment	Reference
N	203	HIS	-	EXPRESSION TAG	UNP P37528
N	204	HIS	-	EXPRESSION TAG	UNP P37528
P	170	ASN	HIS	ENGINEERED	UNP P37528
P	197	LEU	-	EXPRESSION TAG	UNP P37528
P	198	GLU	-	EXPRESSION TAG	UNP P37528
P	199	HIS	-	EXPRESSION TAG	UNP P37528
P	200	HIS	-	EXPRESSION TAG	UNP P37528
P	201	HIS	-	EXPRESSION TAG	UNP P37528
P	202	HIS	-	EXPRESSION TAG	UNP P37528
P	203	HIS	-	EXPRESSION TAG	UNP P37528
P	204	HIS	-	EXPRESSION TAG	UNP P37528
R	170	ASN	HIS	ENGINEERED	UNP P37528
R	197	LEU	-	EXPRESSION TAG	UNP P37528
R	198	GLU	-	EXPRESSION TAG	UNP P37528
R	199	HIS	-	EXPRESSION TAG	UNP P37528
R	200	HIS	-	EXPRESSION TAG	UNP P37528
R	201	HIS	-	EXPRESSION TAG	UNP P37528
R	202	HIS	-	EXPRESSION TAG	UNP P37528
R	203	HIS	-	EXPRESSION TAG	UNP P37528
R	204	HIS	-	EXPRESSION TAG	UNP P37528
T	170	ASN	HIS	ENGINEERED	UNP P37528
T	197	LEU	-	EXPRESSION TAG	UNP P37528
T	198	GLU	-	EXPRESSION TAG	UNP P37528
T	199	HIS	-	EXPRESSION TAG	UNP P37528
T	200	HIS	-	EXPRESSION TAG	UNP P37528
T	201	HIS	-	EXPRESSION TAG	UNP P37528
T	202	HIS	-	EXPRESSION TAG	UNP P37528
T	203	HIS	-	EXPRESSION TAG	UNP P37528
T	204	HIS	-	EXPRESSION TAG	UNP P37528
V	170	ASN	HIS	ENGINEERED	UNP P37528
V	197	LEU	-	EXPRESSION TAG	UNP P37528
V	198	GLU	-	EXPRESSION TAG	UNP P37528
V	199	HIS	-	EXPRESSION TAG	UNP P37528
V	200	HIS	-	EXPRESSION TAG	UNP P37528
V	201	HIS	-	EXPRESSION TAG	UNP P37528
V	202	HIS	-	EXPRESSION TAG	UNP P37528
V	203	HIS	-	EXPRESSION TAG	UNP P37528
V	204	HIS	-	EXPRESSION TAG	UNP P37528
X	170	ASN	HIS	ENGINEERED	UNP P37528
X	197	LEU	-	EXPRESSION TAG	UNP P37528
X	198	GLU	-	EXPRESSION TAG	UNP P37528
X	199	HIS	-	EXPRESSION TAG	UNP P37528

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Chain	Residue	Modelled	Actual	Comment	Reference
X	200	HIS	-	EXPRESSION TAG	UNP P37528
X	201	HIS	-	EXPRESSION TAG	UNP P37528
X	202	HIS	-	EXPRESSION TAG	UNP P37528
X	203	HIS	-	EXPRESSION TAG	UNP P37528
X	204	HIS	-	EXPRESSION TAG	UNP P37528

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0
3	Q	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	W	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	U	1	Total Cl 1 1	0	0
3	O	1	Total Cl 1 1	0	0
3	S	1	Total Cl 1 1	0	0
3	M	1	Total Cl 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



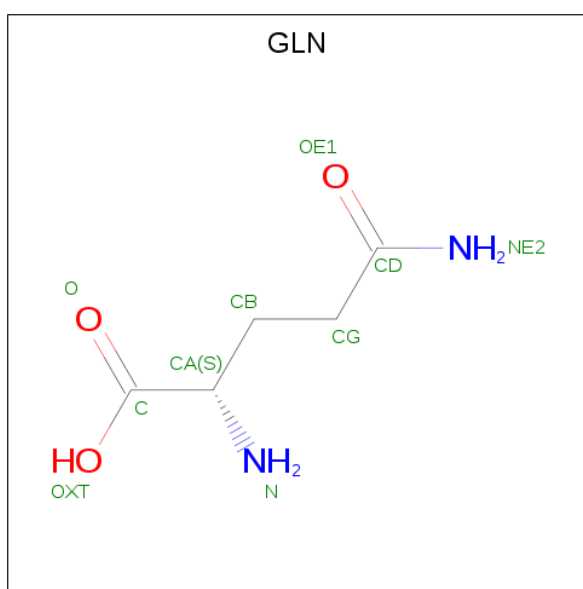
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	Q	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	Q	1	Total	C	O	0	0
			4	2	2		
4	U	1	Total	C	O	0	0
			4	2	2		
4	U	1	Total	C	O	0	0
			4	2	2		
4	W	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			10	5	2	3		
5	D	1	Total	C	N	O	0	0
			10	5	2	3		
5	F	1	Total	C	N	O	0	0
			10	5	2	3		
5	H	1	Total	C	N	O	0	0
			10	5	2	3		
5	J	1	Total	C	N	O	0	0
			10	5	2	3		
5	L	1	Total	C	N	O	0	0
			10	5	2	3		
5	N	1	Total	C	N	O	0	0
			10	5	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	P	1	Total	C	N	O	0	0
			10	5	2	3		
5	R	1	Total	C	N	O	0	0
			10	5	2	3		
5	T	1	Total	C	N	O	0	0
			10	5	2	3		
5	V	1	Total	C	N	O	0	0
			10	5	2	3		
5	X	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	295	Total	O	0	0
			295	295		
6	B	120	Total	O	0	0
			120	120		
6	C	348	Total	O	0	0
			348	348		
6	D	142	Total	O	0	0
			142	142		
6	E	335	Total	O	0	0
			335	335		
6	F	115	Total	O	0	0
			115	115		
6	G	330	Total	O	0	0
			330	330		
6	H	164	Total	O	0	0
			164	164		
6	I	330	Total	O	0	0
			330	330		
6	J	204	Total	O	0	0
			204	204		
6	K	303	Total	O	0	0
			303	303		
6	L	153	Total	O	0	0
			153	153		
6	M	334	Total	O	0	0
			334	334		
6	N	198	Total	O	0	0
			198	198		

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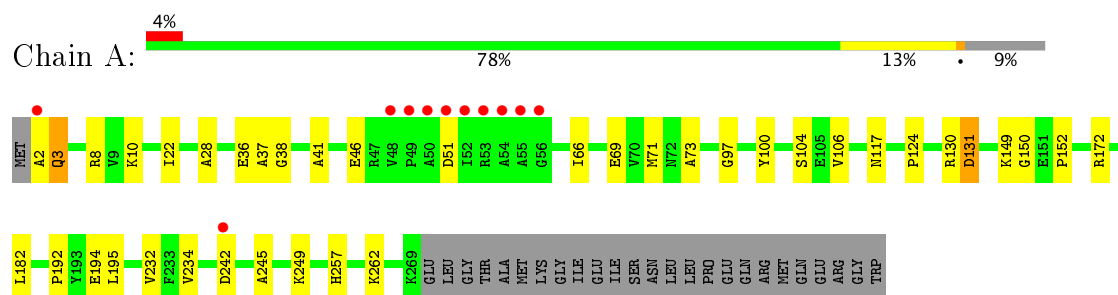
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	O	343	Total 343	O 343	0	0
6	P	177	Total 177	O 177	0	0
6	Q	323	Total 323	O 323	0	0
6	R	173	Total 173	O 173	0	0
6	S	311	Total 311	O 311	0	0
6	T	134	Total 134	O 134	0	0
6	U	285	Total 285	O 285	0	0
6	V	104	Total 104	O 104	0	0
6	W	334	Total 334	O 334	0	0
6	X	219	Total 219	O 219	0	0

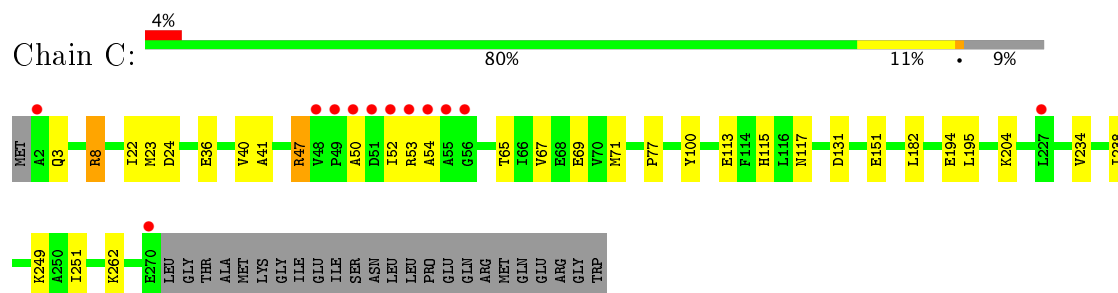
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

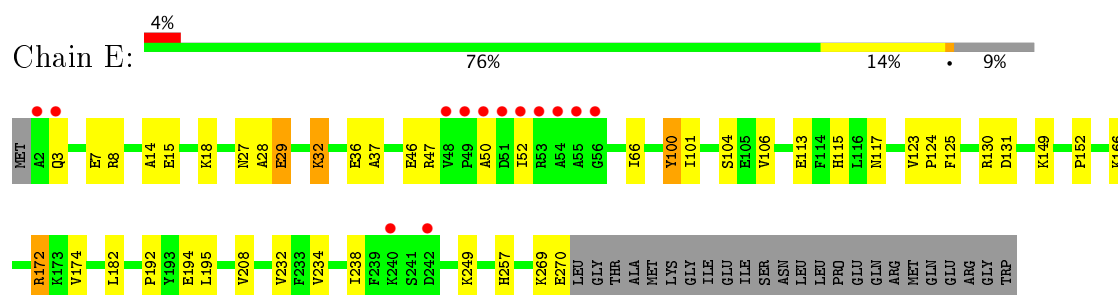
- Molecule 1: Pyridoxal biosynthesis lyase pdxS



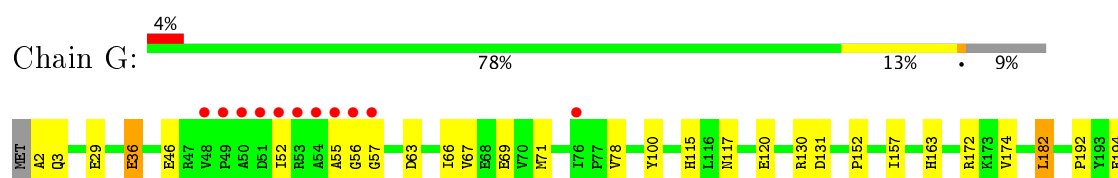
- Molecule 1: Pyridoxal biosynthesis lyase pdxS

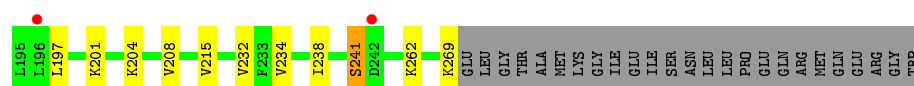


- Molecule 1: Pyridoxal biosynthesis lyase pdxS

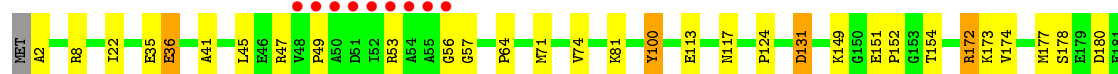
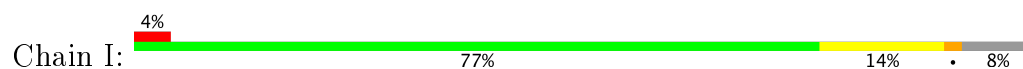


- Molecule 1: Pyridoxal biosynthesis lyase pdxS

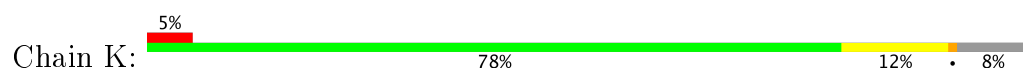




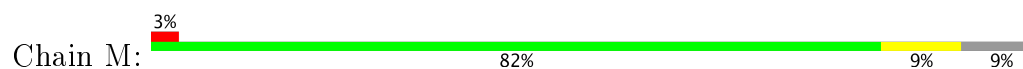
- Molecule 1: Pyridoxal biosynthesis lyase pdxS



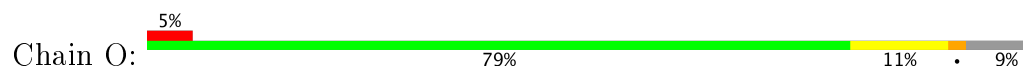
- Molecule 1: Pyridoxal biosynthesis lyase pdxS



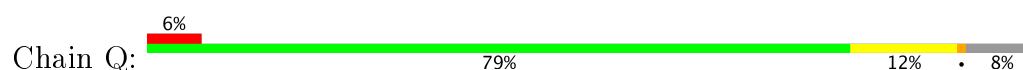
- Molecule 1: Pyridoxal biosynthesis lyase pdxS

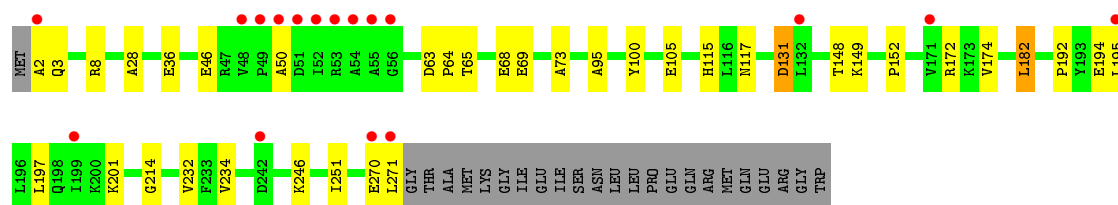


- Molecule 1: Pyridoxal biosynthesis lyase pdxS

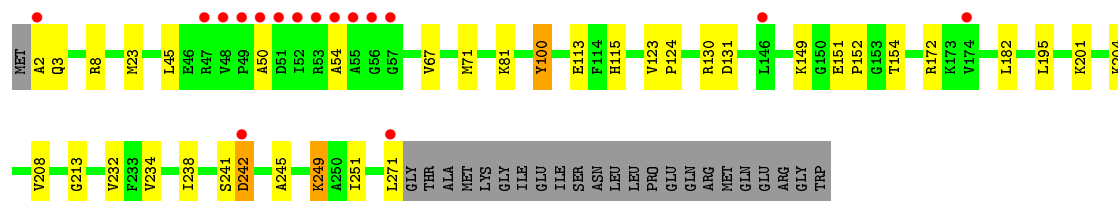
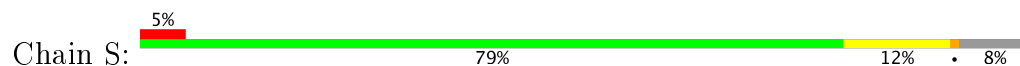


- Molecule 1: Pyridoxal biosynthesis lyase pdxS

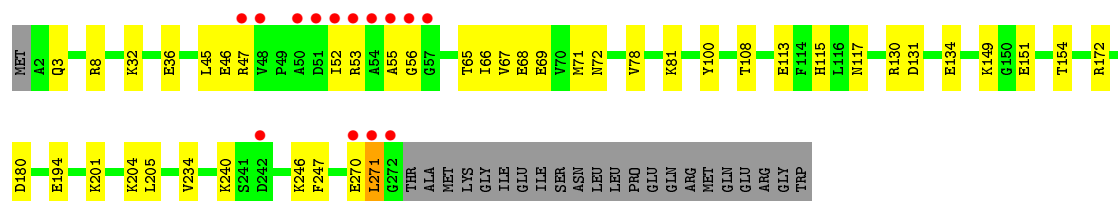
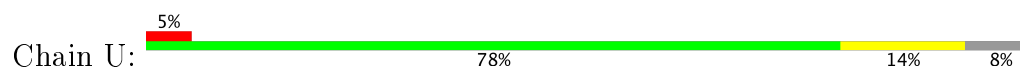




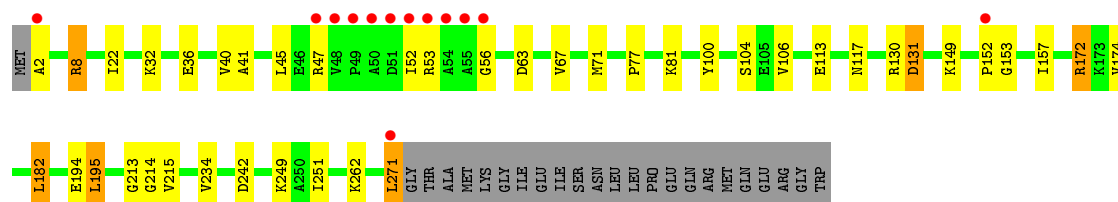
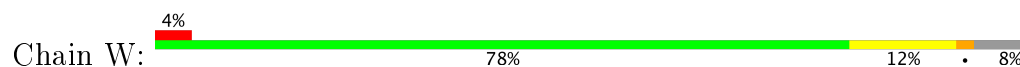
• Molecule 1: Pyridoxal biosynthesis lyase pdxS



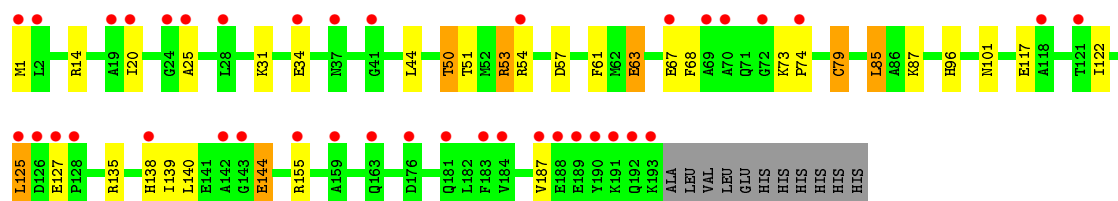
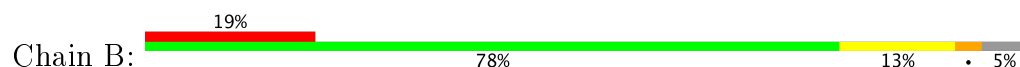
• Molecule 1: Pyridoxal biosynthesis lyase pdxS



• Molecule 1: Pyridoxal biosynthesis lyase pdxS

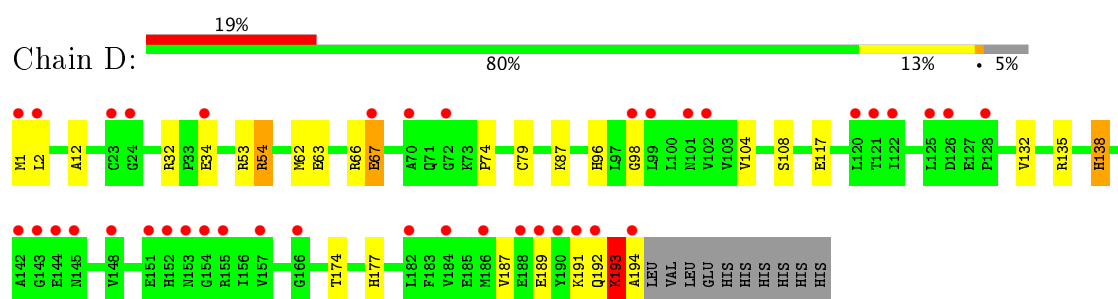


• Molecule 2: Glutamine amidotransferase subunit pdxT

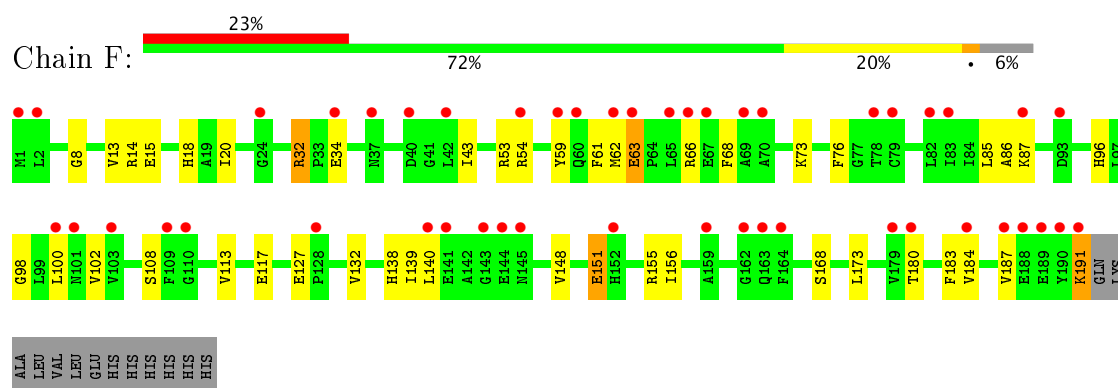


• Molecule 2: Glutamine amidotransferase subunit pdxT

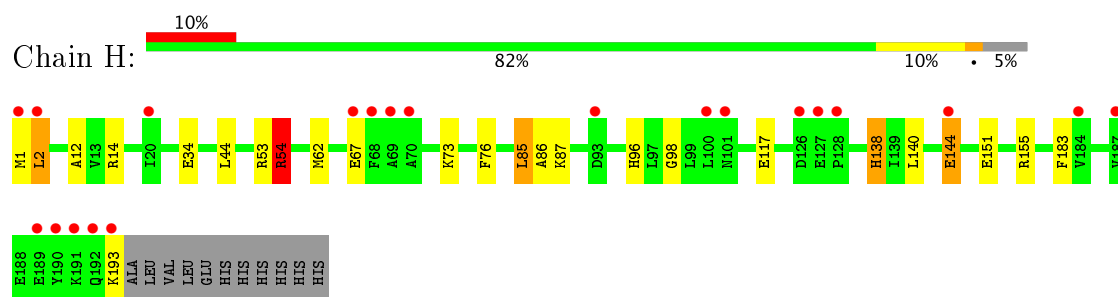




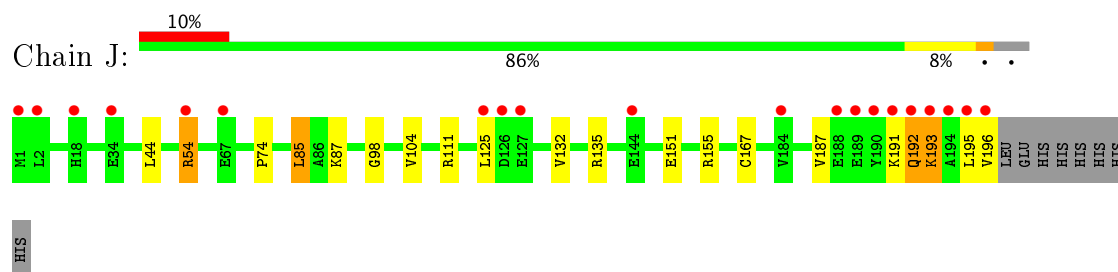
- Molecule 2: Glutamine amidotransferase subunit pdxT



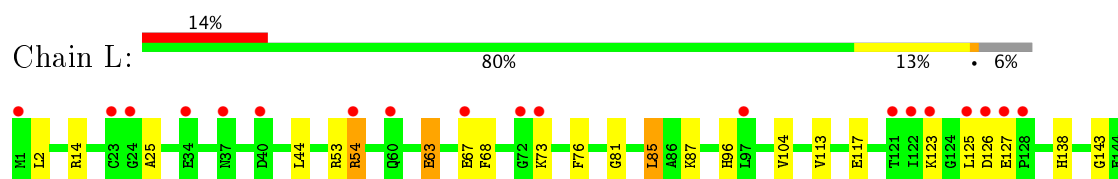
- Molecule 2: Glutamine amidotransferase subunit pdxT

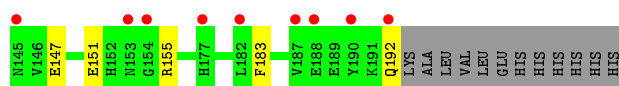


- Molecule 2: Glutamine amidotransferase subunit pdxT

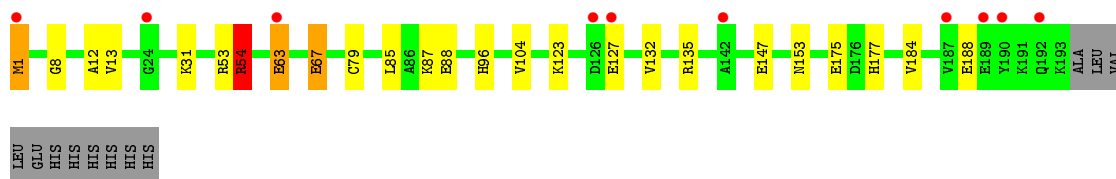
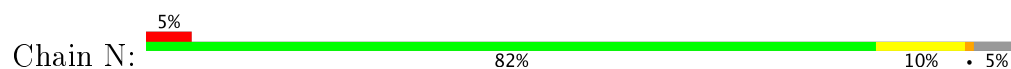


- Molecule 2: Glutamine amidotransferase subunit pdxT

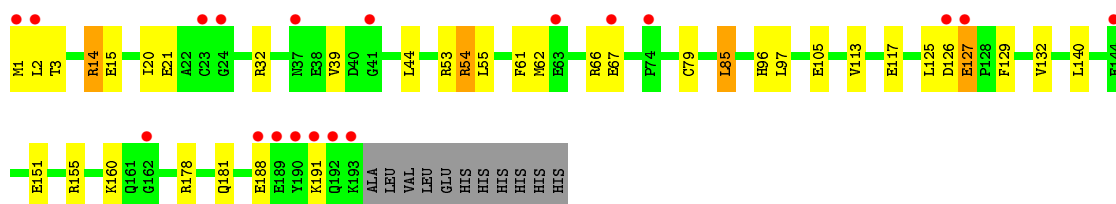
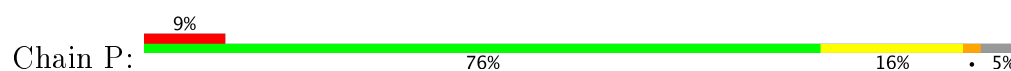




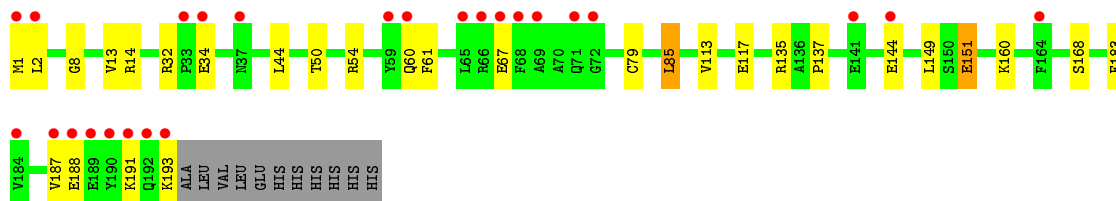
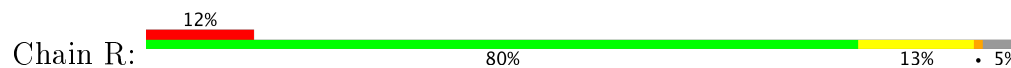
- Molecule 2: Glutamine amidotransferase subunit pdxT



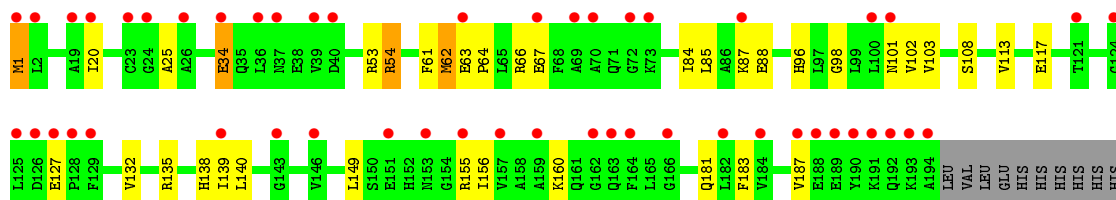
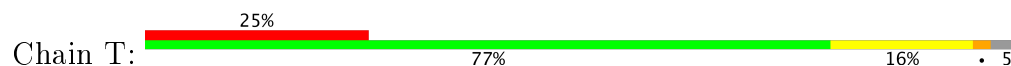
- Molecule 2: Glutamine amidotransferase subunit pdxT



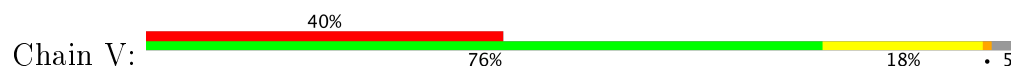
- Molecule 2: Glutamine amidotransferase subunit pdxT

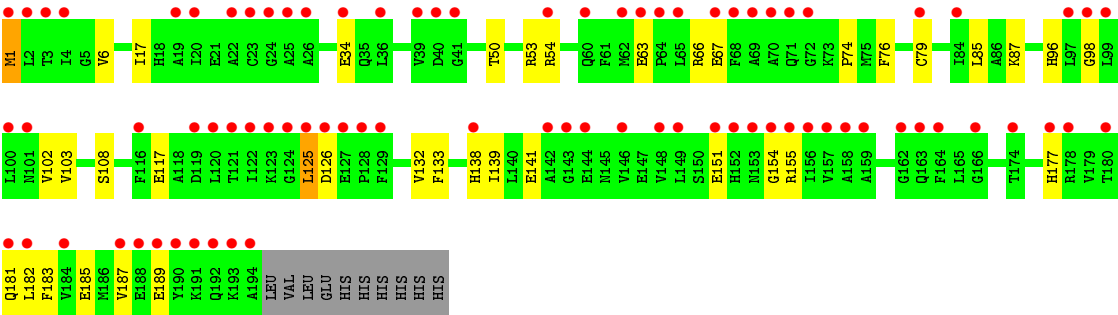


- Molecule 2: Glutamine amidotransferase subunit pdxT

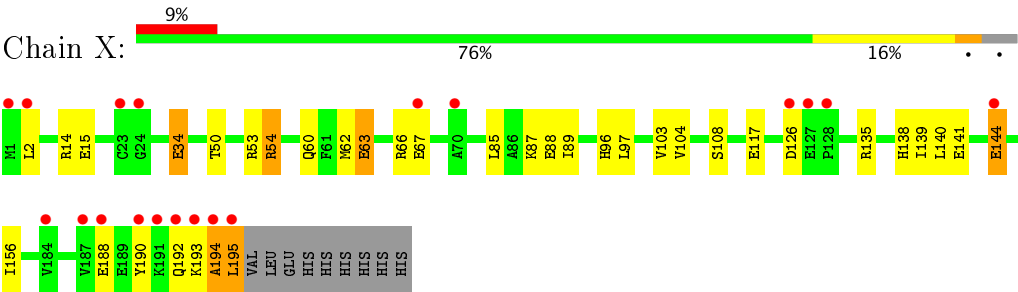


- Molecule 2: Glutamine amidotransferase subunit pdxT





● Molecule 2: Glutamine amidotransferase subunit pdxT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.51Å 259.01Å 144.96Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	50.00 – 2.12 49.62 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.12) 98.2 (49.62-2.12)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.146 , 0.198 0.157 , 0.205	Depositor DCC
$R_{free}$ test set	19065 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	48293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.72	0/2070	0.77	5/2792 (0.2%)
1	C	0.80	0/2076	0.80	2/2799 (0.1%)
1	E	0.76	0/2076	0.79	4/2799 (0.1%)
1	G	0.76	0/2040	0.81	3/2753 (0.1%)
1	I	0.77	0/2078	0.85	4/2802 (0.1%)
1	K	0.75	0/2068	0.78	3/2790 (0.1%)
1	M	0.78	0/2075	0.81	1/2797 (0.0%)
1	O	0.77	0/2060	0.85	4/2777 (0.1%)
1	Q	0.75	0/2061	0.80	5/2780 (0.2%)
1	S	0.73	0/2061	0.79	4/2781 (0.1%)
1	U	0.73	0/2070	0.77	4/2793 (0.1%)
1	W	0.83	0/2086	0.80	4/2814 (0.1%)
2	B	0.56	0/1531	0.71	2/2066 (0.1%)
2	D	0.54	0/1525	0.71	2/2059 (0.1%)
2	F	0.53	0/1502	0.63	0/2029
2	H	0.57	0/1525	0.72	1/2060 (0.0%)
2	J	0.62	1/1540 (0.1%)	0.75	1/2080 (0.0%)
2	L	0.54	0/1511	0.66	0/2041
2	N	0.66	0/1516	0.76	4/2048 (0.2%)
2	P	0.60	0/1527	0.70	0/2062
2	R	0.57	0/1531	0.69	2/2066 (0.1%)
2	T	0.53	0/1521	0.69	1/2054 (0.0%)
2	V	0.48	0/1525	0.69	0/2059
2	X	0.62	0/1533	0.73	2/2070 (0.1%)
All	All	0.69	1/43108 (0.0%)	0.76	58/58171 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	I	0	1
2	D	0	1
2	P	1	0
2	X	0	1
All	All	1	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	167	CYS	CB-SG	-5.57	1.72	1.81

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	8	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	O	172[A]	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	O	172[B]	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	Q	63	ASP	CB-CG-OD2	6.62	124.26	118.30
1	K	63	ASP	CB-CG-OD1	-6.62	112.35	118.30
1	I	172[A]	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	I	172[B]	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	O	172[A]	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	O	172[B]	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	K	63	ASP	CB-CG-OD2	6.34	124.00	118.30
2	B	135	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	H	54	ARG	NE-CZ-NH1	6.13	123.37	120.30
2	N	135	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	G	172	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	8	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	G	63	ASP	CB-CG-OD1	-5.91	112.98	118.30
2	R	135	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	U	180	ASP	CB-CG-OD1	5.79	123.51	118.30
1	E	172[A]	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	E	172[B]	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	X	135	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	R	135	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	G	63	ASP	CB-CG-OD2	5.61	123.35	118.30
1	U	172[A]	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	U	172[B]	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	D	135	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	182	LEU	CB-CG-CD2	-5.56	101.55	111.00
2	T	135	ARG	NE-CZ-NH2	-5.55	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	I	172[A]	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	I	172[B]	ARG	NE-CZ-NH2	-5.47	117.57	120.30
2	J	135	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	S	172[A]	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	S	172[B]	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	172[A]	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	172[B]	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	N	135	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	B	53	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	172[A]	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	E	172[B]	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	D	135	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	X	135	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	Q	63	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	W	63	ASP	CB-CG-OD2	5.21	122.99	118.30
1	K	8	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	W	172[A]	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	W	172[B]	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	Q	172[A]	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	Q	172[B]	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	U	205	LEU	CB-CG-CD1	-5.06	102.41	111.00
1	S	172[A]	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	S	172[B]	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	172[A]	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	172[B]	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	N	54[A]	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	N	54[B]	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	M	24	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	Q	8	ARG	NE-CZ-NH2	-5.01	117.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	P	54[B]	ARG	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	193	LYS	Peptide
1	G	56	GLY	Peptide
1	I	56	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	X	194	ALA	Peptide

## 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	A	2028	0	2078	33	0
1	C	2037	0	2079	39	0
1	E	2037	0	2081	73	0
1	G	2007	0	2041	40	0
1	I	2042	0	2085	54	0
1	K	2032	0	2081	35	0
1	M	2036	0	2084	29	0
1	O	2024	0	2074	46	0
1	Q	2028	0	2072	37	0
1	S	2028	0	2065	34	0
1	U	2034	0	2070	43	0
1	W	2044	0	2095	51	0
2	B	1500	0	1512	35	0
2	D	1497	0	1504	33	0
2	F	1474	0	1478	36	0
2	H	1494	0	1494	21	0
2	J	1512	0	1524	10	0
2	L	1483	0	1486	28	1
2	N	1488	0	1488	28	0
2	P	1496	0	1508	48	0
2	R	1500	0	1512	28	0
2	T	1493	0	1500	57	0
2	V	1497	0	1504	39	0
2	X	1505	0	1515	43	1
3	A	1	0	0	2	0
3	C	1	0	0	2	0
3	E	1	0	0	2	0
3	G	1	0	0	1	0
3	I	1	0	0	2	0
3	K	1	0	0	1	0
3	M	1	0	0	0	0
3	O	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1	0	0	2	0
3	S	1	0	0	2	0
3	U	1	0	0	2	0
3	W	1	0	0	2	0
4	A	12	0	18	8	0
4	C	8	0	12	0	0
4	E	8	0	11	9	0
4	G	4	0	6	9	0
4	I	12	0	17	9	0
4	K	4	0	6	0	0
4	M	4	0	5	5	0
4	Q	8	0	11	11	0
4	U	8	0	12	0	0
4	W	4	0	6	0	0
5	B	10	0	7	1	0
5	D	10	0	7	1	0
5	F	10	0	7	0	0
5	H	10	0	7	0	0
5	J	10	0	7	0	0
5	L	10	0	7	0	0
5	N	10	0	7	0	0
5	P	10	0	7	2	0
5	R	10	0	7	0	0
5	T	10	0	7	0	0
5	V	10	0	7	0	0
5	X	9	0	7	0	0
6	A	295	0	0	13	0
6	B	120	0	0	19	0
6	C	348	0	0	14	0
6	D	142	0	0	14	0
6	E	335	0	0	48	0
6	F	115	0	0	10	0
6	G	330	0	0	22	0
6	H	164	0	0	6	0
6	I	330	0	0	33	0
6	J	204	0	0	1	0
6	K	303	0	0	20	0
6	L	153	0	0	15	0
6	M	334	0	0	17	0
6	N	198	0	0	19	0
6	O	343	0	0	28	0
6	P	177	0	0	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	323	0	0	21	0
6	R	173	0	0	14	1
6	S	311	0	0	25	0
6	T	134	0	0	32	0
6	U	285	0	0	22	0
6	V	104	0	0	16	0
6	W	334	0	0	35	1
6	X	219	0	0	24	0
All	All	48293	0	43118	897	2

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 10.

All (897) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:54[B]:ARG:NH1	6:R:3257:HOH:O	1.57	1.31
1:S:234:VAL:HB	6:S:6294:HOH:O	1.32	1.28
1:E:172[B]:ARG:NH1	6:E:6234:HOH:O	1.67	1.28
1:C:36[B]:GLU:HG3	2:D:54[B]:ARG:NH2	1.48	1.27
6:A:6321:HOH:O	2:B:31:LYS:HB3	1.27	1.27
2:T:34:GLU:HG3	6:T:4725:HOH:O	1.20	1.26
2:N:54[B]:ARG:NH2	6:N:6095:HOH:O	1.64	1.26
1:G:120:GLU:HG2	6:G:6327:HOH:O	1.25	1.26
1:E:113:GLU:HG3	6:E:6324:HOH:O	1.12	1.25
1:E:36[B]:GLU:HG3	6:E:6377:HOH:O	1.26	1.25
1:M:120:GLU:HG2	6:M:6354:HOH:O	1.34	1.23
2:V:151:GLU:HB3	6:V:5669:HOH:O	1.38	1.23
1:Q:152:PRO:HD2	6:Q:6356:HOH:O	1.11	1.23
2:T:155:ARG:HD3	6:T:5384:HOH:O	1.38	1.23
1:I:172[B]:ARG:NH1	6:I:6173:HOH:O	1.66	1.21
2:B:155[B]:ARG:NH1	6:B:5061:HOH:O	1.73	1.19
1:C:234:VAL:HB	6:C:6342:HOH:O	1.39	1.18
1:U:234:VAL:HB	6:U:6316:HOH:O	1.03	1.18
1:U:201:LYS:HE3	6:U:6288:HOH:O	1.43	1.17
2:B:138:HIS:CD2	6:B:5449:HOH:O	1.96	1.16
1:E:36[B]:GLU:CG	6:E:6377:HOH:O	1.80	1.15
2:T:54[A]:ARG:CD	6:T:4784:HOH:O	1.96	1.14
2:P:20:ILE:HG22	6:P:6201:HOH:O	1.45	1.14
1:O:172[B]:ARG:NH1	6:O:6309:HOH:O	1.81	1.13
2:L:54[B]:ARG:NH2	6:L:6170:HOH:O	1.74	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:6320:HOH:O	3:Q:6033:CL:CL	2.05	1.12
2:D:54[B]:ARG:NH2	6:D:6075:HOH:O	1.84	1.10
1:E:29[B]:GLU:OE2	6:E:6338:HOH:O	1.69	1.10
3:E:6009:CL:CL	6:W:6353:HOH:O	2.07	1.09
1:Q:201:LYS:HE3	6:Q:6332:HOH:O	1.51	1.09
1:I:131[B]:ASP:OD1	6:I:6172:HOH:O	1.72	1.07
1:O:67:VAL:HG12	1:O:71:MET:HE2	1.30	1.07
2:T:138:HIS:HB2	6:T:5332:HOH:O	1.55	1.06
1:W:172[B]:ARG:NH1	6:W:6289:HOH:O	1.87	1.06
2:N:147:GLU:HG2	6:N:6225:HOH:O	1.53	1.06
2:N:54[B]:ARG:CZ	6:N:6095:HOH:O	1.90	1.05
2:T:1:MET:HG2	6:T:5143:HOH:O	1.56	1.04
2:X:104:VAL:HB	6:X:6200:HOH:O	1.58	1.03
1:C:194:GLU:HG2	4:M:6007:EDO:H12	1.36	1.03
1:E:234:VAL:HB	6:E:6336:HOH:O	1.57	1.03
1:W:113[B]:GLU:OE2	6:W:6305:HOH:O	1.73	1.03
1:I:234:VAL:HB	6:I:6296:HOH:O	1.56	1.03
1:U:72:ASN:HB3	6:U:6313:HOH:O	1.55	1.03
2:D:54[B]:ARG:CZ	6:D:6075:HOH:O	2.01	1.02
1:G:194:GLU:HB2	4:G:6043:EDO:H11	1.37	1.02
2:T:54[A]:ARG:CG	6:T:4784:HOH:O	2.07	1.02
1:E:36[B]:GLU:OE2	6:E:6278:HOH:O	1.76	1.01
1:I:113[B]:GLU:OE2	6:I:6244:HOH:O	1.78	1.01
1:Q:234:VAL:HB	6:Q:6324:HOH:O	0.84	1.00
1:G:262:LYS:HE2	6:I:6350:HOH:O	1.61	1.00
1:Q:50:ALA:HB2	6:Q:6349:HOH:O	1.59	1.00
1:M:131[A]:ASP:OD2	6:M:6198:HOH:O	1.77	1.00
1:C:113[B]:GLU:OE2	6:C:6292:HOH:O	1.79	1.00
1:E:194:GLU:HB2	4:E:6047:EDO:H11	1.43	0.99
1:Q:197:LEU:HD12	6:Q:6339:HOH:O	1.62	0.99
2:T:155:ARG:HG3	6:T:5723:HOH:O	1.60	0.99
1:A:36[B]:GLU:OE1	6:A:6188:HOH:O	1.80	0.99
2:V:6:VAL:HG23	6:V:5626:HOH:O	1.62	0.98
1:A:131[B]:ASP:OD2	6:A:6181:HOH:O	1.81	0.97
2:B:138:HIS:HD2	6:B:5449:HOH:O	1.36	0.97
1:Q:148:THR:HG22	6:Q:6318:HOH:O	1.64	0.97
2:X:192:GLN:HG3	6:X:6265:HOH:O	1.64	0.97
6:Q:6353:HOH:O	1:S:113:GLU:HG2	1.62	0.96
1:G:192:PRO:HB3	4:G:6043:EDO:H22	1.44	0.96
3:I:6017:CL:CL	6:S:6347:HOH:O	2.18	0.96
1:E:29[A]:GLU:HG2	6:E:6381:HOH:O	1.64	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:67:VAL:HG12	1:M:71:MET:HE3	1.46	0.95
2:X:54[B]:ARG:NH2	6:X:6143:HOH:O	1.99	0.95
2:B:87:LYS:HG3	2:B:101:ASN:HA	1.47	0.95
1:W:131[B]:ASP:OD1	6:W:6210:HOH:O	1.85	0.95
2:T:139:ILE:HG22	6:T:5578:HOH:O	1.67	0.95
2:L:87:LYS:HE3	6:L:6176:HOH:O	1.67	0.94
2:B:144:GLU:CD	2:B:144:GLU:H	1.70	0.94
1:G:234:VAL:HB	6:G:6331:HOH:O	1.68	0.94
6:S:6328:HOH:O	2:T:113:VAL:HB	1.68	0.94
1:O:249:LYS:NZ	2:P:54[A]:ARG:HH21	1.65	0.94
1:K:131[B]:ASP:OD2	6:K:6189:HOH:O	1.83	0.94
1:O:67:VAL:HG12	1:O:71:MET:CE	1.98	0.94
1:A:194:GLU:HB2	4:A:6031:EDO:H12	1.50	0.93
6:E:6262:HOH:O	2:F:113:VAL:HB	1.66	0.93
1:K:32:LYS:HE2	6:K:6296:HOH:O	1.69	0.93
1:O:249:LYS:HZ2	2:P:54[A]:ARG:HH21	1.15	0.92
1:M:45:LEU:HD13	6:M:6331:HOH:O	1.67	0.92
1:I:194:GLU:HB2	4:I:6039:EDO:H11	1.50	0.92
1:I:47:ARG:HG3	6:I:6354:HOH:O	1.68	0.92
1:G:197:LEU:HD12	6:G:6333:HOH:O	1.68	0.92
2:H:144:GLU:CD	2:H:144:GLU:H	1.73	0.91
1:S:152:PRO:HA	6:S:6346:HOH:O	1.70	0.91
1:G:36[B]:GLU:OE1	6:G:6276:HOH:O	1.87	0.90
1:E:36[B]:GLU:OE1	6:E:6220:HOH:O	1.88	0.90
2:T:1:MET:CG	6:T:5143:HOH:O	2.14	0.90
2:X:195:LEU:HG	6:X:6267:HOH:O	1.71	0.90
2:F:191:LYS:C	6:F:5703:HOH:O	2.08	0.89
1:K:245:ALA:O	1:K:249:LYS:HD3	1.73	0.89
2:B:139:ILE:CD1	6:B:5510:HOH:O	2.20	0.89
1:M:67:VAL:HG12	1:M:71:MET:CE	2.03	0.89
3:W:6045:CL:CL	6:W:6141:HOH:O	2.27	0.88
2:R:60:GLN:HG3	6:R:5326:HOH:O	1.74	0.88
3:A:6001:CL:CL	6:O:6244:HOH:O	2.26	0.88
1:S:152:PRO:HD2	6:S:6344:HOH:O	1.71	0.88
2:T:1:MET:CB	6:T:5143:HOH:O	2.21	0.88
1:G:194:GLU:HB2	4:G:6043:EDO:C1	2.04	0.87
1:Q:115:HIS:HD2	6:Q:6346:HOH:O	1.57	0.87
2:V:17:ILE:CD1	6:V:5626:HOH:O	2.21	0.87
1:W:152:PRO:CG	6:W:6343:HOH:O	2.22	0.87
1:E:194:GLU:HB2	4:E:6047:EDO:C1	2.04	0.87
2:D:194:ALA:HA	6:D:6133:HOH:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:GLU:C	6:E:6353:HOH:O	2.13	0.86
6:K:6292:HOH:O	2:L:113:VAL:HB	1.74	0.86
2:X:54[A]:ARG:NH1	6:X:6147:HOH:O	1.64	0.86
1:C:36[B]:GLU:HG3	2:D:54[B]:ARG:HH21	1.33	0.86
1:W:47:ARG:HD2	6:W:6352:HOH:O	1.74	0.86
1:C:67:VAL:HG12	1:C:71:MET:CE	2.05	0.86
1:S:50:ALA:HB2	6:S:6286:HOH:O	1.76	0.86
6:K:6188:HOH:O	3:Q:6033:CL:CL	2.33	0.84
1:S:213:GLY:HA2	6:S:6346:HOH:O	1.77	0.84
1:I:194:GLU:HB2	4:I:6039:EDO:C1	2.08	0.83
1:W:152:PRO:HB2	6:W:6343:HOH:O	1.78	0.83
1:E:29[B]:GLU:CD	6:E:6338:HOH:O	2.11	0.83
1:E:29[B]:GLU:HG3	6:E:6381:HOH:O	1.78	0.83
2:R:54[A]:ARG:CZ	6:R:3513:HOH:O	2.25	0.83
1:E:27:ASN:OD1	1:E:29[B]:GLU:HG2	1.78	0.83
1:W:113[A]:GLU:OE2	6:W:6357:HOH:O	1.97	0.83
2:B:139:ILE:HD12	6:B:5510:HOH:O	1.78	0.83
2:T:139:ILE:CG2	6:T:5578:HOH:O	2.21	0.83
2:T:54[A]:ARG:HG2	6:T:4784:HOH:O	1.71	0.83
1:G:46:GLU:HG3	1:G:66:ILE:HD12	1.62	0.82
2:X:54[B]:ARG:NH1	6:X:6193:HOH:O	2.10	0.82
1:S:67:VAL:HG12	1:S:71:MET:CE	2.10	0.82
3:W:6045:CL:CL	6:W:6307:HOH:O	2.33	0.82
1:U:72:ASN:CB	6:U:6313:HOH:O	2.20	0.81
2:T:54[B]:ARG:HG3	6:T:4784:HOH:O	1.79	0.81
1:C:36[B]:GLU:HG3	2:D:54[B]:ARG:HH22	1.44	0.81
1:W:152:PRO:CB	6:W:6343:HOH:O	2.29	0.81
2:L:125:LEU:HA	6:L:6171:HOH:O	1.81	0.80
3:C:6005:CL:CL	6:C:6144:HOH:O	2.36	0.80
2:X:144:GLU:CD	2:X:144:GLU:H	1.85	0.80
3:A:6001:CL:CL	6:O:6194:HOH:O	2.37	0.80
1:E:130:ARG:HH12	1:E:149:LYS:NZ	1.80	0.80
6:S:6328:HOH:O	2:T:113:VAL:CB	2.27	0.80
2:X:34:GLU:CG	6:X:6094:HOH:O	2.29	0.80
2:X:34:GLU:HG2	6:X:6094:HOH:O	1.81	0.80
1:G:29:GLU:HG2	6:G:6309:HOH:O	1.81	0.79
1:Q:115:HIS:CD2	6:Q:6346:HOH:O	2.34	0.79
1:W:32:LYS:HE2	6:W:6252:HOH:O	1.81	0.79
1:M:270:GLU:HG2	6:O:6362:HOH:O	1.81	0.79
2:V:17:ILE:HD13	6:V:5626:HOH:O	1.82	0.79
2:X:138:HIS:CE1	6:X:6214:HOH:O	2.35	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LYS:HE3	6:E:6351:HOH:O	1.82	0.79
1:C:36[B]:GLU:CG	2:D:54[B]:ARG:NH2	2.39	0.79
1:Q:152:PRO:CD	6:Q:6356:HOH:O	1.87	0.79
1:O:120[A]:GLU:OE2	6:O:6153:HOH:O	2.01	0.79
2:V:1:MET:HB2	6:V:4934:HOH:O	1.83	0.79
2:N:147:GLU:CG	6:N:6225:HOH:O	2.17	0.78
2:F:102:VAL:HG22	6:F:4875:HOH:O	1.81	0.78
1:U:240:LYS:CB	6:U:6314:HOH:O	2.30	0.78
1:G:192:PRO:CB	4:G:6043:EDO:H22	2.13	0.78
2:X:195:LEU:HA	6:X:6225:HOH:O	1.83	0.78
1:G:194:GLU:CB	4:G:6043:EDO:H11	2.13	0.78
2:P:129:PHE:HB2	6:P:6192:HOH:O	1.84	0.78
1:O:113:GLU:HG2	6:O:6344:HOH:O	1.84	0.77
2:R:44:LEU:CD1	2:R:85:LEU:HD13	2.13	0.77
1:U:246:LYS:HD3	6:U:6323:HOH:O	1.84	0.77
1:U:113[B]:GLU:OE1	6:U:6203:HOH:O	2.02	0.77
1:G:197:LEU:CD1	6:G:6333:HOH:O	2.28	0.76
1:U:69:GLU:HG3	6:U:6318:HOH:O	1.85	0.76
2:N:53:ARG:HH11	2:N:96:HIS:HD2	1.33	0.76
1:G:152:PRO:HD2	6:G:6302:HOH:O	1.83	0.76
1:E:270:GLU:CB	6:E:6343:HOH:O	2.33	0.76
1:M:194:GLU:HB2	4:M:6007:EDO:H11	1.67	0.76
1:W:214:GLY:CA	6:W:6367:HOH:O	2.33	0.76
1:W:271:LEU:HD23	6:W:6356:HOH:O	1.86	0.76
2:X:153:ASN:ND2	6:X:6259:HOH:O	2.16	0.75
1:E:130:ARG:NH1	1:E:149:LYS:NZ	2.33	0.75
6:S:6328:HOH:O	2:T:113:VAL:CG2	2.33	0.75
2:R:191:LYS:HE2	6:R:4894:HOH:O	1.85	0.75
3:O:6029:CL:CL	6:O:6307:HOH:O	2.41	0.75
4:A:6031:EDO:H21	1:O:194:GLU:HG2	1.68	0.75
1:Q:131[B]:ASP:OD1	6:Q:6211:HOH:O	2.04	0.75
2:F:100:LEU:HB3	6:F:4875:HOH:O	1.86	0.75
2:B:57:ASP:OD2	6:B:5438:HOH:O	2.04	0.75
1:K:269:LYS:O	1:K:271:LEU:HD13	1.85	0.74
1:S:67:VAL:HG12	1:S:71:MET:HE1	1.69	0.74
2:L:25:ALA:HA	6:L:6172:HOH:O	1.86	0.74
2:B:139:ILE:HG13	6:B:5510:HOH:O	1.87	0.74
1:C:67:VAL:HG12	1:C:71:MET:HE3	1.70	0.74
1:O:214:GLY:CA	6:O:6333:HOH:O	2.34	0.74
2:X:2:LEU:HD21	2:X:188:GLU:HG3	1.70	0.74
1:I:49:PRO:HG3	6:I:6366:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:246:LYS:HE2	6:Q:6354:HOH:O	1.86	0.74
2:X:138:HIS:HB2	6:X:6135:HOH:O	1.87	0.73
1:E:270:GLU:HB3	6:E:6343:HOH:O	1.87	0.73
2:H:53:ARG:HH11	2:H:96:HIS:HD2	1.36	0.73
1:I:197:LEU:HD12	6:I:6364:HOH:O	1.87	0.73
2:P:125:LEU:CD1	6:P:6192:HOH:O	2.35	0.73
1:W:214:GLY:HA3	6:W:6367:HOH:O	1.88	0.73
1:K:245:ALA:O	1:K:249:LYS:CD	2.36	0.73
2:X:138:HIS:ND1	6:X:6214:HOH:O	2.21	0.73
1:O:214:GLY:HA3	6:O:6333:HOH:O	1.89	0.73
1:C:262:LYS:CE	6:E:6351:HOH:O	2.37	0.72
2:X:60:GLN:HG2	6:X:6213:HOH:O	1.87	0.72
1:U:55:ALA:HB3	1:U:56:GLY:HA2	1.70	0.72
2:V:54[B]:ARG:CG	2:V:54[B]:ARG:HH11	2.02	0.72
1:K:29:GLU:CD	6:K:6296:HOH:O	2.27	0.72
1:A:257:HIS:CE1	6:A:6321:HOH:O	2.42	0.72
2:V:54[B]:ARG:HG2	2:V:54[B]:ARG:HH11	1.54	0.72
1:E:50:ALA:HB2	6:E:6364:HOH:O	1.90	0.71
1:A:3:GLN:HA	6:A:6303:HOH:O	1.90	0.71
2:H:144:GLU:CD	2:H:144:GLU:N	2.42	0.71
1:E:130:ARG:HH12	1:E:149:LYS:HZ1	1.36	0.71
1:Q:36:GLU:O	2:R:54[B]:ARG:HD3	1.91	0.71
1:C:67:VAL:HG12	1:C:71:MET:HE2	1.71	0.71
1:O:36:GLU:O	2:P:54[B]:ARG:HD2	1.89	0.71
1:O:47[B]:ARG:HA	6:O:6357:HOH:O	1.90	0.71
2:R:160:LYS:HE2	6:R:5551:HOH:O	1.89	0.71
3:E:6009:CL:CL	6:E:6345:HOH:O	2.45	0.71
1:O:47[B]:ARG:HG3	6:O:6357:HOH:O	1.91	0.71
2:P:188:GLU:HG2	6:P:6209:HOH:O	1.90	0.71
1:E:36[B]:GLU:HG2	6:E:6377:HOH:O	1.65	0.71
2:T:54[A]:ARG:HD2	6:T:4784:HOH:O	1.72	0.71
1:C:194:GLU:CG	4:M:6007:EDO:H12	2.18	0.70
1:O:47[A]:ARG:HA	6:O:6357:HOH:O	1.90	0.70
2:V:17:ILE:HD11	6:V:5626:HOH:O	1.83	0.70
2:N:63:GLU:HG3	6:N:6220:HOH:O	1.88	0.70
2:R:54[B]:ARG:NE	6:R:3929:HOH:O	2.24	0.70
2:F:66:ARG:HD2	6:F:5427:HOH:O	1.90	0.70
2:B:139:ILE:CG1	6:B:5510:HOH:O	2.36	0.70
6:S:6328:HOH:O	2:T:113:VAL:HG23	1.91	0.70
1:U:69:GLU:CG	6:U:6318:HOH:O	2.39	0.70
1:W:152:PRO:CD	6:W:6343:HOH:O	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:192:PRO:HB3	4:Q:6035:EDO:H11	1.72	0.70
3:S:6037:CL:CL	6:S:6243:HOH:O	2.46	0.70
1:W:152:PRO:HD2	6:W:6343:HOH:O	1.91	0.70
1:G:3:GLN:HB3	6:G:6362:HOH:O	1.91	0.70
2:N:67:GLU:CG	6:N:6216:HOH:O	2.40	0.70
2:D:194:ALA:C	6:D:6131:HOH:O	2.30	0.69
1:M:115:HIS:HD2	6:M:6112:HOH:O	1.75	0.69
2:F:62:MET:C	6:F:5427:HOH:O	2.31	0.69
1:E:192:PRO:HB3	4:E:6047:EDO:H22	1.75	0.69
2:B:144:GLU:CD	2:B:144:GLU:N	2.45	0.69
2:V:177:HIS:HD2	6:V:5109:HOH:O	1.75	0.69
1:C:3:GLN:HB3	6:C:6328:HOH:O	1.91	0.69
2:T:87:LYS:HG3	2:T:101:ASN:HA	1.72	0.69
1:E:194:GLU:CB	4:E:6047:EDO:H11	2.21	0.69
1:O:214:GLY:N	6:O:6333:HOH:O	2.26	0.69
1:U:47:ARG:HB2	1:U:52:ILE:HD11	1.74	0.68
1:W:213:GLY:O	6:W:6367:HOH:O	2.10	0.68
3:U:6041:CL:CL	6:U:6242:HOH:O	2.48	0.68
6:M:6287:HOH:O	1:W:262:LYS:CE	2.41	0.68
2:J:44:LEU:HD12	2:J:85:LEU:HD13	1.76	0.67
1:O:36:GLU:CD	6:O:6348:HOH:O	2.31	0.67
2:B:53:ARG:HH11	2:B:96:HIS:HD2	1.42	0.67
2:D:34:GLU:HG2	6:D:6046:HOH:O	1.95	0.67
1:E:113:GLU:CG	6:E:6324:HOH:O	1.89	0.67
2:N:88:GLU:OE1	6:N:6199:HOH:O	2.12	0.67
1:W:271:LEU:CD2	6:W:6356:HOH:O	2.41	0.67
2:F:18:HIS:CD2	6:F:5556:HOH:O	2.47	0.67
1:I:194:GLU:CB	4:I:6039:EDO:H11	2.23	0.67
2:J:44:LEU:CD1	2:J:85:LEU:HD13	2.25	0.67
2:D:194:ALA:CA	6:D:6133:HOH:O	2.37	0.67
1:I:232:VAL:HG12	1:I:234:VAL:HG23	1.76	0.67
1:Q:194:GLU:N	4:Q:6035:EDO:H21	2.10	0.66
1:S:67:VAL:HG12	1:S:71:MET:HE2	1.76	0.66
2:V:50:THR:O	2:V:54[A]:ARG:HG2	1.94	0.66
1:E:36[A]:GLU:OE2	6:E:6301:HOH:O	2.13	0.66
1:G:46:GLU:HG3	1:G:66:ILE:CD1	2.26	0.66
2:F:86:ALA:HA	6:F:4875:HOH:O	1.94	0.66
2:P:129:PHE:HD1	6:P:6192:HOH:O	1.78	0.66
1:A:242:ASP:OD1	6:A:6322:HOH:O	2.13	0.66
2:P:53:ARG:HH11	2:P:96:HIS:HD2	1.42	0.66
2:V:34:GLU:HG2	6:V:3608:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:PRO:CB	4:E:6047:EDO:H22	2.26	0.66
2:L:138:HIS:HB2	6:L:6083:HOH:O	1.94	0.66
1:I:192:PRO:CB	4:I:6039:EDO:H22	2.26	0.65
2:L:54[A]:ARG:CZ	6:L:6107:HOH:O	2.44	0.65
1:Q:201:LYS:CE	6:Q:6332:HOH:O	2.24	0.65
2:B:54[B]:ARG:HD2	6:B:3460:HOH:O	1.95	0.65
2:X:138:HIS:CD2	6:X:6227:HOH:O	2.49	0.65
1:I:197:LEU:CD1	6:I:6364:HOH:O	2.43	0.65
1:A:245:ALA:O	1:A:249:LYS:HG3	1.97	0.64
1:S:152:PRO:O	6:S:6344:HOH:O	2.15	0.64
2:X:53:ARG:HH11	2:X:96:HIS:HD2	1.45	0.64
2:V:66:ARG:HH11	2:V:66:ARG:HG2	1.62	0.64
1:Q:246:LYS:CE	6:Q:6354:HOH:O	2.44	0.64
1:M:48:VAL:HG22	6:M:6331:HOH:O	1.98	0.64
1:G:2:ALA:HA	2:H:117:GLU:O	1.98	0.64
1:I:36:GLU:HG2	6:I:6092:HOH:O	1.97	0.64
1:I:45:LEU:HD21	1:I:81:LYS:HE2	1.79	0.64
1:M:232:VAL:HG12	1:M:234:VAL:HG23	1.78	0.64
1:W:67:VAL:HG12	1:W:71:MET:CE	2.27	0.64
1:G:232:VAL:HG12	1:G:234:VAL:HG23	1.79	0.64
1:K:29:GLU:OE2	6:K:6296:HOH:O	2.15	0.64
2:P:125:LEU:HD13	6:P:6192:HOH:O	1.96	0.64
1:Q:105:GLU:HB3	6:Q:6310:HOH:O	1.98	0.64
2:X:62:MET:SD	2:X:97:LEU:HD23	2.38	0.63
2:L:44:LEU:HD12	2:L:85:LEU:HD13	1.80	0.63
1:U:204:LYS:HD3	6:U:6280:HOH:O	1.99	0.63
1:M:270:GLU:C	6:M:6281:HOH:O	2.36	0.63
1:Q:194:GLU:H	4:Q:6035:EDO:H21	1.64	0.63
2:F:108:SER:OG	2:F:138:HIS:HD2	1.82	0.63
1:I:53:ARG:HD3	6:I:6284:HOH:O	1.98	0.63
2:H:53:ARG:HH11	2:H:96:HIS:CD2	2.17	0.62
2:F:34:GLU:H	2:F:34:GLU:CD	2.03	0.62
2:F:62:MET:HG3	6:F:5427:HOH:O	1.99	0.62
2:N:53:ARG:HH11	2:N:96:HIS:CD2	2.16	0.62
1:W:67:VAL:HG12	1:W:71:MET:HE2	1.82	0.62
2:B:63:GLU:HG3	6:B:4744:HOH:O	2.00	0.62
2:D:138:HIS:HB3	6:D:6113:HOH:O	1.99	0.62
1:O:55:ALA:N	1:O:56:GLY:HA2	2.15	0.62
2:X:144:GLU:N	2:X:144:GLU:CD	2.53	0.62
1:E:270:GLU:C	6:E:6371:HOH:O	2.38	0.61
1:E:8:ARG:HD3	6:E:6359:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:44:LEU:CD1	2:L:85:LEU:HD13	2.30	0.61
2:N:123:LYS:NZ	6:N:6225:HOH:O	2.33	0.61
1:O:213:GLY:C	6:O:6333:HOH:O	2.37	0.61
2:T:54[B]:ARG:HD2	6:T:2551:HOH:O	1.99	0.61
1:M:45:LEU:CD1	6:M:6331:HOH:O	2.36	0.61
1:A:192:PRO:HB3	4:A:6031:EDO:H22	1.82	0.61
2:R:60:GLN:CD	6:R:5326:HOH:O	2.39	0.61
2:X:34:GLU:HG3	6:X:6094:HOH:O	1.97	0.61
2:R:60:GLN:CG	6:R:5326:HOH:O	2.36	0.61
1:E:192:PRO:HB3	4:E:6047:EDO:C2	2.30	0.61
2:P:181:GLN:HG2	6:P:6196:HOH:O	2.01	0.61
3:U:6041:CL:CL	6:U:6205:HOH:O	2.53	0.61
1:C:65:THR:O	1:C:69[A]:GLU:HG3	2.01	0.61
1:W:242:ASP:O	6:W:6181:HOH:O	2.17	0.61
1:I:192:PRO:HB3	4:I:6039:EDO:H22	1.82	0.60
1:C:36[B]:GLU:CG	2:D:54[B]:ARG:HH21	2.11	0.60
1:K:8:ARG:HD2	2:L:117:GLU:OE2	2.00	0.60
4:A:6031:EDO:H21	1:O:194:GLU:H	1.66	0.60
1:M:249[A]:LYS:HG2	2:N:54[A]:ARG:HH21	1.67	0.60
2:N:31:LYS:HG3	6:N:6191:HOH:O	2.01	0.60
2:P:125:LEU:HD12	6:P:6192:HOH:O	2.00	0.60
1:E:130:ARG:NH1	1:E:149:LYS:HZ2	1.99	0.60
1:O:37:ALA:O	2:P:54[A]:ARG:HD2	2.01	0.60
2:X:14:ARG:NH1	2:X:15:GLU:OE2	2.35	0.60
2:F:53:ARG:HH11	2:F:96:HIS:HD2	1.49	0.60
1:K:47:ARG:HG3	1:K:48:VAL:N	2.16	0.60
1:Q:197:LEU:CD1	6:Q:6339:HOH:O	2.34	0.60
2:R:44:LEU:HD12	2:R:85:LEU:HD13	1.82	0.60
1:S:45:LEU:HD21	1:S:81:LYS:HE2	1.83	0.60
1:C:23:MET:HG2	6:C:6342:HOH:O	2.01	0.60
2:H:138:HIS:CE1	2:H:140:LEU:HD23	2.37	0.60
1:Q:194:GLU:HB2	4:Q:6035:EDO:H21	1.83	0.60
2:D:67:GLU:OE2	6:D:6125:HOH:O	2.16	0.60
1:E:232:VAL:HG12	1:E:234:VAL:HG23	1.83	0.60
1:K:8:ARG:NH1	6:K:6321:HOH:O	2.34	0.60
1:M:8:ARG:HD3	2:N:132:VAL:HG21	1.84	0.59
2:N:67:GLU:CB	6:N:6216:HOH:O	2.50	0.59
1:S:232:VAL:HG12	1:S:234:VAL:HG23	1.84	0.59
2:T:87:LYS:HB3	6:T:4753:HOH:O	2.02	0.59
2:T:139:ILE:CB	6:T:5578:HOH:O	2.50	0.59
1:I:173:LYS:HE2	1:I:177:MET:HE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:194:GLU:H	4:Q:6035:EDO:H12	1.68	0.59
2:R:54[B]:ARG:CD	6:R:3929:HOH:O	2.51	0.59
1:C:151:GLU:HB3	6:C:6366:HOH:O	2.03	0.59
1:I:64:PRO:HG3	6:I:6358:HOH:O	2.02	0.59
2:V:87:LYS:HA	2:V:98:GLY:HA2	1.85	0.59
1:W:130:ARG:NE	6:W:6359:HOH:O	2.23	0.59
2:T:156:ILE:HB	6:T:5578:HOH:O	2.02	0.58
1:W:113[B]:GLU:OE1	6:W:6103:HOH:O	2.17	0.58
1:K:123:VAL:HB	6:K:6292:HOH:O	2.04	0.58
1:W:149:LYS:NZ	6:W:6355:HOH:O	2.36	0.58
2:P:126:ASP:HB2	6:P:6155:HOH:O	2.02	0.58
2:D:174:THR:HG21	6:D:6073:HOH:O	2.04	0.58
1:O:253:GLU:OE2	2:P:54[A]:ARG:NH2	2.36	0.58
2:V:54[B]:ARG:CZ	6:V:4748:HOH:O	2.50	0.58
2:P:125:LEU:HD22	6:P:6151:HOH:O	2.04	0.58
2:D:189:GLU:HG2	6:D:6110:HOH:O	2.03	0.58
1:W:152:PRO:HG2	6:W:6343:HOH:O	1.94	0.57
1:K:51:ASP:CG	6:K:6233:HOH:O	2.43	0.57
2:D:177:HIS:HE1	6:D:6144:HOH:O	1.85	0.57
2:D:53:ARG:HH11	2:D:96:HIS:HD2	1.52	0.57
2:H:73:LYS:NZ	6:H:6157:HOH:O	2.16	0.57
3:S:6037:CL:CL	6:S:6321:HOH:O	2.54	0.57
1:M:188[A]:ASN:ND2	6:M:6157:HOH:O	2.37	0.57
2:T:1:MET:HB2	6:T:5143:HOH:O	1.93	0.57
1:A:257:HIS:ND1	6:A:6321:HOH:O	2.32	0.57
1:G:67:VAL:HG12	1:G:71:MET:CE	2.34	0.57
2:T:155:ARG:CG	6:T:5723:HOH:O	2.33	0.57
2:T:54[A]:ARG:NE	6:T:4784:HOH:O	2.25	0.57
2:T:87:LYS:HD2	6:T:4753:HOH:O	2.05	0.57
2:V:108:SER:OG	2:V:138:HIS:CD2	2.58	0.57
2:V:53:ARG:HH11	2:V:96:HIS:HD2	1.51	0.57
2:X:63:GLU:HG3	6:X:6229:HOH:O	2.03	0.57
1:E:130:ARG:HH11	1:E:149:LYS:HD2	1.68	0.57
1:G:69:GLU:HG3	6:G:6336:HOH:O	2.05	0.57
2:F:148:VAL:HG13	2:F:156:ILE:HG23	1.87	0.57
2:V:138:HIS:CD2	2:V:155:ARG:NH1	2.73	0.57
1:M:249[A]:LYS:HG2	2:N:54[A]:ARG:NH2	2.20	0.56
1:O:269:LYS:C	6:O:6335:HOH:O	2.43	0.56
1:O:37:ALA:C	2:P:54[A]:ARG:HD2	2.25	0.56
1:S:238:ILE:O	1:S:241:SER:HB3	2.05	0.56
2:V:54[A]:ARG:NH2	6:V:2884:HOH:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ALA:O	1:E:32:LYS:HG2	2.05	0.56
2:L:123:LYS:NZ	2:L:147:GLU:OE2	2.28	0.56
1:M:270:GLU:CD	6:M:6337:HOH:O	2.42	0.56
1:S:23:MET:HG2	6:S:6294:HOH:O	2.04	0.56
2:B:122:ILE:HB	2:B:125:LEU:HG	1.87	0.56
1:E:46:GLU:HA	1:E:66:ILE:HD13	1.86	0.56
1:I:234:VAL:CB	6:I:6296:HOH:O	2.32	0.56
2:T:63:GLU:HB3	2:T:64:PRO:HD3	1.87	0.56
1:K:270:GLU:O	1:K:271:LEU:HD12	2.05	0.56
1:W:234[A]:VAL:HG21	1:W:251:ILE:HG21	1.87	0.56
1:M:100:TYR:CZ	1:M:124:PRO:HB2	2.41	0.56
2:X:138:HIS:CB	6:X:6135:HOH:O	2.50	0.56
1:O:249:LYS:HZ2	2:P:54[A]:ARG:NH2	1.96	0.56
2:T:139:ILE:HB	6:T:5578:HOH:O	2.06	0.56
1:E:270:GLU:HB2	6:E:6343:HOH:O	2.01	0.56
2:F:32:ARG:HB3	2:F:34:GLU:OE1	2.05	0.56
2:R:34:GLU:H	2:R:34:GLU:CD	2.10	0.56
2:R:54[B]:ARG:HD3	6:R:3929:HOH:O	2.06	0.56
1:K:51:ASP:HA	1:K:54:ALA:HB3	1.88	0.56
2:N:12:ALA:HB3	6:N:6065:HOH:O	2.05	0.56
2:P:2:LEU:HD21	6:P:6209:HOH:O	2.06	0.56
1:Q:192:PRO:HB2	4:Q:6035:EDO:H22	1.87	0.56
2:B:53:ARG:HH11	2:B:96:HIS:CD2	2.23	0.55
1:C:151:GLU:CB	6:C:6366:HOH:O	2.53	0.55
6:K:6292:HOH:O	2:L:113:VAL:CB	2.45	0.55
2:R:2:LEU:CD2	2:R:188:GLU:HG2	2.36	0.55
1:U:204:LYS:HE2	6:U:6211:HOH:O	2.05	0.55
1:I:271:LEU:HD12	6:I:6304:HOH:O	2.06	0.55
1:S:245:ALA:O	1:S:249:LYS:HD3	2.06	0.55
2:X:2:LEU:CD2	2:X:188:GLU:HG3	2.36	0.55
2:L:53:ARG:HH11	2:L:96:HIS:HD2	1.54	0.55
2:R:149:LEU:HD11	2:R:160:LYS:HB2	1.89	0.55
2:X:53:ARG:HH11	2:X:96:HIS:CD2	2.23	0.55
3:K:6021:CL:CL	6:K:6236:HOH:O	2.55	0.55
2:V:108:SER:HB2	2:V:138:HIS:NE2	2.22	0.55
2:X:144:GLU:HB3	6:X:6191:HOH:O	2.05	0.55
1:U:270:GLU:N	6:U:6312:HOH:O	2.39	0.55
1:I:22:ILE:HG12	1:I:41:ALA:HB3	1.89	0.54
2:L:138:HIS:CG	6:L:6132:HOH:O	2.60	0.54
2:P:178:ARG:CZ	6:P:6192:HOH:O	2.55	0.54
2:P:44:LEU:CD1	2:P:85:LEU:HD13	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:152:PRO:HD2	6:O:6323:HOH:O	2.07	0.54
1:C:23:MET:CE	1:C:238:ILE:HD12	2.37	0.54
2:P:53:ARG:HH11	2:P:96:HIS:CD2	2.24	0.54
1:G:29:GLU:HB2	6:G:6361:HOH:O	2.06	0.54
1:G:67:VAL:HG12	1:G:71:MET:HE2	1.90	0.54
2:H:12:ALA:HB3	6:H:6040:HOH:O	2.07	0.54
1:M:249[B]:LYS:NZ	6:M:6318:HOH:O	2.36	0.54
1:O:36:GLU:HB3	6:O:6348:HOH:O	2.05	0.54
2:T:138:HIS:CD2	2:T:155:ARG:HD2	2.42	0.54
1:U:53:ARG:O	1:U:56:GLY:HA3	2.08	0.54
1:S:123:VAL:HB	6:S:6328:HOH:O	2.07	0.54
2:T:138:HIS:HD2	6:T:5384:HOH:O	1.91	0.54
2:T:62:MET:O	2:T:66:ARG:HG3	2.08	0.54
1:K:47:ARG:HG2	1:K:52:ILE:CG1	2.38	0.54
2:P:21:GLU:N	6:P:6201:HOH:O	2.39	0.54
1:I:272:GLY:N	6:I:6360:HOH:O	2.41	0.54
1:Q:232:VAL:HG12	1:Q:234:VAL:HG23	1.90	0.53
2:X:66:ARG:HG2	2:X:66:ARG:HH11	1.73	0.53
1:E:194:GLU:HB2	4:E:6047:EDO:H12	1.89	0.53
1:E:257:HIS:HE1	2:F:59:TYR:CE1	2.27	0.53
1:Q:192:PRO:CB	4:Q:6035:EDO:H22	2.39	0.53
1:S:152:PRO:CD	6:S:6344:HOH:O	2.40	0.53
2:T:156:ILE:HD12	6:T:5578:HOH:O	2.07	0.53
2:F:183:PHE:O	2:F:187:VAL:HG23	2.07	0.53
2:F:66:ARG:HH11	2:F:66:ARG:HG2	1.74	0.53
1:A:3:GLN:HB3	6:A:6279:HOH:O	2.08	0.53
2:N:123:LYS:HD3	6:N:6225:HOH:O	2.08	0.53
1:U:130:ARG:NH1	1:U:149:LYS:NZ	2.57	0.53
2:V:133:PHE:HE2	6:V:5124:HOH:O	1.92	0.53
1:W:8:ARG:HD2	2:X:117:GLU:OE2	2.09	0.53
2:X:50:THR:O	2:X:54[B]:ARG:HG2	2.09	0.53
1:G:192:PRO:HB3	4:G:6043:EDO:C2	2.29	0.53
1:E:8:ARG:HD3	2:F:132:VAL:HG21	1.91	0.52
2:V:125:LEU:CD2	2:V:182:LEU:HD11	2.39	0.52
1:A:150:GLY:O	6:A:6294:HOH:O	2.19	0.52
1:K:8:ARG:CZ	6:K:6321:HOH:O	2.56	0.52
2:V:154:GLY:C	6:V:5669:HOH:O	2.47	0.52
1:W:53:ARG:O	1:W:56:GLY:N	2.32	0.52
1:A:262:LYS:HE3	6:C:6286:HOH:O	2.08	0.52
3:I:6017:CL:CL	6:S:6181:HOH:O	2.56	0.52
4:I:6039:EDO:O1	6:I:6162:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:155:ARG:HG2	2:L:155:ARG:HH11	1.73	0.52
1:S:130:ARG:NH1	1:S:149:LYS:HZ2	2.07	0.52
2:T:155:ARG:CD	6:T:5723:HOH:O	2.56	0.52
2:D:194:ALA:C	6:D:6133:HOH:O	2.47	0.52
2:D:62:MET:O	2:D:66:ARG:HG3	2.09	0.52
2:P:44:LEU:HD12	2:P:85:LEU:HD13	1.91	0.52
1:U:270:GLU:CA	6:U:6312:HOH:O	2.57	0.52
1:A:194:GLU:CB	4:A:6031:EDO:H12	2.33	0.52
1:C:23:MET:HE3	1:C:238:ILE:CD1	2.39	0.52
6:G:6105:HOH:O	2:H:54:ARG:HD2	2.09	0.52
2:V:138:HIS:HB2	6:V:5292:HOH:O	2.10	0.52
1:O:2:ALA:HA	2:P:117:GLU:O	2.09	0.52
2:X:89:ILE:HG12	6:X:6200:HOH:O	2.09	0.52
1:A:46:GLU:HG3	1:A:66:ILE:HD12	1.92	0.52
1:C:50:ALA:O	1:C:54:ALA:CB	2.58	0.52
2:P:127:GLU:H	2:P:127:GLU:CD	2.13	0.52
1:G:269:LYS:C	6:G:6314:HOH:O	2.47	0.51
1:O:117:ASN:ND2	1:O:120[A]:GLU:OE2	2.43	0.51
1:W:174:VAL:HG13	1:W:182:LEU:HD11	1.92	0.51
2:J:193:LYS:HE2	6:J:6222:HOH:O	2.09	0.51
2:L:138:HIS:CD2	6:L:6132:HOH:O	2.62	0.51
1:O:172[B]:ARG:CZ	6:O:6309:HOH:O	2.37	0.51
2:P:129:PHE:CD1	6:P:6192:HOH:O	2.54	0.51
1:A:38:GLY:O	2:B:51:THR:HG23	2.10	0.51
2:B:50:THR:OG1	6:B:2702:HOH:O	2.19	0.51
2:L:2:LEU:O	6:L:6172:HOH:O	2.18	0.51
2:T:155:ARG:CD	6:T:5384:HOH:O	2.19	0.51
1:W:153:GLY:C	6:W:6298:HOH:O	2.49	0.51
1:G:152:PRO:CD	6:G:6302:HOH:O	2.51	0.51
4:M:6007:EDO:O2	6:M:6107:HOH:O	2.19	0.51
2:R:2:LEU:HD22	2:R:188:GLU:HG2	1.93	0.51
1:E:104:SER:OG	1:E:106:VAL:HG22	2.11	0.51
1:I:249:LYS:HG3	2:J:54[A]:ARG:NH1	2.25	0.51
1:O:8:ARG:HD3	2:P:132:VAL:HG21	1.91	0.51
1:W:213:GLY:C	6:W:6367:HOH:O	2.47	0.51
1:A:28:ALA:HB1	1:A:73:ALA:HB2	1.92	0.51
2:F:14:ARG:NH1	2:F:15:GLU:OE2	2.44	0.51
2:P:151:GLU:HA	2:P:155:ARG:O	2.11	0.51
1:K:232:VAL:HG12	1:K:234[A]:VAL:HG23	1.93	0.51
1:K:234[A]:VAL:HG21	1:K:251:ILE:HG21	1.93	0.51
1:C:67:VAL:CG1	1:C:71:MET:HE2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:6359:HOH:O	2:F:132:VAL:HG21	2.09	0.51
2:F:180:THR:O	2:F:184:VAL:HG23	2.11	0.51
2:N:1:MET:HE2	6:N:6223:HOH:O	2.10	0.51
2:H:2:LEU:H	2:H:2:LEU:HD22	1.75	0.51
1:I:49:PRO:HD3	6:I:6366:HOH:O	2.11	0.51
2:B:74:PRO:HG2	2:B:187:VAL:HA	1.92	0.50
2:D:192:GLN:O	2:D:193:LYS:HB2	2.10	0.50
1:O:53:ARG:O	1:O:56:GLY:HA2	2.11	0.50
1:U:246:LYS:NZ	6:U:6323:HOH:O	2.44	0.50
1:W:36:GLU:HG3	6:W:6304:HOH:O	2.11	0.50
1:A:8:ARG:HD2	2:B:117:GLU:OE2	2.11	0.50
2:F:63:GLU:N	6:F:5427:HOH:O	2.43	0.50
1:W:45:LEU:HD21	1:W:81:LYS:HE2	1.93	0.50
1:I:271:LEU:HD11	6:I:6252:HOH:O	2.11	0.50
2:L:68:PHE:CE1	2:L:73:LYS:HD3	2.46	0.50
2:P:3:THR:HG22	2:P:39:VAL:HG12	1.93	0.50
1:I:272:GLY:C	6:I:6368:HOH:O	2.50	0.50
6:K:6292:HOH:O	2:L:113:VAL:CG2	2.59	0.50
6:O:6271:HOH:O	2:P:113[B]:VAL:HG11	2.10	0.50
2:V:54[B]:ARG:HG2	2:V:54[B]:ARG:NH1	2.20	0.50
2:X:108:SER:HG	2:X:138:HIS:CE1	2.30	0.50
1:C:115:HIS:HD2	6:C:6240:HOH:O	1.95	0.50
1:A:46:GLU:HG3	1:A:66:ILE:CD1	2.41	0.50
1:A:37:ALA:O	2:B:54[B]:ARG:HD3	2.11	0.50
2:D:192:GLN:O	2:D:193:LYS:CB	2.59	0.50
1:I:269:LYS:O	1:I:271:LEU:HD13	2.11	0.50
1:O:115:HIS:HE1	6:O:6094:HOH:O	1.95	0.50
1:E:269:LYS:O	1:E:270:GLU:HB2	2.12	0.50
1:I:238:ILE:HD11	6:I:6296:HOH:O	2.12	0.50
2:N:67:GLU:HG2	6:N:6216:HOH:O	2.10	0.50
1:K:47:ARG:HG2	1:K:52:ILE:HG13	1.93	0.50
1:O:2:ALA:N	6:O:6173:HOH:O	2.44	0.50
1:A:36[B]:GLU:HB2	6:B:5598:HOH:O	2.12	0.50
1:I:234:VAL:CG1	6:I:6296:HOH:O	2.57	0.50
1:W:2:ALA:N	6:W:6320:HOH:O	2.45	0.50
1:E:8:ARG:HG2	6:E:6359:HOH:O	2.11	0.49
1:Q:149:LYS:HE2	6:Q:6310:HOH:O	2.11	0.49
1:U:36:GLU:HG3	6:V:5545:HOH:O	2.12	0.49
1:E:47:ARG:HB2	1:E:52:ILE:HD11	1.92	0.49
1:W:47:ARG:HG3	1:W:52:ILE:HD11	1.94	0.49
2:B:44:LEU:CD1	2:B:85:LEU:HD13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:HIS:CE1	2:F:140:LEU:HD23	2.47	0.49
1:G:130:ARG:NE	6:G:6332:HOH:O	2.44	0.49
2:H:54:ARG:HG2	6:H:6135:HOH:O	2.12	0.49
2:B:20:ILE:HG23	2:B:25:ALA:HB3	1.92	0.49
3:C:6005:CL:CL	6:C:6284:HOH:O	2.57	0.49
1:I:232:VAL:CG1	1:I:234:VAL:HG23	2.42	0.49
2:V:53:ARG:HH11	2:V:96:HIS:CD2	2.28	0.49
2:D:53:ARG:HH11	2:D:96:HIS:CD2	2.29	0.49
1:E:50:ALA:CB	6:E:6364:HOH:O	2.52	0.49
2:P:2:LEU:HD21	2:P:188:GLU:HG2	1.95	0.49
2:H:193:LYS:C	6:H:6179:HOH:O	2.50	0.49
2:H:86:ALA:O	2:H:98:GLY:HA2	2.13	0.49
1:I:197:LEU:HG	6:I:6364:HOH:O	2.12	0.49
2:P:105:GLU:HB2	2:P:140:LEU:HD11	1.95	0.49
1:A:130[A]:ARG:NH1	1:A:149:LYS:NZ	2.61	0.49
2:D:32:ARG:HE	2:D:34:GLU:CD	2.16	0.49
1:G:130:ARG:HG2	1:G:163:HIS:CE1	2.48	0.49
1:A:22:ILE:HG12	1:A:41:ALA:HB3	1.94	0.49
1:C:3:GLN:NE2	6:C:6234:HOH:O	2.45	0.49
1:I:173:LYS:HE3	6:Q:6066:HOH:O	2.12	0.49
1:I:262:LYS:NZ	1:K:95:ALA:O	2.45	0.49
2:P:178:ARG:NH2	6:P:6192:HOH:O	2.45	0.49
1:E:152:PRO:HG2	6:E:6363:HOH:O	2.13	0.49
1:M:72:ASN:HB3	6:M:6328:HOH:O	2.12	0.49
2:P:66:ARG:HG2	2:P:66:ARG:HH11	1.78	0.49
1:Q:194:GLU:CB	4:Q:6035:EDO:H21	2.43	0.48
1:U:65:THR:HB	6:U:6303:HOH:O	2.12	0.48
2:X:88:GLU:HG2	2:X:103:VAL:HG13	1.95	0.48
1:K:53:ARG:HD3	6:K:6272:HOH:O	2.14	0.48
1:I:192:PRO:HB3	4:I:6039:EDO:C2	2.42	0.48
2:X:151:GLU:HG3	6:X:6236:HOH:O	2.13	0.48
1:G:234:VAL:CB	6:G:6331:HOH:O	2.43	0.48
2:N:127:GLU:HG2	6:N:6204:HOH:O	2.13	0.48
2:D:96:HIS:HE1	6:D:6028:HOH:O	1.95	0.48
1:E:8:ARG:CG	6:E:6359:HOH:O	2.62	0.48
2:P:14:ARG:NH1	2:P:15:GLU:OE2	2.46	0.48
1:U:8:ARG:HD3	2:V:132:VAL:HG21	1.95	0.48
1:C:234:VAL:HG21	1:C:251:ILE:HG21	1.95	0.48
2:P:127:GLU:HG3	6:P:6198:HOH:O	2.13	0.48
1:Q:271:LEU:C	6:Q:6289:HOH:O	2.52	0.48
1:S:2:ALA:HA	2:T:117:GLU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:53:ARG:HH11	2:T:96:HIS:HD2	1.60	0.48
1:W:271:LEU:C	6:W:6338:HOH:O	2.51	0.48
2:B:138:HIS:NE2	2:B:140:LEU:HD23	2.29	0.48
1:I:174:VAL:HG13	1:I:182:LEU:HD11	1.96	0.48
1:I:8:ARG:HD3	2:J:132:VAL:HG21	1.96	0.48
1:K:269:LYS:O	1:K:271:LEU:CD1	2.61	0.48
1:M:48:VAL:HA	6:M:6331:HOH:O	2.14	0.48
1:O:238:ILE:HD13	1:O:247:PHE:HD2	1.79	0.48
1:U:201:LYS:CE	6:U:6288:HOH:O	2.25	0.48
1:U:67:VAL:HG12	1:U:71:MET:HE2	1.96	0.48
1:M:67:VAL:HG12	1:M:71:MET:HE2	1.92	0.48
1:U:45:LEU:HD21	1:U:81:LYS:HE2	1.96	0.48
1:O:152:PRO:HB2	6:O:6323:HOH:O	2.14	0.47
4:A:6031:EDO:H21	1:O:194:GLU:CG	2.40	0.47
1:E:123:VAL:HB	6:E:6262:HOH:O	2.14	0.47
1:I:100:TYR:CZ	1:I:124:PRO:HB2	2.50	0.47
2:T:20:ILE:HG23	2:T:25:ALA:HB3	1.96	0.47
1:K:249:LYS:HE3	6:K:6123:HOH:O	2.12	0.47
1:C:53:ARG:HB2	6:C:6344:HOH:O	2.13	0.47
1:K:130:ARG:NH1	1:K:149:LYS:NZ	2.63	0.47
1:U:46:GLU:HA	1:U:66:ILE:HD13	1.95	0.47
1:E:152:PRO:HB3	6:E:6327:HOH:O	2.15	0.47
2:F:87:LYS:HA	2:F:98:GLY:HA2	1.95	0.47
1:I:197:LEU:CG	6:I:6364:HOH:O	2.61	0.47
1:S:242:ASP:OD1	6:S:6334:HOH:O	2.20	0.47
1:U:68:GLU:CG	6:U:6293:HOH:O	2.63	0.47
1:U:151:GLU:OE2	1:U:154:THR:HG21	2.14	0.47
2:V:125:LEU:HD21	2:V:182:LEU:HD11	1.96	0.47
2:P:32:ARG:NH2	6:P:6178:HOH:O	2.47	0.47
2:R:2:LEU:HD11	2:R:187:VAL:HG12	1.95	0.47
2:R:32:ARG:HB3	2:R:34:GLU:OE1	2.15	0.47
2:T:87:LYS:HD3	2:T:98:GLY:O	2.15	0.47
1:C:22:ILE:HG12	1:C:41:ALA:HB3	1.97	0.47
1:E:15:GLU:OE1	1:E:18:LYS:NZ	2.47	0.47
2:R:183:PHE:O	2:R:187:VAL:HG23	2.14	0.47
2:F:20:ILE:HD11	2:F:43:ILE:HD12	1.96	0.47
1:G:204:LYS:HE2	6:G:6310:HOH:O	2.13	0.47
1:Q:65:THR:O	1:Q:69:GLU:HG3	2.14	0.47
1:C:50:ALA:O	1:C:54:ALA:HB3	2.15	0.47
1:E:174:VAL:HG13	1:E:182:LEU:HD11	1.96	0.47
1:E:238:ILE:HD11	6:E:6336:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:152:PRO:HB3	6:I:6330:HOH:O	2.15	0.47
1:O:240:LYS:NZ	6:O:6316:HOH:O	2.43	0.47
1:O:35:GLU:OE2	1:O:74:VAL:HB	2.15	0.47
1:O:36:GLU:CB	6:O:6348:HOH:O	2.61	0.47
1:O:262:LYS:HE3	1:Q:95:ALA:HB1	1.97	0.47
1:G:152:PRO:HB2	6:G:6302:HOH:O	2.14	0.47
2:P:191:LYS:HE2	6:P:6186:HOH:O	2.15	0.47
1:I:71:MET:HE2	2:J:111:ARG:CZ	2.44	0.46
2:X:54[B]:ARG:CZ	6:X:6143:HOH:O	2.48	0.46
4:E:6047:EDO:H12	1:W:194:GLU:HG2	1.96	0.46
2:V:74:PRO:HG2	2:V:187:VAL:HA	1.96	0.46
1:I:194:GLU:HB2	4:I:6039:EDO:H12	1.91	0.46
1:U:67:VAL:HG12	1:U:71:MET:CE	2.46	0.46
1:W:172[B]:ARG:CZ	6:W:6289:HOH:O	2.47	0.46
1:E:8:ARG:HD2	2:F:117:GLU:OE2	2.15	0.46
1:S:204:LYS:HE2	6:S:6305:HOH:O	2.14	0.46
1:G:201:LYS:HG3	6:G:6333:HOH:O	2.16	0.46
1:S:201:LYS:NZ	6:S:6260:HOH:O	2.47	0.46
2:F:68:PHE:CE1	2:F:73:LYS:HD2	2.50	0.46
1:K:28:ALA:HB2	1:K:69:GLU:HG2	1.97	0.46
1:S:151:GLU:HB3	6:S:6248:HOH:O	2.15	0.46
1:U:134:GLU:OE2	1:U:149:LYS:HE3	2.16	0.46
1:U:115:HIS:HE1	6:U:6106:HOH:O	1.98	0.46
1:W:104:SER:OG	1:W:106:VAL:HG22	2.16	0.46
2:X:54[A]:ARG:NH2	6:X:6147:HOH:O	2.46	0.46
2:D:74:PRO:HG2	2:D:187:VAL:HA	1.97	0.46
1:E:14:ALA:HB1	1:E:208:VAL:HG22	1.96	0.46
6:E:6359:HOH:O	2:F:173:LEU:HB3	2.15	0.46
1:G:29:GLU:OE1	6:G:6205:HOH:O	2.21	0.46
4:A:6031:EDO:C2	1:O:194:GLU:H	2.29	0.46
1:A:104:SER:OG	1:A:106:VAL:HG22	2.15	0.46
1:E:7:GLU:CD	6:E:6372:HOH:O	2.54	0.46
6:E:6359:HOH:O	2:F:132:VAL:HG11	2.15	0.46
1:Q:28:ALA:HB1	1:Q:73:ALA:HB2	1.97	0.46
1:A:2:ALA:HA	2:B:117:GLU:O	2.16	0.46
1:C:23:MET:HE2	1:C:238:ILE:HD12	1.98	0.46
2:P:160:LYS:HE2	6:P:6176:HOH:O	2.15	0.46
1:E:257:HIS:CE1	2:F:59:TYR:CE1	3.04	0.45
1:M:8:ARG:HD3	2:N:132:VAL:CG2	2.45	0.45
1:Q:192:PRO:HB3	4:Q:6035:EDO:C1	2.42	0.45
2:B:67:GLU:HG3	6:B:4729:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:194:GLU:CA	4:I:6039:EDO:H11	2.46	0.45
2:N:87:LYS:NZ	6:N:6132:HOH:O	2.48	0.45
1:O:249:LYS:HZ3	2:P:54[A]:ARG:HH21	1.57	0.45
2:R:191:LYS:C	6:R:4702:HOH:O	2.54	0.45
1:I:2:ALA:N	6:I:6303:HOH:O	2.49	0.45
1:M:192:PRO:HB3	4:M:6007:EDO:H21	1.97	0.45
1:Q:2:ALA:HA	2:R:117:GLU:O	2.16	0.45
1:A:106:VAL:HG12	1:A:152:PRO:HG2	1.99	0.45
1:E:101:ILE:CD1	1:E:123:VAL:HG11	2.46	0.45
2:F:66:ARG:CD	6:F:5427:HOH:O	2.58	0.45
2:R:50:THR:HB	2:R:54[B]:ARG:NH1	2.31	0.45
2:T:156:ILE:CD1	6:T:5578:HOH:O	2.64	0.45
2:D:66:ARG:HG2	2:D:66:ARG:HH11	1.81	0.45
1:G:194:GLU:CA	4:G:6043:EDO:H11	2.46	0.45
2:V:1:MET:HE2	2:V:1:MET:O	2.17	0.45
1:I:238:ILE:CD1	6:I:6296:HOH:O	2.64	0.45
2:T:88:GLU:HG3	2:T:103:VAL:HG13	1.98	0.45
1:I:271:LEU:CD1	6:I:6304:HOH:O	2.62	0.45
2:J:151:GLU:HB2	2:J:155:ARG:O	2.17	0.45
1:C:204:LYS:HE2	6:C:6202:HOH:O	2.15	0.45
2:L:151:GLU:CD	6:L:6162:HOH:O	2.55	0.45
2:L:151:GLU:HA	2:L:155:ARG:O	2.17	0.45
1:S:234:VAL:HG21	1:S:251:ILE:HG21	1.99	0.45
1:U:151:GLU:HG2	1:U:154:THR:CG2	2.47	0.45
6:M:6287:HOH:O	1:W:262:LYS:HE2	2.13	0.45
2:B:54[A]:ARG:NH2	6:B:3835:HOH:O	2.51	0.44
6:O:6271:HOH:O	2:P:113[A]:VAL:HG21	2.16	0.44
1:U:71:MET:HA	1:U:78:VAL:HG21	1.99	0.44
1:W:157:ILE:HD13	1:W:215:VAL:HA	1.98	0.44
3:G:6013:CL:CL	6:G:6293:HOH:O	2.59	0.44
2:N:177:HIS:HD2	6:N:6066:HOH:O	2.00	0.44
2:R:32:ARG:NH2	6:R:5656:HOH:O	2.50	0.44
2:V:1:MET:CE	2:V:1:MET:O	2.65	0.44
1:W:40:VAL:O	1:W:77:PRO:HD2	2.17	0.44
1:I:270:GLU:HB2	6:I:6367:HOH:O	2.17	0.44
1:M:115:HIS:CD2	6:M:6112:HOH:O	2.60	0.44
2:T:88:GLU:HG2	2:T:103:VAL:HG22	2.00	0.44
1:W:67:VAL:HG12	1:W:71:MET:HE1	1.97	0.44
1:E:238:ILE:CD1	6:E:6336:HOH:O	2.65	0.44
1:G:115:HIS:HE1	6:G:6087:HOH:O	2.00	0.44
1:G:174:VAL:HG13	1:G:182:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:76:PHE:HB2	2:H:183:PHE:CD1	2.52	0.44
1:K:104:SER:OG	1:K:106:VAL:HG22	2.17	0.44
2:L:53:ARG:HH11	2:L:96:HIS:CD2	2.34	0.44
2:P:62:MET:SD	2:P:97:LEU:HD23	2.58	0.44
1:A:36[B]:GLU:CD	6:A:6188:HOH:O	2.43	0.44
4:A:6031:EDO:O1	6:A:6169:HOH:O	2.21	0.44
2:F:53:ARG:HH11	2:F:96:HIS:CD2	2.32	0.44
1:W:153:GLY:CA	6:W:6298:HOH:O	2.65	0.44
1:C:47:ARG:HG3	1:C:52:ILE:HD11	1.99	0.44
2:F:102:VAL:HB	2:F:139:ILE:HG23	2.00	0.44
1:G:238:ILE:O	1:G:241:SER:HB3	2.17	0.44
2:N:31:LYS:HB2	6:N:6191:HOH:O	2.17	0.43
1:O:100:TYR:CZ	1:O:124:PRO:HB2	2.53	0.43
1:S:50:ALA:O	1:S:54:ALA:HB3	2.18	0.43
2:B:155[A]:ARG:HD3	6:B:5018:HOH:O	2.17	0.43
2:B:68:PHE:CE1	2:B:73:LYS:HD3	2.53	0.43
1:I:149:LYS:NZ	6:I:6292:HOH:O	2.49	0.43
1:C:36[A]:GLU:HG3	6:C:6281:HOH:O	2.18	0.43
1:E:194:GLU:CA	4:E:6047:EDO:H11	2.49	0.43
1:K:115:HIS:HD2	6:K:6212:HOH:O	2.00	0.43
1:U:247:PHE:CE1	1:U:271:LEU:HG	2.54	0.43
1:U:8:ARG:HD2	2:V:117:GLU:OE2	2.18	0.43
2:V:125:LEU:HA	6:V:5630:HOH:O	2.19	0.43
2:H:151:GLU:HA	2:H:155:ARG:O	2.19	0.43
1:S:8:ARG:HD2	2:T:117:GLU:OE2	2.19	0.43
1:S:8:ARG:HD3	2:T:132:VAL:HG21	2.01	0.43
2:V:54[B]:ARG:NH1	2:V:54[B]:ARG:CG	2.69	0.43
1:C:262:LYS:HE2	6:E:6351:HOH:O	2.12	0.43
1:G:262:LYS:CE	6:I:6350:HOH:O	2.38	0.43
1:I:151:GLU:OE2	1:I:154:THR:OG1	2.32	0.43
1:I:35:GLU:OE2	1:I:74:VAL:HB	2.18	0.43
2:P:54[A]:ARG:HG2	6:P:6109:HOH:O	2.18	0.43
2:R:54[B]:ARG:NH2	6:R:3386:HOH:O	2.52	0.43
2:D:108:SER:HB2	2:D:138:HIS:CE1	2.54	0.43
1:E:115:HIS:HD2	6:E:6237:HOH:O	2.01	0.43
2:H:44:LEU:CD1	2:H:85:LEU:HD13	2.49	0.43
1:A:10:LYS:HB3	1:A:124:PRO:HB3	2.01	0.43
1:C:23:MET:HE3	1:C:238:ILE:HD12	1.99	0.43
2:D:87:LYS:HA	2:D:98:GLY:HA2	2.01	0.43
2:H:2:LEU:HD23	6:H:6138:HOH:O	2.19	0.43
2:T:138:HIS:CE1	6:T:4026:HOH:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:MET:HE1	1:A:97:GLY:C	2.39	0.43
2:B:54[B]:ARG:CD	6:B:3460:HOH:O	2.62	0.43
1:K:40:VAL:O	1:K:77:PRO:HD2	2.19	0.43
2:P:54[A]:ARG:NH1	2:P:55:LEU:HD23	2.34	0.43
2:T:87:LYS:HA	2:T:98:GLY:HA2	2.01	0.43
2:L:76:PHE:HB2	2:L:183:PHE:CE1	2.54	0.42
2:N:8:GLY:HA2	2:N:13:VAL:HG21	2.00	0.42
1:Q:105:GLU:CG	6:Q:6310:HOH:O	2.66	0.42
1:Q:174:VAL:HG13	1:Q:182:LEU:HD11	2.01	0.42
1:Q:64:PRO:O	1:Q:68:GLU:HG3	2.19	0.42
4:G:6043:EDO:H21	1:U:194:GLU:H	1.84	0.42
2:L:143:GLY:HA2	6:L:6169:HOH:O	2.18	0.42
2:X:192:GLN:O	2:X:194:ALA:N	2.52	0.42
1:E:100:TYR:CZ	1:E:124:PRO:HB2	2.53	0.42
2:P:96:HIS:HE1	6:P:6052:HOH:O	2.01	0.42
2:T:88:GLU:CG	2:T:103:VAL:HG13	2.49	0.42
2:V:181:GLN:HE21	2:V:185:GLU:HG3	1.84	0.42
2:B:79:CYS:SG	5:B:6004:GLN:NE2	2.92	0.42
1:G:71:MET:HA	1:G:78:VAL:HG21	2.01	0.42
1:Q:46:GLU:O	6:Q:6315:HOH:O	2.22	0.42
1:W:157:ILE:HD12	6:W:6367:HOH:O	2.20	0.42
1:C:8:ARG:HD3	2:D:132:VAL:HG21	2.02	0.42
2:P:79:CYS:SG	5:P:6032:GLN:CD	2.98	0.42
1:U:247:PHE:HE1	1:U:271:LEU:HG	1.84	0.42
2:V:125:LEU:CD2	2:V:125:LEU:N	2.82	0.42
2:X:138:HIS:CD2	2:X:140:LEU:HD23	2.55	0.42
1:E:8:ARG:CD	6:E:6359:HOH:O	2.61	0.42
1:S:130:ARG:HD3	6:S:6211:HOH:O	2.19	0.42
1:W:195:LEU:HA	1:W:195:LEU:HD12	1.96	0.42
1:E:3[B]:GLN:NE2	6:E:6256:HOH:O	2.53	0.42
2:T:87:LYS:CB	6:T:4753:HOH:O	2.64	0.42
1:E:172[B]:ARG:CZ	6:E:6234:HOH:O	2.40	0.42
2:F:151:GLU:HA	2:F:155:ARG:O	2.20	0.42
2:J:192:GLN:O	2:J:193:LYS:C	2.57	0.42
2:L:192:GLN:C	6:L:6177:HOH:O	2.58	0.42
1:O:115:HIS:HD2	6:O:6176:HOH:O	2.03	0.42
2:T:108:SER:CB	2:T:138:HIS:HD1	2.33	0.42
2:V:66:ARG:CG	2:V:66:ARG:HH11	2.31	0.42
1:A:36[A]:GLU:HG2	6:B:5598:HOH:O	2.20	0.42
1:E:152:PRO:CD	6:E:6363:HOH:O	2.68	0.42
2:J:74:PRO:HG2	2:J:187:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:238:ILE:O	1:K:241:SER:HB3	2.20	0.42
1:M:232:VAL:CG1	1:M:234:VAL:HG23	2.49	0.42
2:N:175:GLU:OE2	2:N:175:GLU:HA	2.20	0.42
2:T:149:LEU:HD11	2:T:160:LYS:HB2	2.00	0.42
2:V:103:VAL:HG23	2:V:141:GLU:HG3	2.02	0.42
2:B:14:ARG:HD3	6:B:3011:HOH:O	2.20	0.41
1:C:40:VAL:O	1:C:77:PRO:HD2	2.20	0.41
1:C:8:ARG:HD2	2:D:117:GLU:OE2	2.20	0.41
1:E:36[A]:GLU:HG3	6:E:6282:HOH:O	2.19	0.41
1:I:49:PRO:CD	6:I:6366:HOH:O	2.68	0.41
1:I:81:LYS:NZ	6:I:6163:HOH:O	2.52	0.41
1:Q:194:GLU:CA	4:Q:6035:EDO:H21	2.50	0.41
1:S:115:HIS:HE1	6:S:6073:HOH:O	2.03	0.41
1:S:130:ARG:NH1	1:S:149:LYS:NZ	2.68	0.41
2:X:139:ILE:HB	2:X:156:ILE:HB	2.02	0.41
4:G:6043:EDO:H12	1:U:194:GLU:HG2	2.01	0.41
1:I:178:SER:OG	1:I:180:ASP:OD1	2.34	0.41
2:T:181:GLN:HG2	6:T:5402:HOH:O	2.19	0.41
2:X:151:GLU:HA	2:X:155:ARG:O	2.20	0.41
1:G:157:ILE:HD13	1:G:215:VAL:HA	2.02	0.41
1:W:22:ILE:HG12	1:W:41:ALA:HB3	2.03	0.41
1:A:232:VAL:HG12	1:A:234[B]:VAL:HG23	2.03	0.41
2:D:12:ALA:HB3	6:D:6037:HOH:O	2.21	0.41
1:E:270:GLU:O	6:E:6343:HOH:O	2.22	0.41
1:W:152:PRO:HG3	6:W:6373:HOH:O	2.19	0.41
1:W:153:GLY:HA2	6:W:6298:HOH:O	2.20	0.41
1:A:3:GLN:CA	6:A:6303:HOH:O	2.61	0.41
2:B:155[A]:ARG:HG2	6:B:5449:HOH:O	2.21	0.41
1:C:23:MET:HE3	1:C:238:ILE:HD13	2.01	0.41
2:H:87:LYS:HA	2:H:98:GLY:HA2	2.02	0.41
2:L:126:ASP:N	6:L:6171:HOH:O	2.32	0.41
1:S:151:GLU:HG2	1:S:154:THR:CG2	2.50	0.41
2:T:102:VAL:HB	2:T:139:ILE:HG23	2.03	0.41
6:M:6287:HOH:O	1:W:262:LYS:HE3	2.17	0.41
2:X:66:ARG:NH1	2:X:97:LEU:O	2.47	0.41
2:D:191:LYS:O	2:D:194:ALA:HB3	2.21	0.41
1:E:101:ILE:HD12	1:E:123:VAL:HG11	2.02	0.41
1:E:166:LYS:HG2	6:G:6348:HOH:O	2.21	0.41
1:I:262:LYS:NZ	6:I:6319:HOH:O	2.53	0.41
1:S:271:LEU:HD12	6:S:6267:HOH:O	2.20	0.41
2:T:138:HIS:NE2	2:T:140:LEU:HD23	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:3:GLN:HB3	6:U:6292:HOH:O	2.19	0.41
2:X:54[A]:ARG:CZ	6:X:6147:HOH:O	2.34	0.41
2:F:76:PHE:HB2	2:F:183:PHE:CD1	2.56	0.41
1:M:61:MET:HB2	1:M:89:GLU:CD	2.41	0.41
2:X:53:ARG:HD3	2:X:96:HIS:HD2	1.85	0.41
1:E:37:ALA:HA	1:E:249:LYS:HE2	2.02	0.41
1:E:36[A]:GLU:CD	6:E:6301:HOH:O	2.56	0.41
1:G:52:ILE:O	1:G:55:ALA:HB3	2.21	0.41
2:J:87:LYS:HA	2:J:98:GLY:HA2	2.01	0.41
1:O:174:VAL:HG13	1:O:182:LEU:HD11	2.03	0.41
2:R:137:PRO:O	2:R:168:SER:HB2	2.21	0.41
1:E:101:ILE:O	1:E:125:PHE:HA	2.21	0.41
2:F:8:GLY:HA2	2:F:13:VAL:HG21	2.03	0.41
1:S:100:TYR:CZ	1:S:124:PRO:HB2	2.56	0.41
2:V:102:VAL:HB	2:V:139:ILE:HG23	2.02	0.41
2:L:81:GLY:HA2	6:L:6111:HOH:O	2.21	0.41
2:T:183:PHE:O	2:T:187:VAL:HG23	2.20	0.41
2:T:53:ARG:HH11	2:T:96:HIS:CD2	2.38	0.41
2:V:76:PHE:HB2	2:V:183:PHE:CD1	2.55	0.41
1:W:47:ARG:HB3	1:W:47:ARG:HE	1.63	0.41
2:H:76:PHE:HB2	2:H:183:PHE:CE1	2.56	0.41
1:K:194:GLU:HG2	4:Q:6035:EDO:H12	2.02	0.41
1:M:71:MET:HA	1:M:78:VAL:HG21	2.03	0.41
2:R:151:GLU:CD	6:R:3363:HOH:O	2.59	0.41
2:T:63:GLU:HB2	6:T:4130:HOH:O	2.19	0.41
2:D:79:CYS:SG	5:D:6008:GLN:CD	2.99	0.40
1:K:204:LYS:HE2	6:K:6249:HOH:O	2.21	0.40
1:O:249:LYS:HG3	6:O:6272:HOH:O	2.21	0.40
1:Q:234:VAL:HG21	1:Q:251:ILE:HG21	2.04	0.40
1:U:130:ARG:NE	6:U:6223:HOH:O	2.53	0.40
1:U:53:ARG:HD3	1:U:108:THR:OG1	2.21	0.40
1:W:262:LYS:HG3	6:W:6378:HOH:O	2.21	0.40
1:E:50:ALA:CA	6:E:6364:HOH:O	2.69	0.40
2:P:79:CYS:SG	5:P:6032:GLN:NE2	2.94	0.40
2:T:84:ILE:O	2:T:96:HIS:HB2	2.22	0.40
1:K:115:HIS:HE1	6:K:6040:HOH:O	2.04	0.40
2:N:184:VAL:O	2:N:188:GLU:HG3	2.21	0.40
2:N:54[B]:ARG:NH1	6:N:6095:HOH:O	2.31	0.40
2:R:8:GLY:HA2	2:R:13:VAL:HG21	2.03	0.40
1:U:130:ARG:NH1	1:U:149:LYS:HZ1	2.19	0.40
1:U:3:GLN:NE2	6:V:2913:HOH:O	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:HG3	6:A:6232:HOH:O	2.21	0.40
1:A:38:GLY:HA3	2:B:54[B]:ARG:HG2	2.04	0.40
1:E:249:LYS:NZ	6:E:6278:HOH:O	2.53	0.40
2:H:14[A]:ARG:NH2	6:H:6176:HOH:O	2.54	0.40
1:M:238:ILE:O	1:M:241:SER:HB3	2.20	0.40
1:S:152:PRO:N	6:S:6344:HOH:O	2.53	0.40
1:K:113:GLU:HB3	6:K:6210:HOH:O	2.20	0.40
1:K:67:VAL:HG12	1:K:71:MET:HE2	2.02	0.40
2:L:63:GLU:HB2	6:L:6152:HOH:O	2.20	0.40
1:U:130:ARG:HH12	1:U:149:LYS:NZ	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:87:LYS:NZ	2:X:141:GLU:OE1[1_656]	1.83	0.37
6:R:1160:HOH:O	6:W:6293:HOH:O[1_556]	2.16	0.04

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/294 (92%)	269 (99%)	3 (1%)	0	100	100
1	C	272/294 (92%)	266 (98%)	6 (2%)	0	100	100
1	E	272/294 (92%)	266 (98%)	6 (2%)	0	100	100
1	G	269/294 (92%)	264 (98%)	4 (2%)	1 (0%)	38	35
1	I	273/294 (93%)	265 (97%)	7 (3%)	1 (0%)	38	35
1	K	272/294 (92%)	265 (97%)	7 (3%)	0	100	100
1	M	272/294 (92%)	270 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	270/294 (92%)	266 (98%)	2 (1%)	2 (1%)	25	19
1	Q	271/294 (92%)	266 (98%)	3 (1%)	2 (1%)	25	19
1	S	271/294 (92%)	265 (98%)	6 (2%)	0	100	100
1	U	273/294 (93%)	269 (98%)	4 (2%)	0	100	100
1	W	274/294 (93%)	269 (98%)	5 (2%)	0	100	100
2	B	193/204 (95%)	186 (96%)	6 (3%)	1 (0%)	32	28
2	D	193/204 (95%)	187 (97%)	5 (3%)	1 (0%)	32	28
2	F	190/204 (93%)	183 (96%)	7 (4%)	0	100	100
2	H	193/204 (95%)	187 (97%)	6 (3%)	0	100	100
2	J	195/204 (96%)	187 (96%)	7 (4%)	1 (0%)	32	28
2	L	191/204 (94%)	183 (96%)	8 (4%)	0	100	100
2	N	192/204 (94%)	185 (96%)	6 (3%)	1 (0%)	32	28
2	P	193/204 (95%)	188 (97%)	5 (3%)	0	100	100
2	R	193/204 (95%)	189 (98%)	3 (2%)	1 (0%)	32	28
2	T	193/204 (95%)	188 (97%)	5 (3%)	0	100	100
2	V	193/204 (95%)	183 (95%)	9 (5%)	1 (0%)	32	28
2	X	194/204 (95%)	186 (96%)	7 (4%)	1 (0%)	32	28
All	All	5574/5976 (93%)	5432 (98%)	129 (2%)	13 (0%)	51	51

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	193	LYS
1	G	57	GLY
1	I	57	GLY
1	O	57	GLY
2	J	192	GLN
1	Q	270	GLU
2	X	193	LYS
2	B	79	CYS
2	V	79	CYS
2	N	79	CYS
2	R	79	CYS
1	O	214	GLY
1	Q	214	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/227 (92%)	203 (97%)	7 (3%)	43	44
1	C	211/227 (93%)	204 (97%)	7 (3%)	43	44
1	E	211/227 (93%)	204 (97%)	7 (3%)	43	44
1	G	207/227 (91%)	198 (96%)	9 (4%)	33	32
1	I	211/227 (93%)	203 (96%)	8 (4%)	38	37
1	K	210/227 (92%)	203 (97%)	7 (3%)	43	44
1	M	211/227 (93%)	207 (98%)	4 (2%)	62	67
1	O	209/227 (92%)	203 (97%)	6 (3%)	48	50
1	Q	209/227 (92%)	202 (97%)	7 (3%)	43	44
1	S	209/227 (92%)	200 (96%)	9 (4%)	33	32
1	U	209/227 (92%)	203 (97%)	6 (3%)	48	50
1	W	212/227 (93%)	204 (96%)	8 (4%)	38	37
2	B	160/168 (95%)	151 (94%)	9 (6%)	25	21
2	D	159/168 (95%)	151 (95%)	8 (5%)	28	25
2	F	157/168 (94%)	147 (94%)	10 (6%)	20	17
2	H	159/168 (95%)	149 (94%)	10 (6%)	21	17
2	J	161/168 (96%)	152 (94%)	9 (6%)	25	21
2	L	158/168 (94%)	150 (95%)	8 (5%)	28	25
2	N	158/168 (94%)	150 (95%)	8 (5%)	28	25
2	P	160/168 (95%)	152 (95%)	8 (5%)	28	25
2	R	160/168 (95%)	150 (94%)	10 (6%)	21	17
2	T	158/168 (94%)	149 (94%)	9 (6%)	24	20
2	V	159/168 (95%)	152 (96%)	7 (4%)	33	31
2	X	160/168 (95%)	149 (93%)	11 (7%)	18	14
All	All	4428/4740 (93%)	4236 (96%)	192 (4%)	37	32

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	51	ASP
1	A	100	TYR
1	A	117	ASN
1	A	131[A]	ASP
1	A	131[B]	ASP
1	A	195	LEU
2	B	1	MET
2	B	34	GLU
2	B	50	THR
2	B	61	PHE
2	B	63	GLU
2	B	85	LEU
2	B	125	LEU
2	B	127	GLU
2	B	144	GLU
1	C	47	ARG
1	C	100	TYR
1	C	117	ASN
1	C	131	ASP
1	C	182	LEU
1	C	195	LEU
1	C	249	LYS
2	D	1	MET
2	D	2	LEU
2	D	54[A]	ARG
2	D	54[B]	ARG
2	D	63	GLU
2	D	67	GLU
2	D	104	VAL
2	D	138	HIS
1	E	29[A]	GLU
1	E	29[B]	GLU
1	E	32	LYS
1	E	100	TYR
1	E	117	ASN
1	E	131	ASP
1	E	195	LEU
2	F	32	ARG
2	F	54[A]	ARG
2	F	54[B]	ARG
2	F	61	PHE
2	F	63	GLU

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Mol	Chain	Res	Type
2	F	85	LEU
2	F	127	GLU
2	F	151	GLU
2	F	168	SER
2	F	191	LYS
1	G	36[A]	GLU
1	G	36[B]	GLU
1	G	100	TYR
1	G	117	ASN
1	G	131[A]	ASP
1	G	131[B]	ASP
1	G	182	LEU
1	G	208	VAL
1	G	241	SER
2	H	1	MET
2	H	2	LEU
2	H	34[A]	GLU
2	H	34[B]	GLU
2	H	54	ARG
2	H	62	MET
2	H	67	GLU
2	H	85	LEU
2	H	138	HIS
2	H	144	GLU
1	I	36	GLU
1	I	100	TYR
1	I	117	ASN
1	I	131[A]	ASP
1	I	131[B]	ASP
1	I	182	LEU
1	I	195	LEU
1	I	242	ASP
2	J	54[A]	ARG
2	J	54[B]	ARG
2	J	85	LEU
2	J	104	VAL
2	J	125	LEU
2	J	191	LYS
2	J	193	LYS
2	J	195	LEU
2	J	196	VAL
1	K	51	ASP

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Mol	Chain	Res	Type
1	K	100	TYR
1	K	113	GLU
1	K	131[A]	ASP
1	K	131[B]	ASP
1	K	195	LEU
1	K	208	VAL
2	L	14	ARG
2	L	54[A]	ARG
2	L	54[B]	ARG
2	L	63	GLU
2	L	67	GLU
2	L	85	LEU
2	L	104	VAL
2	L	127	GLU
1	M	100	TYR
1	M	117	ASN
1	M	182	LEU
1	M	195	LEU
2	N	1	MET
2	N	54[A]	ARG
2	N	54[B]	ARG
2	N	63	GLU
2	N	67	GLU
2	N	85	LEU
2	N	104	VAL
2	N	153	ASN
1	O	51	ASP
1	O	100	TYR
1	O	131	ASP
1	O	182	LEU
1	O	195	LEU
1	O	262	LYS
2	P	1	MET
2	P	14	ARG
2	P	54[A]	ARG
2	P	54[B]	ARG
2	P	61	PHE
2	P	67	GLU
2	P	85	LEU
2	P	127	GLU
1	Q	3	GLN
1	Q	100	TYR

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Mol	Chain	Res	Type
1	Q	117	ASN
1	Q	131[A]	ASP
1	Q	131[B]	ASP
1	Q	182	LEU
1	Q	195	LEU
2	R	1	MET
2	R	14[A]	ARG
2	R	14[B]	ARG
2	R	61	PHE
2	R	67	GLU
2	R	85	LEU
2	R	113	VAL
2	R	144	GLU
2	R	151	GLU
2	R	193	LYS
1	S	3	GLN
1	S	100	TYR
1	S	131[A]	ASP
1	S	131[B]	ASP
1	S	182	LEU
1	S	195	LEU
1	S	208	VAL
1	S	242	ASP
1	S	249	LYS
2	T	1	MET
2	T	34	GLU
2	T	54[A]	ARG
2	T	54[B]	ARG
2	T	61	PHE
2	T	62	MET
2	T	67	GLU
2	T	85	LEU
2	T	127	GLU
1	U	32	LYS
1	U	100	TYR
1	U	117	ASN
1	U	131[A]	ASP
1	U	131[B]	ASP
1	U	271	LEU
2	V	1	MET
2	V	63	GLU
2	V	67	GLU

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Mol	Chain	Res	Type
2	V	85	LEU
2	V	125	LEU
2	V	126	ASP
2	V	189	GLU
1	W	100	TYR
1	W	117	ASN
1	W	131[A]	ASP
1	W	131[B]	ASP
1	W	182	LEU
1	W	195	LEU
1	W	249	LYS
1	W	271	LEU
2	X	34	GLU
2	X	54[A]	ARG
2	X	54[B]	ARG
2	X	63	GLU
2	X	67	GLU
2	X	85	LEU
2	X	87	LYS
2	X	126	ASP
2	X	144	GLU
2	X	190	TYR
2	X	195	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	72	ASN
1	A	117	ASN
2	B	96	HIS
2	B	153	ASN
2	B	192	GLN
1	C	115	HIS
1	C	117	ASN
2	D	96	HIS
2	D	153	ASN
2	D	181	GLN
1	E	115	HIS
1	E	117	ASN
1	E	257	HIS
2	F	96	HIS

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Mol	Chain	Res	Type
2	F	138	HIS
2	F	153	ASN
2	F	181	GLN
1	G	115	HIS
1	G	117	ASN
2	H	96	HIS
2	H	138	HIS
1	I	115	HIS
1	I	117	ASN
1	I	257	HIS
1	K	115	HIS
2	L	96	HIS
2	L	153	ASN
1	M	115	HIS
1	M	117	ASN
2	N	96	HIS
2	N	153	ASN
2	P	96	HIS
2	P	138	HIS
1	Q	117	ASN
2	R	153	ASN
1	S	115	HIS
2	T	96	HIS
2	T	153	ASN
1	U	117	ASN
2	V	96	HIS
2	V	138	HIS
2	V	153	ASN
2	V	181	GLN
1	W	117	ASN
2	X	96	HIS
2	X	153	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

Of 42 ligands modelled in this entry, 12 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	A	6002	-	3,3,3	0.61	0	2,2,2	0.53	0
4	EDO	A	6030	-	3,3,3	0.27	0	2,2,2	0.79	0
4	EDO	A	6031	-	3,3,3	0.60	0	2,2,2	0.20	0
5	GLN	B	6004	-	4,9,9	0.50	0	5,11,11	0.22	0
4	EDO	C	6006	-	3,3,3	0.28	0	2,2,2	0.15	0
4	EDO	C	6026	-	3,3,3	0.22	0	2,2,2	0.30	0
5	GLN	D	6008	-	4,9,9	0.61	0	5,11,11	0.27	0
4	EDO	E	6010	-	3,3,3	0.38	0	2,2,2	0.28	0
4	EDO	E	6047	-	3,3,3	0.75	0	2,2,2	0.29	0
5	GLN	F	6012	-	4,9,9	0.34	0	5,11,11	0.37	0
4	EDO	G	6043	-	3,3,3	0.60	0	2,2,2	0.07	0
5	GLN	H	6016	-	4,9,9	0.37	0	5,11,11	0.29	0
4	EDO	I	6018	-	3,3,3	0.29	0	2,2,2	0.90	0
4	EDO	I	6038	-	3,3,3	0.26	0	2,2,2	0.32	0
4	EDO	I	6039	-	3,3,3	0.66	0	2,2,2	0.15	0
5	GLN	J	6020	-	4,9,9	0.57	0	5,11,11	0.57	0
4	EDO	K	6022	-	3,3,3	0.27	0	2,2,2	0.25	0
5	GLN	L	6024	-	4,9,9	0.12	0	5,11,11	0.08	0
4	EDO	M	6007	-	3,3,3	0.89	0	2,2,2	0.51	0
5	GLN	N	6028	-	4,9,9	0.43	0	5,11,11	0.69	0
5	GLN	P	6032	-	4,9,9	0.42	0	5,11,11	0.33	0
4	EDO	Q	6034	-	3,3,3	0.28	0	2,2,2	0.13	0
4	EDO	Q	6035	-	3,3,3	1.01	0	2,2,2	0.88	0
5	GLN	R	6036	-	4,9,9	0.65	0	5,11,11	0.15	0
5	GLN	T	6040	-	4,9,9	0.35	0	5,11,11	0.19	0
4	EDO	U	6014	-	3,3,3	0.22	0	2,2,2	0.43	0
4	EDO	U	6042	-	3,3,3	0.46	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GLN	V	6044	-	4,9,9	0.44	0	5,11,11	0.37	0
4	EDO	W	6046	-	3,3,3	0.24	0	2,2,2	0.03	0
5	GLN	X	6048	-	8,8,9	1.98	1 (12%)	6,9,11	2.15	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	6002	-	-	0/1/1/1	0/0/0/0
4	EDO	A	6030	-	-	0/1/1/1	0/0/0/0
4	EDO	A	6031	-	-	0/1/1/1	0/0/0/0
5	GLN	B	6004	-	-	0/5/9/9	0/0/0/0
4	EDO	C	6006	-	-	0/1/1/1	0/0/0/0
4	EDO	C	6026	-	-	0/1/1/1	0/0/0/0
5	GLN	D	6008	-	-	0/5/9/9	0/0/0/0
4	EDO	E	6010	-	-	0/1/1/1	0/0/0/0
4	EDO	E	6047	-	-	0/1/1/1	0/0/0/0
5	GLN	F	6012	-	-	0/5/9/9	0/0/0/0
4	EDO	G	6043	-	-	0/1/1/1	0/0/0/0
5	GLN	H	6016	-	-	0/5/9/9	0/0/0/0
4	EDO	I	6018	-	-	0/1/1/1	0/0/0/0
4	EDO	I	6038	-	-	0/1/1/1	0/0/0/0
4	EDO	I	6039	-	-	0/1/1/1	0/0/0/0
5	GLN	J	6020	-	-	0/5/9/9	0/0/0/0
4	EDO	K	6022	-	-	0/1/1/1	0/0/0/0
5	GLN	L	6024	-	-	0/5/9/9	0/0/0/0
4	EDO	M	6007	-	-	0/1/1/1	0/0/0/0
5	GLN	N	6028	-	-	0/5/9/9	0/0/0/0
5	GLN	P	6032	-	-	0/5/9/9	0/0/0/0
4	EDO	Q	6034	-	-	0/1/1/1	0/0/0/0
4	EDO	Q	6035	-	-	0/1/1/1	0/0/0/0
5	GLN	R	6036	-	-	0/5/9/9	0/0/0/0
5	GLN	T	6040	-	-	0/5/9/9	0/0/0/0
4	EDO	U	6014	-	-	0/1/1/1	0/0/0/0
4	EDO	U	6042	-	-	0/1/1/1	0/0/0/0
5	GLN	V	6044	-	-	0/5/9/9	0/0/0/0
4	EDO	W	6046	-	-	0/1/1/1	0/0/0/0
5	GLN	X	6048	-	-	0/5/7/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	6048	GLN	CA-C	5.21	1.57	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	X	6048	GLN	O-C-CA	-5.23	110.58	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	6031	EDO	8	0
5	B	6004	GLN	1	0
5	D	6008	GLN	1	0
4	E	6047	EDO	9	0
4	G	6043	EDO	9	0
4	I	6039	EDO	9	0
4	M	6007	EDO	5	0
5	P	6032	GLN	2	0
4	Q	6035	EDO	11	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	268/294 (91%)	0.59	11 (4%) 38 44	29, 38, 55, 83	0
1	C	269/294 (91%)	0.75	12 (4%) 34 40	29, 34, 52, 81	0
1	E	269/294 (91%)	0.59	13 (4%) 31 37	30, 38, 54, 80	0
1	G	268/294 (91%)	0.54	13 (4%) 30 36	30, 36, 55, 87	0
1	I	271/294 (92%)	0.60	12 (4%) 35 41	28, 34, 57, 79	0
1	K	270/294 (91%)	0.66	16 (5%) 23 28	29, 36, 61, 79	0
1	M	269/294 (91%)	0.57	10 (3%) 42 49	28, 34, 52, 74	0
1	O	268/294 (91%)	0.62	14 (5%) 28 34	28, 35, 53, 73	0
1	Q	270/294 (91%)	0.71	17 (6%) 21 26	28, 36, 58, 76	0
1	S	270/294 (91%)	0.73	16 (5%) 23 28	30, 38, 62, 82	0
1	U	271/294 (92%)	0.63	14 (5%) 28 34	30, 39, 61, 82	0
1	W	270/294 (91%)	0.62	13 (4%) 31 37	28, 34, 53, 83	0
2	B	193/204 (94%)	1.18	39 (20%) 1 1	44, 55, 65, 83	0
2	D	194/204 (95%)	1.10	39 (20%) 1 1	40, 51, 60, 70	0
2	F	191/204 (93%)	1.47	47 (24%) 1 1	46, 60, 69, 78	0
2	H	193/204 (94%)	0.64	21 (10%) 6 8	37, 48, 58, 78	0
2	J	196/204 (96%)	0.48	20 (10%) 7 9	36, 45, 57, 63	0
2	L	192/204 (94%)	0.92	28 (14%) 3 4	40, 51, 60, 74	0
2	N	193/204 (94%)	0.46	10 (5%) 28 34	34, 44, 55, 76	0
2	P	193/204 (94%)	0.63	19 (9%) 8 11	38, 48, 59, 70	0
2	R	193/204 (94%)	0.83	25 (12%) 4 5	39, 49, 60, 82	0
2	T	194/204 (95%)	1.43	50 (25%) 1 1	46, 55, 65, 71	0
2	V	194/204 (95%)	1.97	82 (42%) 0 0	47, 62, 70, 78	0
2	X	195/204 (95%)	0.53	19 (9%) 8 11	35, 44, 57, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5554/5976 (92%)	0.77	560 (10%) 8 10	28, 42, 64, 87	0

All (560) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	54	ALA	10.0
1	S	54	ALA	9.7
1	K	50	ALA	9.0
1	A	56	GLY	8.4
1	I	54	ALA	8.4
2	T	194	ALA	7.9
1	S	50	ALA	7.9
2	L	1	MET	7.7
1	G	56	GLY	7.6
1	A	54	ALA	7.6
1	C	52	ILE	7.5
1	I	50	ALA	7.4
1	W	54	ALA	7.4
1	G	52	ILE	7.3
1	U	54	ALA	7.3
1	C	48	VAL	7.2
1	E	54	ALA	7.1
1	C	55	ALA	7.1
1	K	54	ALA	7.0
1	G	51	ASP	7.0
2	X	195	LEU	6.8
1	E	50	ALA	6.7
2	V	192	GLN	6.6
1	Q	54	ALA	6.6
2	J	196	VAL	6.6
2	D	194	ALA	6.5
2	V	190	TYR	6.4
1	C	56	GLY	6.3
1	S	48	VAL	6.2
2	V	194	ALA	6.1
2	B	191	LYS	6.1
2	F	1	MET	6.1
2	V	125	LEU	6.0
2	V	100	LEU	6.0
2	V	41	GLY	6.0
1	G	50	ALA	6.0
1	U	51	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	49	PRO	5.9
1	A	55	ALA	5.8
1	O	52	ILE	5.8
2	X	194	ALA	5.8
2	J	195	LEU	5.8
1	M	54	ALA	5.7
2	F	187	VAL	5.7
1	O	54	ALA	5.7
1	W	50	ALA	5.7
2	T	125	LEU	5.7
1	O	50	ALA	5.7
1	W	55	ALA	5.7
2	V	154	GLY	5.7
2	V	184	VAL	5.7
1	I	51	ASP	5.6
2	V	182	LEU	5.6
1	G	54	ALA	5.6
2	T	1	MET	5.6
1	S	55	ALA	5.5
2	T	101	ASN	5.5
2	F	162	GLY	5.5
2	T	192	GLN	5.4
2	V	144	GLU	5.4
2	B	187	VAL	5.4
2	B	189	GLU	5.4
2	P	2	LEU	5.3
2	J	194	ALA	5.3
2	B	1	MET	5.3
2	D	192	GLN	5.3
2	R	67	GLU	5.3
2	T	188	GLU	5.3
1	U	52	ILE	5.2
2	J	192	GLN	5.2
1	U	55	ALA	5.1
1	S	56	GLY	5.1
2	V	187	VAL	5.1
1	A	50	ALA	5.1
2	B	125	LEU	5.1
2	F	190	TYR	5.0
2	R	1	MET	5.0
1	C	50	ALA	5.0
2	D	2	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	M	52	ILE	5.0
1	G	55	ALA	4.9
2	T	190	TYR	4.9
2	D	143	GLY	4.9
1	U	56	GLY	4.9
1	S	271	LEU	4.9
1	E	52	ILE	4.9
2	V	126	ASP	4.8
2	B	192	GLN	4.8
2	B	126	ASP	4.8
2	R	192	GLN	4.8
2	D	70	ALA	4.8
2	L	128	PRO	4.8
2	T	127	GLU	4.7
1	I	52	ILE	4.7
2	V	2	LEU	4.7
1	W	51	ASP	4.7
2	D	24	GLY	4.6
1	O	56	GLY	4.6
2	L	187	VAL	4.6
2	V	191	LYS	4.6
1	U	271	LEU	4.5
2	T	184	VAL	4.5
2	V	143	GLY	4.5
1	K	56	GLY	4.5
2	L	126	ASP	4.5
2	V	122	ILE	4.5
1	U	50	ALA	4.5
1	E	53	ARG	4.5
2	T	40	ASP	4.5
2	T	126	ASP	4.4
2	D	1	MET	4.4
2	H	1	MET	4.4
2	H	192	GLN	4.3
2	T	128	PRO	4.3
1	I	272	GLY	4.3
2	P	190	TYR	4.3
2	V	129	PHE	4.3
2	V	1	MET	4.3
1	W	56	GLY	4.3
2	T	193	LYS	4.3
2	V	121	THR	4.3

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Mol	Chain	Res	Type	RSRZ
2	V	188	GLU	4.2
2	L	72	GLY	4.2
2	T	143	GLY	4.2
2	V	72	GLY	4.2
2	L	153	ASN	4.2
2	F	101	ASN	4.2
2	H	190	TYR	4.2
2	P	1	MET	4.2
1	A	51	ASP	4.2
2	R	189	GLU	4.2
1	I	271	LEU	4.2
2	L	127	GLU	4.1
1	K	52	ILE	4.1
2	V	24	GLY	4.1
1	Q	56	GLY	4.1
2	F	2	LEU	4.1
1	I	55	ALA	4.1
2	T	187	VAL	4.1
1	E	51	ASP	4.1
2	V	67	GLU	4.0
2	F	189	GLU	4.0
2	D	125	LEU	4.0
2	F	40	ASP	4.0
2	L	23	CYS	4.0
2	V	23	CYS	4.0
2	V	189	GLU	4.0
2	V	149	LEU	4.0
1	K	51	ASP	4.0
2	L	67	GLU	4.0
1	C	2	ALA	4.0
1	W	52	ILE	4.0
2	F	67	GLU	4.0
2	D	191	LYS	4.0
1	Q	55	ALA	4.0
2	V	148	VAL	4.0
1	I	56	GLY	3.9
1	K	55	ALA	3.9
1	Q	52	ILE	3.9
1	G	242	ASP	3.9
2	B	121	THR	3.9
2	P	192	GLN	3.9
1	Q	53	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
2	L	190	TYR	3.9
2	F	184	VAL	3.9
2	N	190	TYR	3.9
1	S	52	ILE	3.9
1	S	2	ALA	3.8
2	H	126	ASP	3.8
2	T	162	GLY	3.8
2	B	2	LEU	3.8
1	U	48	VAL	3.8
2	T	164	PHE	3.8
2	D	145	ASN	3.8
1	S	51	ASP	3.8
1	Q	271	LEU	3.8
2	R	191	LYS	3.8
2	B	188	GLU	3.7
2	P	189	GLU	3.7
2	T	189	GLU	3.7
2	R	193	LYS	3.7
2	X	24	GLY	3.7
2	V	127	GLU	3.7
1	W	49	PRO	3.7
2	X	126	ASP	3.7
2	B	138	HIS	3.7
2	V	65	LEU	3.7
1	W	48	VAL	3.7
2	V	128	PRO	3.7
2	B	190	TYR	3.7
2	F	65	LEU	3.7
1	G	53	ARG	3.7
2	H	187	VAL	3.6
2	F	191	LYS	3.6
2	X	190	TYR	3.6
2	F	62	MET	3.6
2	V	71	GLN	3.6
1	Q	50	ALA	3.6
2	L	192	GLN	3.6
2	X	192	GLN	3.6
2	D	128	PRO	3.5
2	V	138	HIS	3.5
1	O	55	ALA	3.5
2	F	82	LEU	3.5
2	V	63	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	J	1	MET	3.5
1	A	52	ILE	3.5
2	T	72	GLY	3.5
1	Q	270	GLU	3.5
2	N	189	GLU	3.5
1	M	48	VAL	3.5
2	D	148	VAL	3.5
2	V	193	LYS	3.5
2	H	193	LYS	3.4
2	V	181	GLN	3.4
2	B	143	GLY	3.4
2	H	127	GLU	3.4
2	D	126	ASP	3.4
2	H	69	ALA	3.4
1	E	242	ASP	3.4
1	E	56	GLY	3.4
2	X	193	LYS	3.4
2	F	144	GLU	3.4
2	L	125	LEU	3.4
2	D	144	GLU	3.4
1	C	51	ASP	3.4
2	T	39	VAL	3.4
2	T	34	GLU	3.3
2	L	60	GLN	3.3
2	B	127	GLU	3.3
1	Q	51	ASP	3.3
2	D	23	CYS	3.3
2	V	163	GLN	3.3
1	K	53	ARG	3.3
2	F	188	GLU	3.3
1	A	48	VAL	3.3
2	V	22	ALA	3.3
2	F	79	CYS	3.3
2	R	190	TYR	3.3
2	V	98	GLY	3.3
2	F	100	LEU	3.3
2	T	2	LEU	3.3
2	N	126	ASP	3.3
2	D	122	ILE	3.3
2	V	153	ASN	3.3
2	R	144	GLU	3.2
2	B	184	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	V	68	PHE	3.2
2	F	24	GLY	3.2
1	M	50	ALA	3.2
2	X	70	ALA	3.2
2	V	101	ASN	3.2
2	V	4	ILE	3.2
1	A	49	PRO	3.2
1	K	57	GLY	3.2
2	B	24	GLY	3.2
1	M	55	ALA	3.2
2	J	127	GLU	3.2
2	R	37	ASN	3.2
2	T	19	ALA	3.2
2	V	19	ALA	3.2
2	T	121	THR	3.2
2	V	151	GLU	3.1
2	F	37	ASN	3.1
2	F	93	ASP	3.1
2	V	36	LEU	3.1
2	D	121	THR	3.1
2	R	60	GLN	3.1
2	V	180	THR	3.1
1	A	2	ALA	3.1
1	M	56	GLY	3.1
2	X	127	GLU	3.1
2	L	123	LYS	3.1
1	U	270	GLU	3.1
2	D	153	ASN	3.1
2	V	164	PHE	3.1
2	V	40	ASP	3.1
1	U	53	ARG	3.1
2	J	67	GLU	3.0
2	V	3	THR	3.0
2	T	159	ALA	3.0
2	V	158	ALA	3.0
2	F	60	GLN	3.0
2	V	142	ALA	3.0
1	C	53	ARG	3.0
2	L	122	ILE	3.0
2	V	157	VAL	3.0
2	R	59	TYR	3.0
2	L	37	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	R	72	GLY	3.0
2	V	178	ARG	3.0
1	K	49	PRO	3.0
2	D	99	LEU	3.0
2	P	191	LYS	3.0
2	T	73	LYS	3.0
2	D	154	GLY	3.0
1	S	242	ASP	3.0
2	T	191	LYS	3.0
2	J	189	GLU	3.0
2	F	70	ALA	3.0
1	S	47	ARG	2.9
1	K	242	ASP	2.9
2	H	144	GLU	2.9
2	V	155	ARG	2.9
2	H	70	ALA	2.9
2	V	166	GLY	2.9
2	N	1	MET	2.9
2	T	163	GLN	2.9
2	D	189	GLU	2.9
2	F	63	GLU	2.9
2	P	144	GLU	2.9
2	X	191	LYS	2.9
2	V	162	GLY	2.9
1	E	3[A]	GLN	2.9
1	M	53	ARG	2.9
2	T	166	GLY	2.9
2	H	100	LEU	2.9
2	V	152	HIS	2.9
1	K	271	LEU	2.9
2	P	63	GLU	2.9
2	R	187	VAL	2.8
1	E	55	ALA	2.8
2	B	70	ALA	2.8
2	F	59	TYR	2.8
2	V	34	GLU	2.8
2	T	100	LEU	2.8
2	V	177	HIS	2.8
2	J	193	LYS	2.8
2	T	26	ALA	2.8
2	V	124	GLY	2.8
1	O	139	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	T	69	ALA	2.8
2	T	67	GLU	2.8
2	T	70	ALA	2.8
2	J	2	LEU	2.8
2	T	63	GLU	2.8
1	A	53	ARG	2.8
2	F	66	ARG	2.8
2	B	193	LYS	2.8
2	P	67	GLU	2.7
2	R	34	GLU	2.7
2	F	69	ALA	2.7
2	F	140	LEU	2.7
2	R	33	PRO	2.7
2	V	120	LEU	2.7
1	G	48	VAL	2.7
2	H	67	GLU	2.7
1	G	57	GLY	2.7
2	T	24	GLY	2.7
1	M	51	ASP	2.7
2	R	2	LEU	2.7
1	K	48	VAL	2.7
2	T	37	ASN	2.7
2	T	139	ILE	2.7
1	W	152	PRO	2.7
2	D	72	GLY	2.7
2	F	159	ALA	2.7
2	D	182	LEU	2.7
2	J	190	TYR	2.6
2	D	188	GLU	2.6
1	E	49	PRO	2.6
1	I	49	PRO	2.6
1	O	51	ASP	2.6
2	N	192	GLN	2.6
2	P	126	ASP	2.6
2	F	164	PHE	2.6
2	H	191	LYS	2.6
1	I	53	ARG	2.6
1	O	53	ARG	2.6
1	S	49	PRO	2.6
2	B	74	PRO	2.6
2	F	128	PRO	2.6
2	L	188	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	187	VAL	2.6
1	E	2	ALA	2.6
2	V	20	ILE	2.6
2	J	34	GLU	2.6
2	L	34	GLU	2.6
2	T	155	ARG	2.6
2	V	174	THR	2.6
1	W	271	LEU	2.6
2	F	103	VAL	2.6
2	X	184	VAL	2.6
2	R	66	ARG	2.6
1	K	240	LYS	2.6
1	S	57	GLY	2.6
2	P	127	GLU	2.6
1	Q	171	VAL	2.5
2	R	184	VAL	2.5
2	D	186	MET	2.5
2	V	156	ILE	2.5
2	B	128	PRO	2.5
2	V	39	VAL	2.5
2	P	24	GLY	2.5
2	B	176	ASP	2.5
2	B	25	ALA	2.5
2	J	191	LYS	2.5
2	X	128	PRO	2.5
2	P	188	GLU	2.5
2	F	152	HIS	2.5
1	Q	242	ASP	2.5
2	F	180	THR	2.5
2	F	141	GLU	2.5
2	B	37	ASN	2.5
2	P	37	ASN	2.5
2	F	83	ILE	2.5
2	N	24	GLY	2.5
1	Q	2	ALA	2.5
2	R	65	LEU	2.4
1	W	47	ARG	2.4
2	B	54[A]	ARG	2.4
2	V	54[A]	ARG	2.4
1	A	242	ASP	2.4
2	L	24	GLY	2.4
2	V	79	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	190	TYR	2.4
2	V	26	ALA	2.4
1	U	47	ARG	2.4
2	H	68	PHE	2.4
1	G	196	LEU	2.4
2	N	127	GLU	2.4
2	R	188	GLU	2.4
2	T	87	LYS	2.4
2	H	93	ASP	2.4
2	L	40	ASP	2.4
2	D	102	VAL	2.4
2	J	184	VAL	2.4
2	X	188	GLU	2.4
1	K	153	GLY	2.4
2	J	188	GLU	2.4
2	V	99	LEU	2.4
2	T	124	GLY	2.4
2	T	36	LEU	2.4
2	N	142	ALA	2.4
2	V	60	GLN	2.4
2	J	126	ASP	2.4
2	L	182	LEU	2.3
2	T	129	PHE	2.3
2	T	151	GLU	2.3
1	E	240	LYS	2.3
2	B	19	ALA	2.3
1	E	48	VAL	2.3
2	B	69	ALA	2.3
2	F	34	GLU	2.3
2	V	69	ALA	2.3
1	Q	199	ILE	2.3
1	Q	132	LEU	2.3
2	J	125	LEU	2.3
1	M	270	GLU	2.3
2	R	68	PHE	2.3
2	X	2	LEU	2.3
2	L	154	GLY	2.3
2	V	146	VAL	2.3
2	R	69	ALA	2.3
2	B	181	GLN	2.3
2	V	119	ASP	2.3
2	B	183	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	142	ALA	2.3
2	F	78	THR	2.3
2	J	144	GLU	2.3
1	K	241	SER	2.3
1	W	2	ALA	2.3
2	F	179	VAL	2.3
2	H	184	VAL	2.3
1	O	195	LEU	2.2
1	O	171	VAL	2.2
1	Q	48	VAL	2.2
2	T	146	VAL	2.2
1	Q	49	PRO	2.2
2	B	163	GLN	2.2
2	B	118	ALA	2.2
2	V	70	ALA	2.2
2	J	18	HIS	2.2
1	M	92	VAL	2.2
1	W	53	ARG	2.2
2	T	153	ASN	2.2
2	B	41	GLY	2.2
2	D	67	GLU	2.2
2	T	20	ILE	2.2
2	D	120	LEU	2.2
2	F	87	LYS	2.2
2	P	193	LYS	2.2
1	I	270	GLU	2.2
2	X	144	GLU	2.2
2	L	73	LYS	2.2
2	V	123	LYS	2.2
2	L	121	THR	2.2
1	C	227	LEU	2.2
2	L	97	LEU	2.2
2	V	97	LEU	2.2
2	R	164	PHE	2.2
2	F	145	ASN	2.2
2	X	1	MET	2.2
1	U	272	GLY	2.2
2	B	34	GLU	2.2
1	K	67	VAL	2.2
2	F	109	PHE	2.2
2	X	187	VAL	2.2
1	C	270	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	67	GLU	2.1
2	X	67	GLU	2.1
2	D	101	ASN	2.1
2	V	116	PHE	2.1
2	X	23	CYS	2.1
1	O	242	ASP	2.1
1	O	213	GLY	2.1
2	B	72	GLY	2.1
2	D	155	ARG	2.1
2	F	110	GLY	2.1
2	V	64	PRO	2.1
2	D	34	GLU	2.1
2	D	152	HIS	2.1
2	D	184	VAL	2.1
1	S	53	ARG	2.1
2	R	71	GLN	2.1
2	B	20	ILE	2.1
2	F	54[A]	ARG	2.1
2	R	141	GLU	2.1
2	B	142	ALA	2.1
2	H	128	PRO	2.1
2	P	23	CYS	2.1
2	T	23	CYS	2.1
2	V	84	ILE	2.1
2	D	157	VAL	2.1
2	T	157	VAL	2.1
2	V	62	MET	2.1
2	B	159	ALA	2.1
2	V	159	ALA	2.1
2	N	63	GLU	2.1
1	U	57	GLY	2.1
1	S	146	LEU	2.1
2	F	42	LEU	2.1
2	T	182	LEU	2.1
1	I	48	VAL	2.1
1	S	174	VAL	2.1
1	U	242	ASP	2.1
2	D	151	GLU	2.1
2	P	74	PRO	2.1
2	F	163	GLN	2.1
2	F	143	GLY	2.1
2	P	41	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	189	GLU	2.0
2	B	28	LEU	2.0
2	H	20	ILE	2.0
2	J	54[A]	ARG	2.0
2	L	145	ASN	2.0
2	D	98	GLY	2.0
2	P	162	GLY	2.0
2	B	155[A]	ARG	2.0
2	H	101	ASN	2.0
1	G	49	PRO	2.0
1	G	76	ILE	2.0
1	Q	195	LEU	2.0
2	L	54[A]	ARG	2.0
2	L	177	HIS	2.0
1	O	199	ILE	2.0
2	H	2	LEU	2.0
2	V	25	ALA	2.0
1	O	126	VAL	2.0
2	D	166	GLY	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
4	EDO	G	6043	4/4	0.91	0.25	5.18	31,37,44,50	0
4	EDO	I	6039	4/4	0.93	0.22	2.86	34,39,46,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	6030	4/4	0.91	0.18	2.37	35,43,46,51	0
4	EDO	M	6007	4/4	0.91	0.20	2.28	28,37,41,43	0
5	GLN	R	6036	10/10	0.91	0.17	2.10	36,37,39,40	0
4	EDO	E	6047	4/4	0.93	0.19	1.51	30,40,44,47	0
4	EDO	A	6002	4/4	0.91	0.16	0.47	37,43,45,51	0
4	EDO	Q	6035	4/4	0.92	0.19	0.39	32,34,43,46	0
4	EDO	A	6031	4/4	0.93	0.19	0.16	32,39,44,49	0
5	GLN	H	6016	10/10	0.94	0.12	0.01	34,36,36,38	0
5	GLN	L	6024	10/10	0.93	0.13	-0.21	39,41,42,43	0
5	GLN	F	6012	10/10	0.94	0.17	-0.27	43,46,47,49	0
5	GLN	T	6040	10/10	0.92	0.13	-0.44	41,42,43,43	0
4	EDO	U	6014	4/4	0.95	0.13	-0.72	38,42,44,46	0
4	EDO	I	6018	4/4	0.94	0.15	-0.74	35,40,44,49	0
4	EDO	U	6042	4/4	0.94	0.12	-0.80	38,43,46,51	0
5	GLN	V	6044	10/10	0.92	0.12	-1.20	45,46,47,49	0
4	EDO	W	6046	4/4	0.96	0.13	-1.54	36,42,43,45	0
4	EDO	E	6010	4/4	0.96	0.12	-1.65	35,43,44,48	0
5	GLN	B	6004	10/10	0.92	0.12	-1.71	43,44,45,46	0
5	GLN	N	6028	10/10	0.95	0.10	-1.72	32,32,34,34	0
5	GLN	X	6048	9/10	0.95	0.10	-1.79	32,34,36,37	0
4	EDO	I	6038	4/4	0.94	0.13	-1.96	37,42,43,46	0
4	EDO	C	6026	4/4	0.94	0.14	-1.99	37,43,44,51	0
5	GLN	D	6008	10/10	0.96	0.10	-2.16	33,35,35,35	0
4	EDO	C	6006	4/4	0.96	0.12	-2.47	38,41,43,50	0
5	GLN	P	6032	10/10	0.96	0.08	-3.21	37,38,39,40	0
5	GLN	J	6020	10/10	0.96	0.07	-3.43	33,34,35,35	0
4	EDO	Q	6034	4/4	0.97	0.10	-3.81	35,39,39,48	0
4	EDO	K	6022	4/4	0.97	0.10	-3.82	33,39,39,45	0
3	CL	A	6001	1/1	0.75	0.08	-	73,73,73,73	0
3	CL	Q	6033	1/1	0.95	0.13	-	79,79,79,79	0
3	CL	C	6005	1/1	0.85	0.09	-	75,75,75,75	0
3	CL	S	6037	1/1	0.94	0.07	-	72,72,72,72	0
3	CL	U	6041	1/1	0.80	0.08	-	80,80,80,80	0
3	CL	M	6025	1/1	0.93	0.07	-	65,65,65,65	0
3	CL	I	6017	1/1	0.92	0.09	-	65,65,65,65	0
3	CL	E	6009	1/1	0.93	0.07	-	67,67,67,67	0
3	CL	K	6021	1/1	0.97	0.09	-	70,70,70,70	0
3	CL	O	6029	1/1	0.81	0.12	-	83,83,83,83	0
3	CL	G	6013	1/1	0.85	0.11	-	74,74,74,74	0
3	CL	W	6045	1/1	0.91	0.05	-	65,65,65,65	0

## 6.5 Other polymers

There are no such residues in this entry.