



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 05:34 PM BST

PDB ID : 2XSO
Title : CRYSTAL STRUCTURE OF P4 VARIANT OF BIPHENYL DIOXYGENASE FROM BURKHOLDERIA XENOVORANS LB400
Authors : Kumar, P.; Bolin, J.T.
Deposited on : 2010-09-29
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

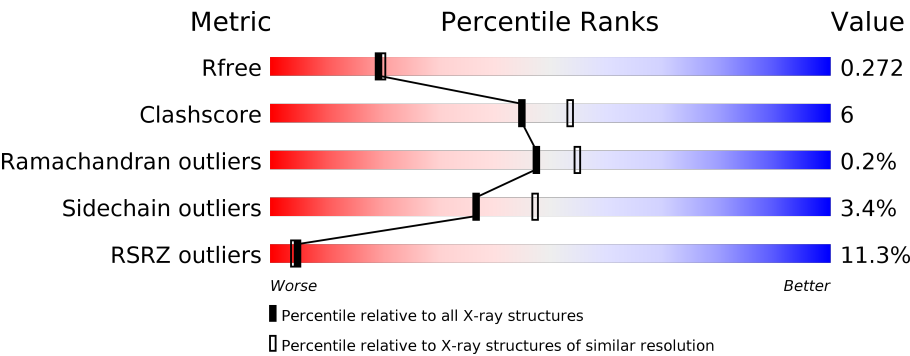
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	459	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%81%13%• 6%</div>
1	C	459	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%83%10%• 6%</div>
1	E	459	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%80%14%• 6%</div>
1	G	459	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>3%80%13%• 6%</div>
1	I	459	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>9%76%18%• 6%</div>
1	K	459	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>4%78%14%• 6%</div>

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Mol	Chain	Length	Quality of chain
1	M	459	
1	O	459	
1	Q	459	
1	S	459	
1	U	459	
1	W	459	
2	B	188	
2	D	188	
2	F	188	
2	H	188	
2	J	188	
2	L	188	
2	N	188	
2	P	188	
2	R	188	
2	T	188	
2	V	188	
2	X	188	

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	FES	K	900	-	-	X	-
3	FES	O	900	-	-	X	-
3	FES	S	900	-	-	X	-
3	FES	W	900	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 61911 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 BIPHENYL DIOXYGENASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	C	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	E	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	G	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	I	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	K	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	M	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	O	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	Q	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	S	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	U	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			
1	W	433	Total	C	N	O	S	0	0	0
			3427	2179	602	622	24			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ALA	THR	engineered mutation	UNP P37333
A	336	MET	PHE	engineered mutation	UNP P37333
C	335	ALA	THR	engineered mutation	UNP P37333
C	336	MET	PHE	engineered mutation	UNP P37333
E	335	ALA	THR	engineered mutation	UNP P37333

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Chain	Residue	Modelled	Actual	Comment	Reference
E	336	MET	PHE	engineered mutation	UNP P37333
G	335	ALA	THR	engineered mutation	UNP P37333
G	336	MET	PHE	engineered mutation	UNP P37333
I	335	ALA	THR	engineered mutation	UNP P37333
I	336	MET	PHE	engineered mutation	UNP P37333
K	335	ALA	THR	engineered mutation	UNP P37333
K	336	MET	PHE	engineered mutation	UNP P37333
M	335	ALA	THR	engineered mutation	UNP P37333
M	336	MET	PHE	engineered mutation	UNP P37333
O	335	ALA	THR	engineered mutation	UNP P37333
O	336	MET	PHE	engineered mutation	UNP P37333
Q	335	ALA	THR	engineered mutation	UNP P37333
Q	336	MET	PHE	engineered mutation	UNP P37333
S	335	ALA	THR	engineered mutation	UNP P37333
S	336	MET	PHE	engineered mutation	UNP P37333
U	335	ALA	THR	engineered mutation	UNP P37333
U	336	MET	PHE	engineered mutation	UNP P37333
W	335	ALA	THR	engineered mutation	UNP P37333
W	336	MET	PHE	engineered mutation	UNP P37333

- Molecule 2 is a protein called BIPHENYL DIOXYGENASE SUBUNIT BETA.

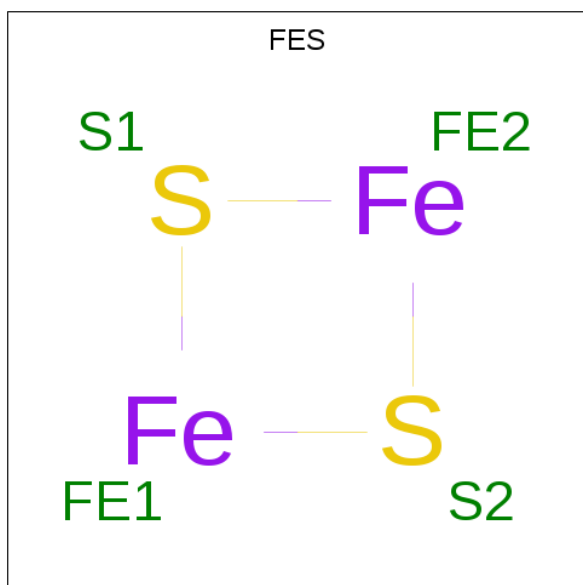
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	D	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	F	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	H	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	J	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	L	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	N	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	P	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	R	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	T	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	X	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total 4	Fe 2	S 2	0	0
3	U	1	Total 4	Fe 2	S 2	0	0
3	W	1	Total 4	Fe 2	S 2	0	0

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	185	Total 185	O 185	0	0
5	B	122	Total 122	O 122	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	147	Total 147	O 147	0	0
5	D	113	Total 113	O 113	0	0
5	E	210	Total 210	O 210	0	0
5	F	131	Total 131	O 131	0	0
5	G	181	Total 181	O 181	0	0
5	H	122	Total 122	O 122	0	0
5	I	88	Total 88	O 88	0	0
5	J	48	Total 48	O 48	0	0
5	K	123	Total 123	O 123	0	0
5	L	88	Total 88	O 88	0	0
5	M	96	Total 96	O 96	0	0
5	N	76	Total 76	O 76	0	0
5	O	106	Total 106	O 106	0	0
5	P	38	Total 38	O 38	0	0
5	Q	90	Total 90	O 90	0	0
5	R	89	Total 89	O 89	0	0
5	S	116	Total 116	O 116	0	0
5	T	69	Total 69	O 69	0	0
5	U	115	Total 115	O 115	0	0
5	V	45	Total 45	O 45	0	0
5	W	89	Total 89	O 89	0	0

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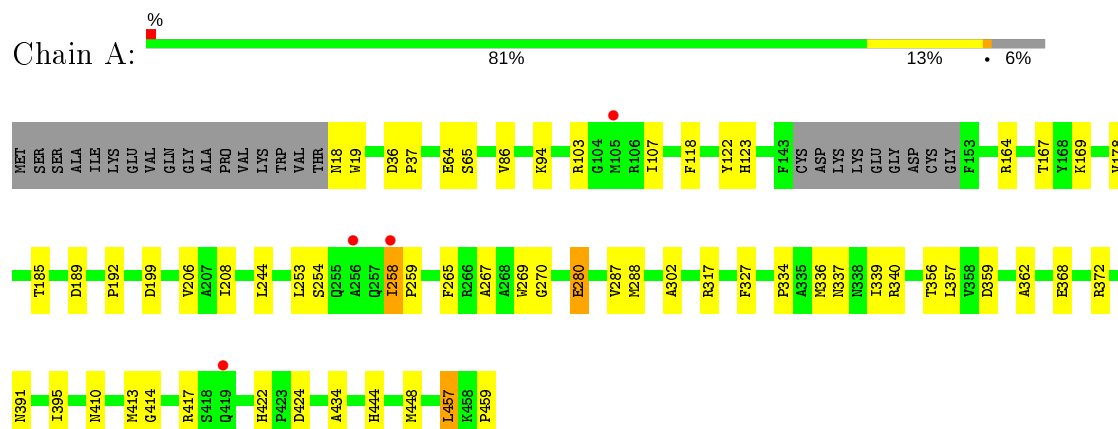
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	37	Total	O	0	0
			37	37		

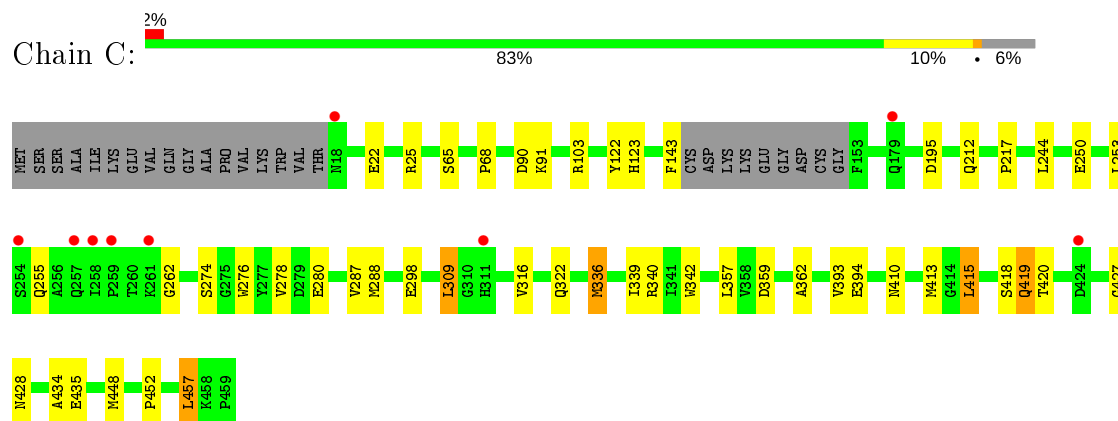
3 Residue-property plots [i](#)

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

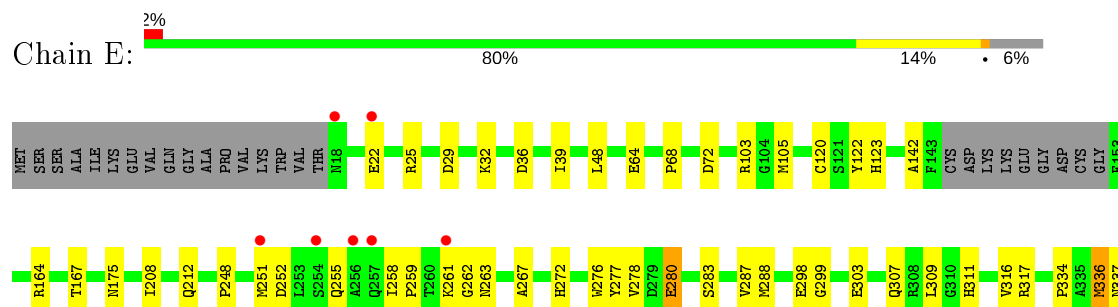
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

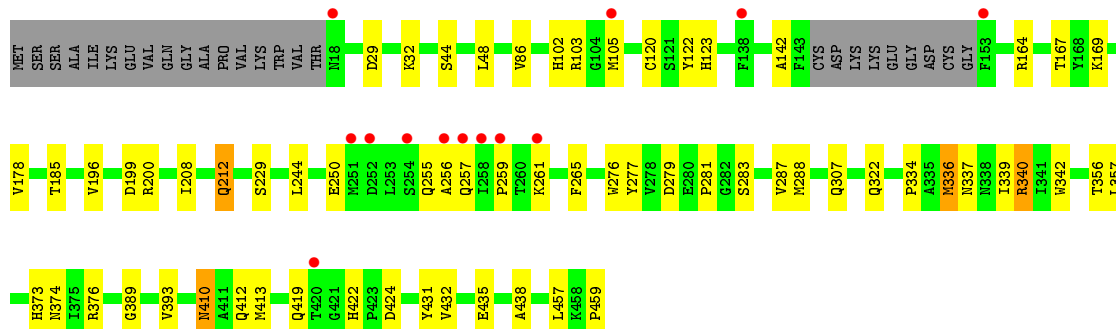
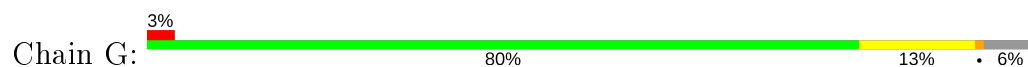


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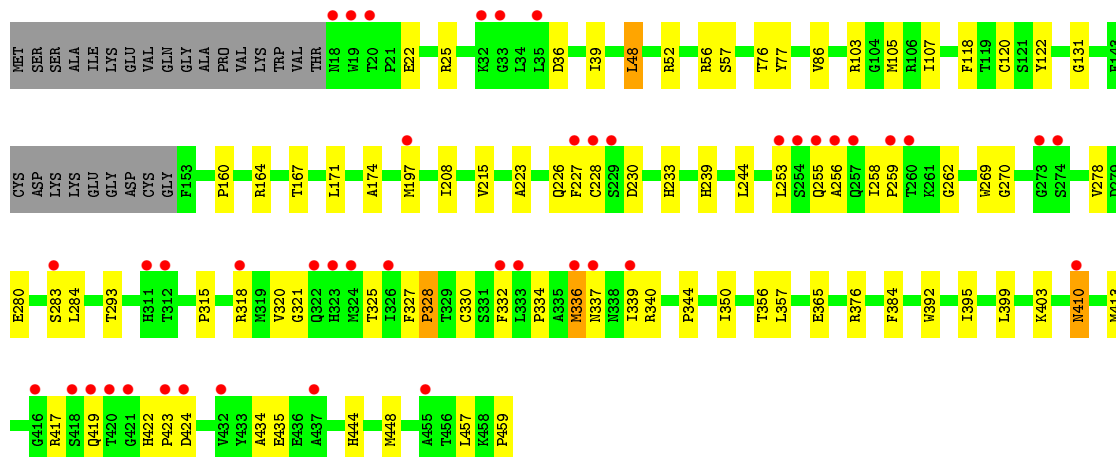
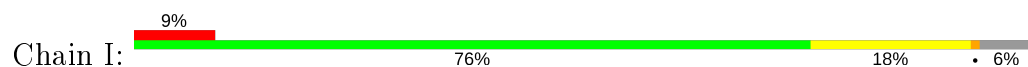




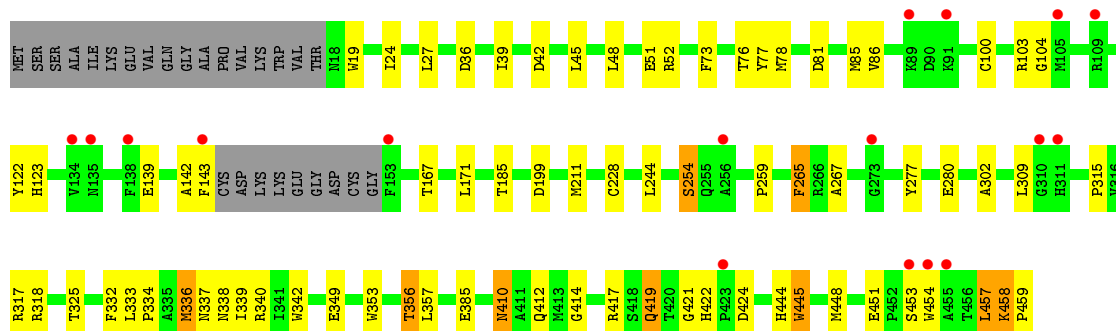
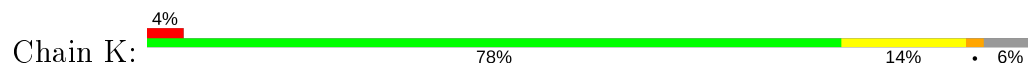
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



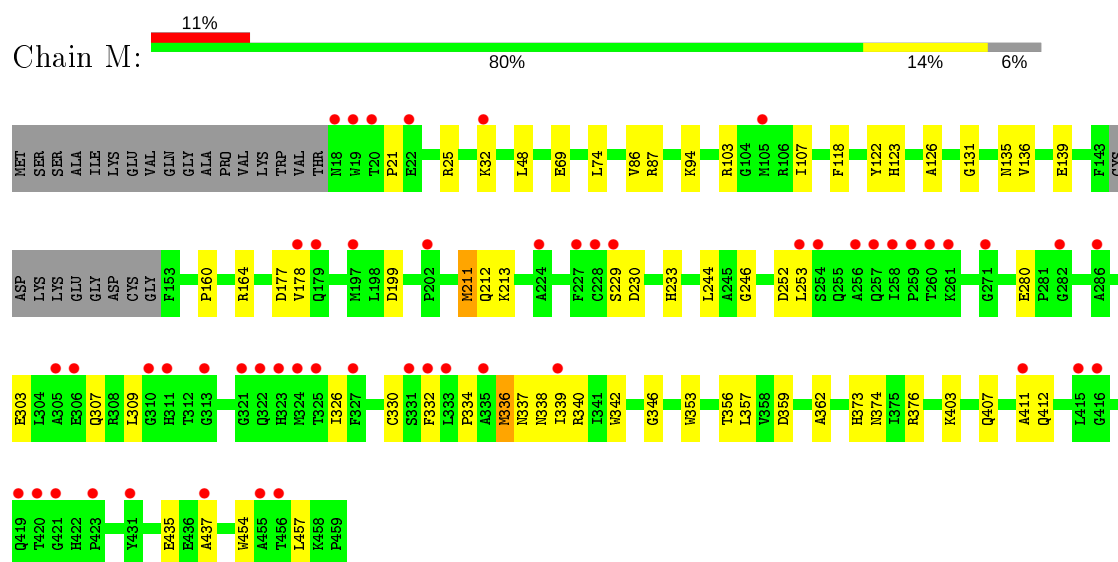
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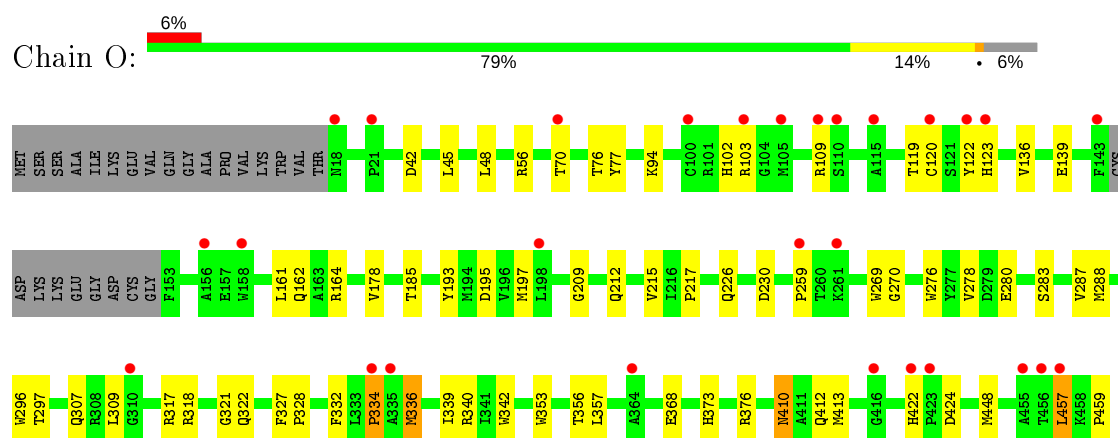
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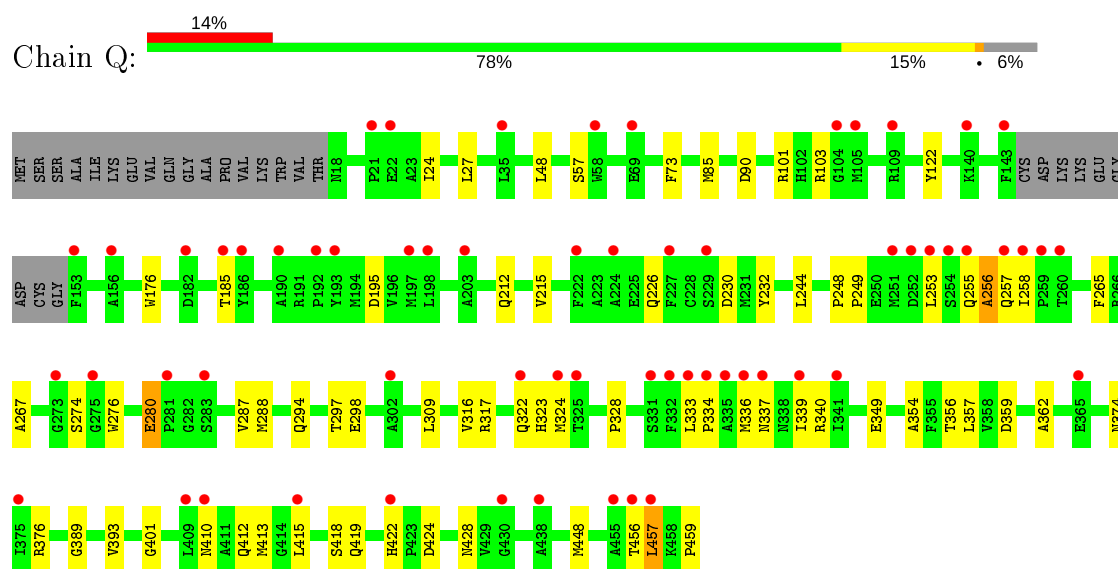
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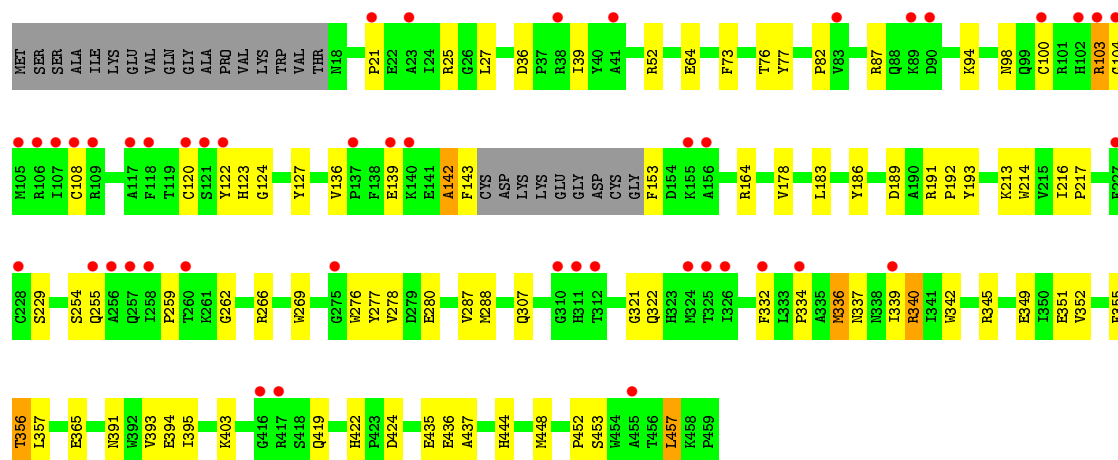
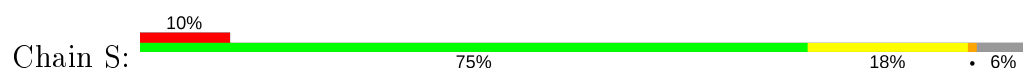
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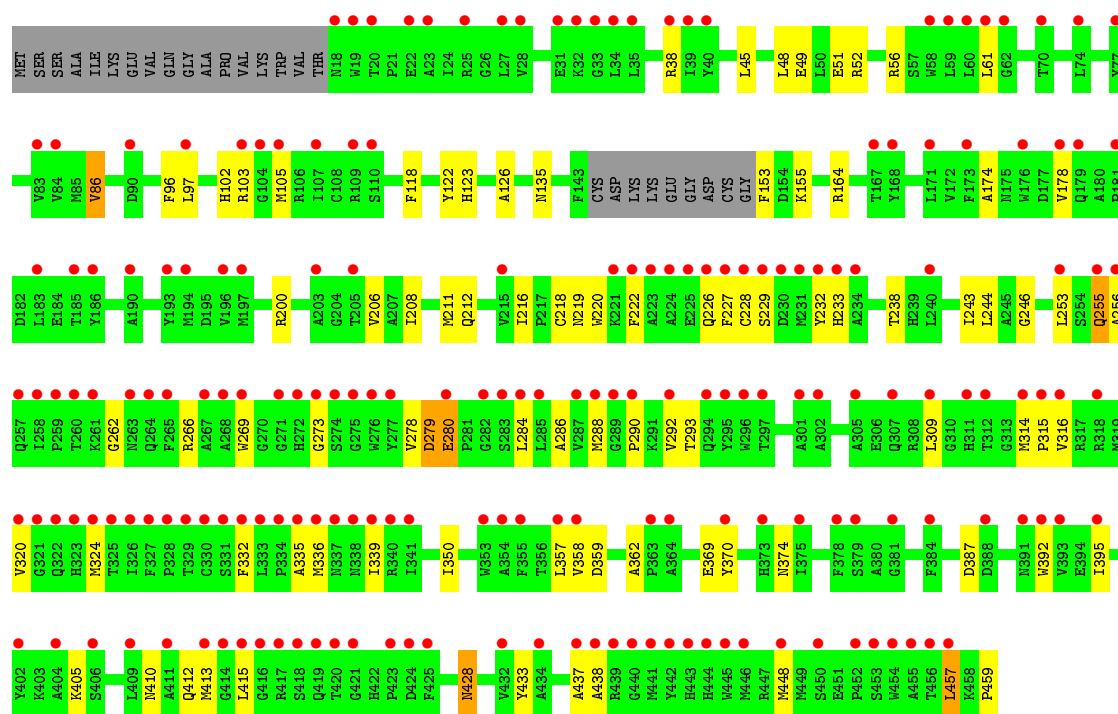
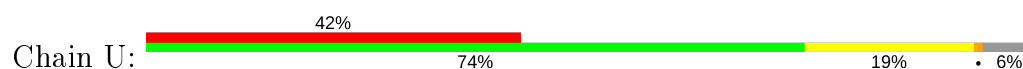
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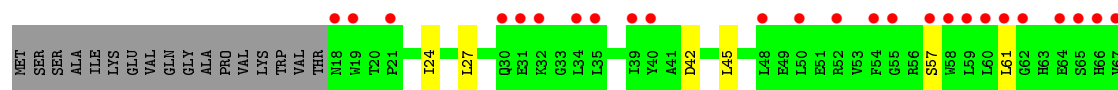
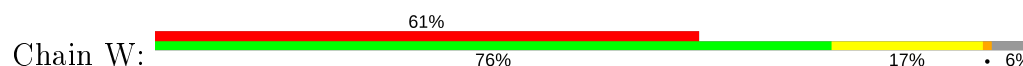
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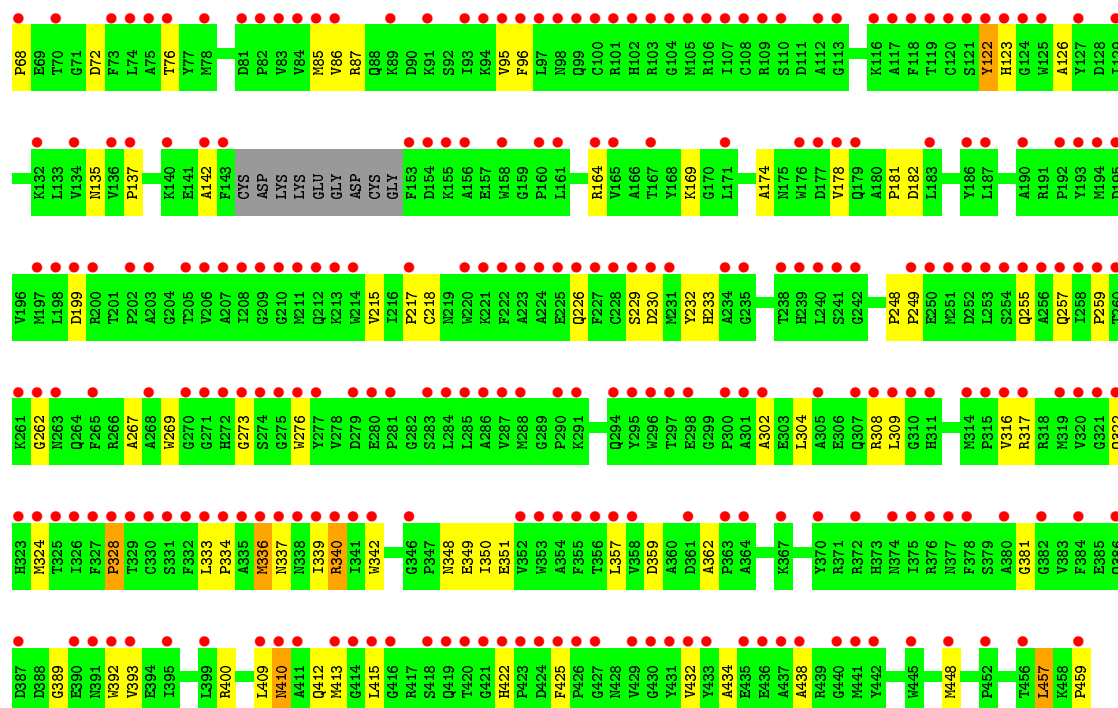


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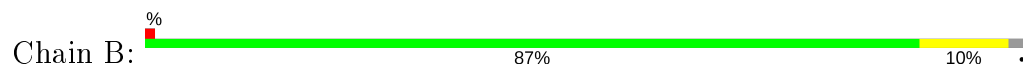


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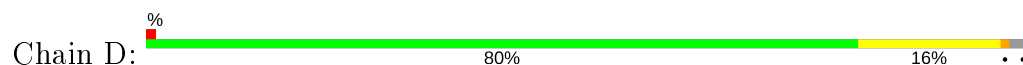




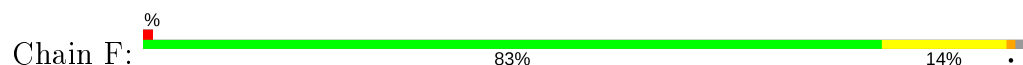
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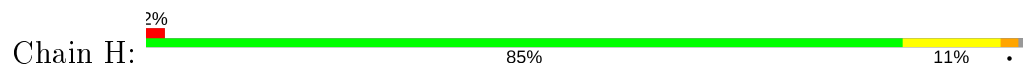
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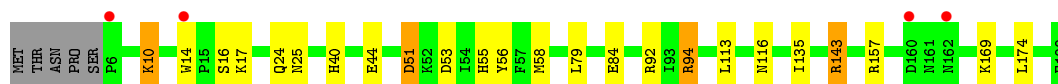


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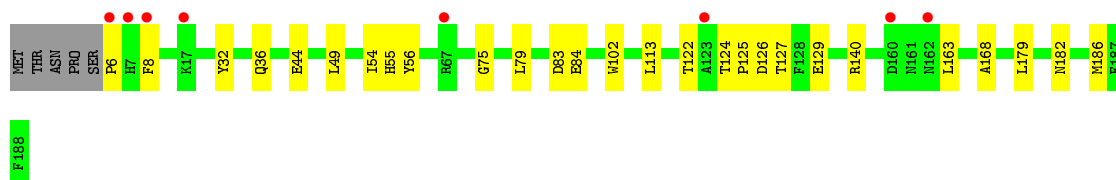
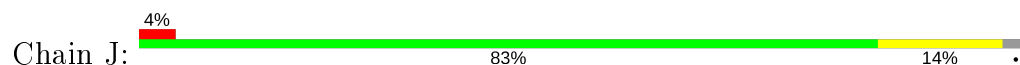


● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

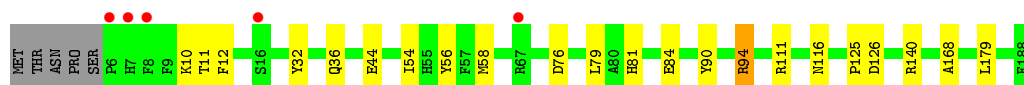
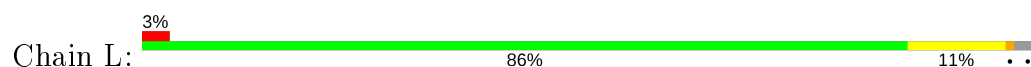




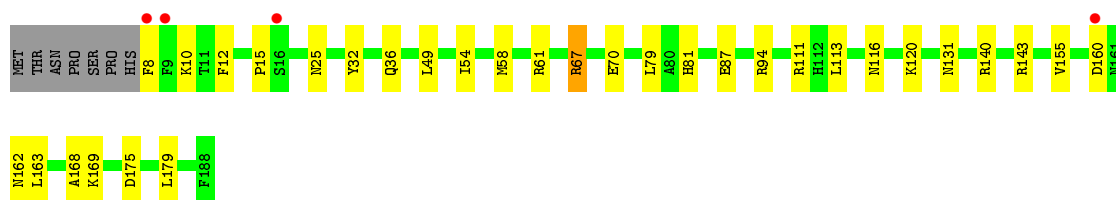
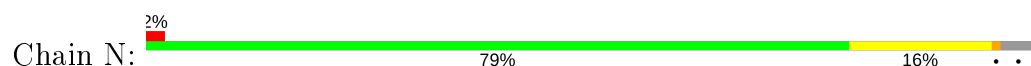
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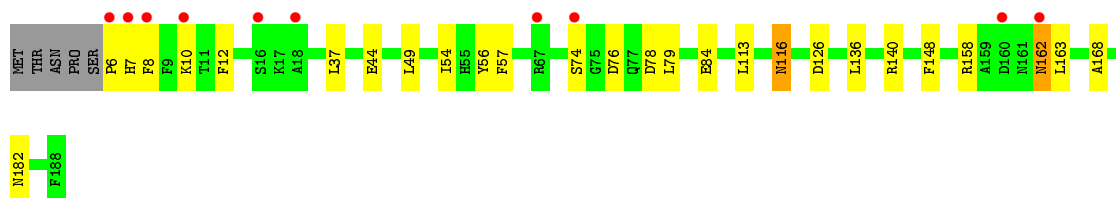
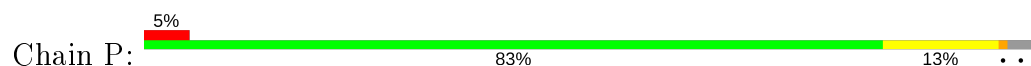
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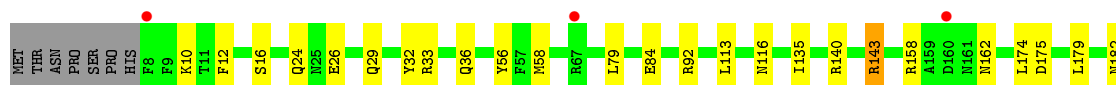
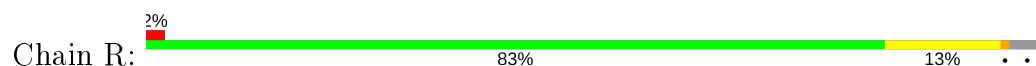
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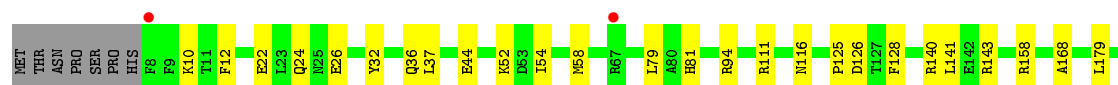
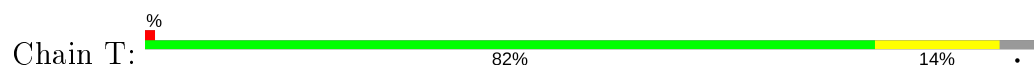


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

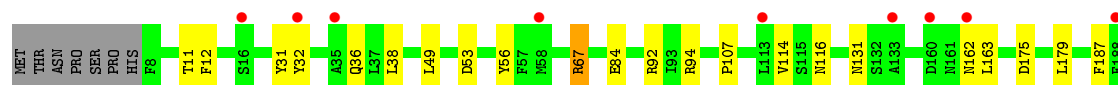
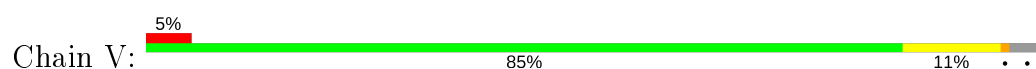




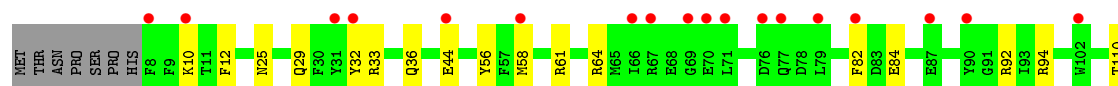
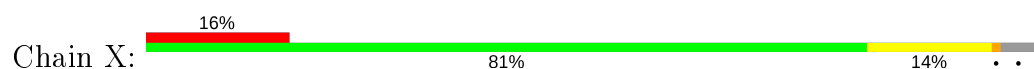
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	133.47Å 133.59Å 133.23Å 102.51° 104.99° 102.75°	Depositor
Resolution (Å)	125.00 – 2.20 28.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.0 (125.00-2.20) 81.0 (28.40-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.266 0.234 , 0.272	Depositor DCC
R_{free} test set	17060 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.080 for k,l,h 0.080 for l,h,k 0.018 for -l,-k,-h 0.022 for -h,-l,-k 0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	61911	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, FES

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	0.51	0/3529	0.63	0/4791
1	C	0.47	0/3529	0.59	1/4791 (0.0%)
1	E	0.52	0/3529	0.64	1/4791 (0.0%)
1	G	0.52	0/3529	0.64	0/4791
1	I	0.43	0/3529	0.57	0/4791
1	K	0.46	0/3529	0.59	0/4791
1	M	0.44	0/3529	0.57	0/4791
1	O	0.43	0/3529	0.58	0/4791
1	Q	0.43	0/3529	0.56	0/4791
1	S	0.43	0/3529	0.56	0/4791
1	U	0.41	0/3529	0.54	0/4791
1	W	0.39	0/3529	0.52	0/4791
2	B	0.60	0/1561	0.68	0/2110
2	D	0.57	0/1561	0.69	1/2110 (0.0%)
2	F	0.59	0/1561	0.69	0/2110
2	H	0.60	0/1561	0.68	1/2110 (0.0%)
2	J	0.42	0/1561	0.54	0/2110
2	L	0.50	0/1561	0.63	0/2110
2	N	0.49	0/1542	0.60	0/2084
2	P	0.44	0/1561	0.59	0/2110
2	R	0.48	0/1542	0.61	0/2084
2	T	0.49	0/1542	0.60	0/2084
2	V	0.43	0/1542	0.55	0/2084
2	X	0.41	0/1542	0.54	0/2084
All	All	0.47	0/60985	0.59	4/82682 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	415	LEU	CA-CB-CG	5.98	129.06	115.30
1	E	340	ARG	NE-CZ-NH1	-5.56	117.52	120.30
2	D	143	ARG	NE-CZ-NH2	-5.53	117.54	120.30
2	H	143	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3427	0	3276	41	0
1	C	3427	0	3276	30	0
1	E	3427	0	3276	45	0
1	G	3427	0	3276	42	0
1	I	3427	0	3276	52	0
1	K	3427	0	3276	51	0
1	M	3427	0	3276	36	0
1	O	3427	0	3276	52	0
1	Q	3427	0	3276	51	0
1	S	3427	0	3276	61	0
1	U	3427	0	3276	61	0
1	W	3427	0	3276	58	0
2	B	1524	0	1471	15	0
2	D	1524	0	1471	25	0
2	F	1524	0	1471	33	0
2	H	1524	0	1471	29	0
2	J	1524	0	1471	17	0
2	L	1524	0	1471	20	0
2	N	1507	0	1456	34	0
2	P	1524	0	1471	16	0
2	R	1507	0	1456	22	0
2	T	1507	0	1456	24	0
2	V	1507	0	1456	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	1507	0	1456	21	0
3	A	4	0	0	1	0
3	C	4	0	0	1	0
3	E	4	0	0	1	0
3	G	4	0	0	1	0
3	I	4	0	0	0	0
3	K	4	0	0	2	0
3	M	4	0	0	1	0
3	O	4	0	0	3	0
3	Q	4	0	0	0	0
3	S	4	0	0	4	0
3	U	4	0	0	1	0
3	W	4	0	0	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
4	S	1	0	0	0	0
4	U	1	0	0	0	0
4	W	1	0	0	0	0
5	A	185	0	0	5	0
5	B	122	0	0	4	0
5	C	147	0	0	1	0
5	D	113	0	0	4	0
5	E	210	0	0	6	0
5	F	131	0	0	2	0
5	G	181	0	0	1	0
5	H	122	0	0	10	0
5	I	88	0	0	4	0
5	J	48	0	0	2	0
5	K	123	0	0	3	0
5	L	88	0	0	3	0
5	M	96	0	0	2	0
5	N	76	0	0	5	0
5	O	106	0	0	7	0
5	P	38	0	0	0	0
5	Q	90	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	89	0	0	1	0
5	S	116	0	0	13	0
5	T	69	0	0	2	0
5	U	115	0	0	10	0
5	V	45	0	0	1	0
5	W	89	0	0	9	0
5	X	37	0	0	2	0
All	All	61911	0	56889	753	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (753) 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:H:58:MET:HE3	2:H:174:LEU:HD22	1.15	1.14
1:G:287:VAL:HG12	1:G:288:MET:CE	1.87	1.03
2:H:58:MET:CE	2:H:174:LEU:HD22	1.91	1.00
2:B:188:PHE:C	5:B:2106:HOH:O	2.03	0.97
1:A:339:ILE:HD11	1:A:357:LEU:HG	1.49	0.93
1:I:197:MET:SD	5:I:2068:HOH:O	2.27	0.92
1:G:287:VAL:HG12	1:G:288:MET:HE2	1.47	0.92
2:N:67:ARG:HE	2:N:67:ARG:HA	1.31	0.92
2:N:8:PHE:HE2	2:N:70:GLU:HB2	1.34	0.92
2:B:58:MET:HE2	2:B:81:HIS:HB2	1.50	0.91
3:O:900:FES:S2	5:O:2036:HOH:O	2.28	0.90
1:S:259:PRO:HB3	1:S:280:GLU:HG2	1.54	0.89
2:B:58:MET:HE2	2:B:81:HIS:CB	2.03	0.88
2:D:55:HIS:NE2	2:D:83:ASP:OD2	2.07	0.87
1:U:233:HIS:HE1	5:U:2073:HOH:O	1.58	0.87
1:E:287:VAL:HG12	1:E:288:MET:HE3	1.57	0.86
2:L:12:PHE:H	2:R:36:GLN:HE21	1.20	0.85
1:C:394:GLU:HG3	5:G:2045:HOH:O	1.76	0.84
1:E:287:VAL:HG12	1:E:288:MET:CE	2.07	0.84
1:G:208:ILE:HD12	1:G:356:THR:OG1	1.78	0.83
1:I:422:HIS:HD2	1:I:424:ASP:H	1.27	0.83
1:S:103:ARG:CB	5:S:2028:HOH:O	2.26	0.83
1:C:287:VAL:HG12	1:C:288:MET:CE	2.10	0.82
1:O:356:THR:HG23	2:P:79:LEU:HD11	1.61	0.81
1:U:339:ILE:HD11	1:U:357:LEU:HG	1.61	0.81
1:O:339:ILE:HD11	1:O:357:LEU:HG	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:VAL:HG12	1:G:288:MET:HE3	1.60	0.81
1:K:142:ALA:HB1	1:Q:413:MET:HG3	1.62	0.81
1:U:413:MET:HG3	1:W:142:ALA:HB1	1.63	0.81
1:S:339:ILE:HD13	1:S:357:LEU:HG	1.64	0.80
1:S:142:ALA:HB1	1:W:413:MET:HG3	1.64	0.80
1:A:339:ILE:CD1	1:A:357:LEU:HG	2.11	0.79
1:A:356:THR:HB	5:A:2142:HOH:O	1.82	0.79
2:B:169:LYS:HE3	5:E:2167:HOH:O	1.83	0.79
1:I:337:ASN:HA	5:I:2068:HOH:O	1.84	0.78
2:R:58:MET:HE3	2:R:174:LEU:HD22	1.65	0.78
1:S:103:ARG:HB3	5:S:2028:HOH:O	1.83	0.78
2:T:36:GLN:HE21	2:V:12:PHE:H	1.28	0.77
2:N:8:PHE:CE2	2:N:70:GLU:HB2	2.18	0.77
1:E:339:ILE:HD11	1:E:357:LEU:HG	1.65	0.77
2:N:113:LEU:HD22	2:R:135:ILE:HG13	1.66	0.75
2:H:10:LYS:HD2	1:S:254:SER:HB3	1.66	0.75
1:C:287:VAL:HG12	1:C:288:MET:HE3	1.66	0.75
1:A:356:THR:CB	5:A:2142:HOH:O	2.34	0.75
1:K:259:PRO:HB3	1:K:280:GLU:HG2	1.68	0.75
1:O:287:VAL:HG12	1:O:288:MET:HE3	1.69	0.74
1:A:208:ILE:HD12	1:A:356:THR:HG1	1.52	0.74
5:A:2110:HOH:O	2:H:40:HIS:HD2	1.69	0.74
1:I:422:HIS:CD2	1:I:424:ASP:H	2.04	0.74
1:U:448:MET:HA	1:U:457:LEU:HD11	1.69	0.74
1:S:255:GLN:OE1	5:S:2066:HOH:O	2.06	0.74
1:Q:185:THR:HG22	1:Q:459:PRO:HG2	1.69	0.73
1:O:422:HIS:HD2	1:O:424:ASP:H	1.36	0.73
2:T:36:GLN:NE2	2:V:12:PHE:H	1.86	0.73
1:C:418:SER:HB3	1:C:428:ASN:OD1	1.89	0.72
1:W:400:ARG:HD3	5:W:2079:HOH:O	1.89	0.72
3:K:900:FES:S1	5:K:2024:HOH:O	2.47	0.72
1:E:142:ALA:HB1	1:G:413:MET:HG2	1.72	0.72
1:M:339:ILE:HD11	1:M:357:LEU:HG	1.71	0.72
1:A:254:SER:HB3	2:F:10:LYS:HD2	1.71	0.72
2:N:67:ARG:NE	2:N:67:ARG:HA	2.05	0.71
1:S:403:LYS:HB3	5:S:2110:HOH:O	1.90	0.71
1:W:273:GLY:HA2	5:W:2059:HOH:O	1.90	0.71
2:F:151:GLU:OE2	2:H:40:HIS:HE1	1.73	0.71
1:Q:274:SER:HB2	1:Q:324:MET:HG3	1.72	0.71
2:V:36:GLN:HE21	2:X:12:PHE:H	1.39	0.70
1:O:123:HIS:N	5:O:2035:HOH:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:VAL:HG12	1:A:288:MET:CE	2.22	0.70
1:A:334:PRO:O	1:A:337:ASN:OD1	2.10	0.69
1:O:287:VAL:HG12	1:O:288:MET:CE	2.22	0.69
2:T:58:MET:HE2	2:T:81:HIS:HB2	1.74	0.69
1:Q:448:MET:HA	1:Q:457:LEU:HD11	1.73	0.69
2:X:143:ARG:O	5:X:2029:HOH:O	2.10	0.69
2:T:12:PHE:H	2:X:36:GLN:HE21	1.41	0.69
1:W:123:HIS:N	3:W:900:FES:S2	2.64	0.69
1:U:232:TYR:HA	1:U:433:TYR:CD1	2.27	0.69
3:S:900:FES:S1	5:S:2021:HOH:O	2.51	0.69
2:J:113:LEU:HD21	2:P:113:LEU:HD23	1.75	0.69
5:H:2056:HOH:O	2:T:52:LYS:HB3	1.92	0.69
1:Q:244:LEU:HD13	1:Q:253:LEU:HG	1.75	0.69
1:K:334:PRO:O	1:K:337:ASN:OD1	2.11	0.68
1:A:287:VAL:HG12	1:A:288:MET:HE3	1.75	0.68
5:H:2056:HOH:O	2:T:52:LYS:HD2	1.94	0.68
2:L:76:ASP:HB2	5:L:2036:HOH:O	1.94	0.68
1:O:259:PRO:HB3	1:O:280:GLU:HB3	1.76	0.68
2:L:12:PHE:H	2:R:36:GLN:NE2	1.92	0.67
1:Q:412:GLN:O	1:Q:415:LEU:HB2	1.94	0.67
1:E:422:HIS:HD2	1:E:424:ASP:H	1.42	0.67
1:G:422:HIS:HD2	1:G:424:ASP:H	1.42	0.67
1:G:276:TRP:HB3	1:G:322:GLN:HG3	1.75	0.66
1:U:232:TYR:HA	1:U:433:TYR:HD1	1.59	0.66
1:W:122:TYR:HB3	3:W:900:FES:S2	2.35	0.66
1:G:287:VAL:CG1	1:G:288:MET:CE	2.70	0.66
1:S:422:HIS:CD2	1:S:424:ASP:H	2.14	0.66
1:A:422:HIS:HD2	1:A:424:ASP:H	1.44	0.66
1:G:422:HIS:CD2	1:G:424:ASP:H	2.14	0.66
1:A:372:ARG:NH1	5:A:2156:HOH:O	2.13	0.65
1:M:107:ILE:HG22	1:M:118:PHE:HB3	1.77	0.65
1:A:259:PRO:HB3	1:A:280:GLU:CG	2.26	0.65
1:C:309:LEU:HD12	1:C:316:VAL:HG11	1.79	0.65
1:Q:389:GLY:O	1:Q:393:VAL:HG23	1.97	0.65
1:E:356:THR:HG23	2:F:79:LEU:HD11	1.79	0.64
1:C:143:PHE:C	1:E:417:ARG:HH21	2.01	0.64
2:F:58:MET:HE3	2:F:81:HIS:CB	2.27	0.64
1:M:340:ARG:HD3	1:M:342:TRP:CH2	2.33	0.64
1:K:142:ALA:HB1	1:Q:413:MET:CG	2.28	0.64
1:S:332:PHE:HB3	1:S:339:ILE:HG13	1.79	0.63
1:C:435:GLU:OE1	1:G:102:HIS:NE2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:339:ILE:CD1	1:M:357:LEU:HG	2.27	0.63
1:U:266:ARG:HB3	1:U:428:ASN:HD22	1.63	0.63
1:A:208:ILE:HD12	1:A:356:THR:OG1	1.99	0.63
2:F:17:LYS:HE2	2:F:121:GLU:HB2	1.79	0.63
1:Q:297:THR:O	1:Q:317:ARG:HD2	1.99	0.63
2:R:26:GLU:OE1	2:R:158:ARG:NH2	2.31	0.63
2:V:107:PRO:HD2	2:X:64:ARG:O	1.98	0.63
1:I:356:THR:HG23	2:J:79:LEU:HD11	1.80	0.62
1:Q:276:TRP:HB3	1:Q:322:GLN:HG3	1.80	0.62
2:T:44:GLU:HG3	5:T:2011:HOH:O	1.99	0.62
1:W:126:ALA:HB3	1:W:135:ASN:HB3	1.81	0.62
2:N:54:ILE:HA	2:N:168:ALA:O	1.99	0.62
1:E:339:ILE:CD1	1:E:357:LEU:HG	2.29	0.62
2:H:58:MET:HE3	2:H:174:LEU:CD2	2.10	0.62
1:U:200:ARG:HG3	5:U:2065:HOH:O	1.98	0.62
1:C:413:MET:HG3	1:G:142:ALA:HB1	1.82	0.62
2:F:58:MET:HE3	2:F:81:HIS:CG	2.35	0.62
1:I:259:PRO:HG2	1:I:283:SER:HB3	1.82	0.62
1:U:123:HIS:HB2	3:U:900:FES:S2	2.39	0.62
1:K:414:GLY:HA2	1:K:417:ARG:HD2	1.81	0.61
1:G:287:VAL:CG1	1:G:288:MET:HE3	2.29	0.61
2:L:32:TYR:CD1	2:N:116:ASN:HA	2.35	0.61
1:U:45:LEU:O	1:U:49:GLU:HG3	2.01	0.61
1:U:233:HIS:CE1	5:U:2073:HOH:O	2.39	0.61
1:U:279:ASP:O	1:U:280:GLU:HB2	2.00	0.61
2:F:24:GLN:HG2	2:H:25:ASN:HD21	1.65	0.61
2:H:169:LYS:CE	5:H:2110:HOH:O	2.49	0.61
1:K:451:GLU:HB2	1:K:457:LEU:HD12	1.82	0.61
1:E:309:LEU:HD22	1:E:316:VAL:HG11	1.81	0.61
1:C:448:MET:HA	1:C:457:LEU:HD11	1.81	0.61
2:H:53:ASP:OD2	2:H:157:ARG:NH2	2.31	0.61
1:C:287:VAL:HG12	1:C:288:MET:HE2	1.81	0.61
2:D:151:GLU:OE2	2:F:40:HIS:HE1	1.84	0.61
1:A:413:MET:HG2	1:A:434:ALA:HA	1.83	0.61
1:C:298:GLU:HG3	5:C:2103:HOH:O	2.00	0.61
2:T:58:MET:HE2	2:T:81:HIS:CB	2.30	0.61
1:W:337:ASN:HA	5:W:2067:HOH:O	2.00	0.60
2:D:58:MET:HE2	2:D:81:HIS:CB	2.31	0.60
1:U:339:ILE:CD1	1:U:357:LEU:HG	2.31	0.60
1:S:123:HIS:HB2	3:S:900:FES:S2	2.40	0.60
1:U:228:CYS:SG	1:U:273:GLY:HA3	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:ILE:HD13	1:G:357:LEU:HG	1.82	0.60
1:I:315:PRO:HB2	1:I:318:ARG:HD3	1.82	0.60
1:M:411:ALA:HA	1:M:435:GLU:OE2	2.01	0.60
1:K:454:TRP:O	1:K:458:LYS:HG3	2.02	0.60
1:A:422:HIS:CD2	1:A:424:ASP:H	2.20	0.60
1:O:103:ARG:N	3:O:900:FES:S1	2.75	0.60
1:U:359:ASP:HB2	1:U:362:ALA:HB2	1.85	0.59
1:U:126:ALA:HB3	1:U:135:ASN:HB3	1.84	0.59
1:C:420:THR:HA	1:C:427:GLY:O	2.03	0.59
1:Q:287:VAL:HG12	1:Q:288:MET:CE	2.33	0.59
1:C:420:THR:OG1	1:O:94:LYS:HD3	2.02	0.59
1:E:422:HIS:CD2	1:E:424:ASP:H	2.21	0.59
2:T:116:ASN:HA	2:X:32:TYR:CD1	2.38	0.59
1:C:340:ARG:HD3	1:C:342:TRP:CH2	2.37	0.59
2:F:113:LEU:HD23	2:H:113:LEU:HD21	1.84	0.59
1:U:219:ASN:HA	5:U:2096:HOH:O	2.02	0.59
1:M:356:THR:HG23	2:N:79:LEU:HD11	1.84	0.59
1:W:164:ARG:HD2	1:W:178:VAL:HA	1.84	0.58
1:A:259:PRO:HB3	1:A:280:GLU:HG2	1.85	0.58
1:C:123:HIS:HB2	3:C:900:FES:S2	2.43	0.58
1:W:86:VAL:HG11	1:W:96:PHE:HE2	1.67	0.58
1:A:356:THR:HG23	2:B:79:LEU:HD11	1.84	0.58
1:G:105:MET:HB3	1:G:120:CYS:SG	2.43	0.58
1:G:334:PRO:O	1:G:337:ASN:OD1	2.20	0.58
1:S:103:ARG:HB2	5:S:2028:HOH:O	1.99	0.58
1:U:244:LEU:HD13	1:U:253:LEU:HG	1.85	0.58
2:P:6:PRO:HG2	2:P:76:ASP:OD1	2.02	0.58
2:H:169:LYS:NZ	5:H:2111:HOH:O	2.34	0.58
1:Q:309:LEU:HD13	1:Q:316:VAL:HG11	1.85	0.57
1:O:422:HIS:CD2	1:O:424:ASP:H	2.21	0.57
1:A:391:ASN:O	1:A:395:ILE:HG13	2.04	0.57
1:A:414:GLY:HA2	1:A:417:ARG:HD2	1.86	0.57
2:B:58:MET:HE2	2:B:81:HIS:CG	2.39	0.57
1:E:22:GLU:HG3	1:E:25:ARG:NH2	2.20	0.57
1:I:344:PRO:HA	1:I:350:ILE:HG22	1.86	0.57
1:K:228:CYS:HB2	1:K:325:THR:HB	1.86	0.57
1:W:304:LEU:O	1:W:308:ARG:HG3	2.04	0.57
2:F:58:MET:CE	2:F:81:HIS:CB	2.82	0.57
1:I:262:GLY:HA2	1:I:278:VAL:HG23	1.86	0.57
2:P:6:PRO:HA	2:P:57:PHE:HE2	1.69	0.57
1:Q:226:GLN:HA	1:Q:230:ASP:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:321:GLY:HA2	1:I:336:MET:HE1	1.86	0.57
1:Q:339:ILE:N	1:Q:339:ILE:HD12	2.20	0.57
1:U:324:MET:HB3	1:U:332:PHE:CE1	2.40	0.57
1:U:266:ARG:HB3	1:U:428:ASN:ND2	2.19	0.57
1:S:276:TRP:HB3	1:S:322:GLN:HG3	1.87	0.56
1:S:349:GLU:OE2	2:X:143:ARG:NH2	2.37	0.56
2:V:84:GLU:CD	2:V:92:ARG:HE	2.09	0.56
1:C:90:ASP:O	1:C:91:LYS:HB2	2.04	0.56
1:Q:356:THR:HG21	1:Q:374:ASN:CB	2.35	0.56
1:I:259:PRO:HG3	1:I:280:GLU:HG2	1.87	0.56
1:W:273:GLY:O	1:W:324:MET:HG3	2.06	0.56
1:E:287:VAL:HG12	1:E:288:MET:HE2	1.84	0.56
2:N:8:PHE:HE2	2:N:70:GLU:CB	2.13	0.56
1:O:164:ARG:HD2	1:O:178:VAL:HA	1.87	0.56
2:T:54:ILE:HA	2:T:168:ALA:O	2.05	0.56
1:G:123:HIS:HB2	3:G:900:FES:S2	2.46	0.56
1:C:276:TRP:HB3	1:C:322:GLN:HG3	1.88	0.56
1:U:243:ILE:HB	5:U:2075:HOH:O	2.04	0.56
1:E:29:ASP:OD1	1:E:32:LYS:HD2	2.06	0.56
1:E:208:ILE:HD12	1:E:356:THR:OG1	2.05	0.55
2:H:169:LYS:HE2	5:H:2110:HOH:O	2.05	0.55
1:A:123:HIS:HB2	3:A:900:FES:S2	2.46	0.55
2:D:33:ARG:CZ	5:D:2100:HOH:O	2.55	0.55
2:J:6:PRO:N	2:J:75:GLY:HA3	2.21	0.55
1:G:339:ILE:CD1	1:G:357:LEU:HG	2.36	0.55
2:B:158:ARG:NE	5:B:2101:HOH:O	2.16	0.55
2:N:32:TYR:CD1	2:R:116:ASN:HA	2.41	0.55
2:R:162:ASN:HB3	5:R:2081:HOH:O	2.06	0.55
1:U:164:ARG:O	1:U:174:ALA:HA	2.07	0.55
2:F:58:MET:CE	2:F:81:HIS:HB2	2.37	0.55
2:L:111:ARG:HB2	2:N:175:ASP:OD2	2.07	0.55
2:V:49:LEU:HD21	2:V:163:LEU:HD13	1.88	0.55
2:T:12:PHE:H	2:X:36:GLN:NE2	2.02	0.55
1:E:283:SER:O	1:E:287:VAL:HG23	2.07	0.55
2:D:51:ASP:OD2	2:D:166:SER:OG	2.24	0.54
1:S:340:ARG:HD3	1:S:342:TRP:CH2	2.43	0.54
1:W:348:ASN:ND2	5:W:2070:HOH:O	2.34	0.54
2:V:36:GLN:NE2	2:X:12:PHE:H	2.05	0.54
1:O:283:SER:O	1:O:287:VAL:HG23	2.07	0.54
1:K:356:THR:HG23	2:L:79:LEU:HD11	1.89	0.54
2:F:58:MET:HE1	2:F:184:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:373:HIS:CD2	1:O:376:ARG:HH21	2.26	0.54
1:I:422:HIS:HD2	1:I:424:ASP:N	2.02	0.54
1:M:229:SER:HB2	1:M:437:ALA:HB3	1.90	0.54
1:O:448:MET:HA	1:O:457:LEU:HD11	1.89	0.54
1:U:412:GLN:O	1:U:415:LEU:HB2	2.08	0.54
1:U:56:ARG:NH2	1:U:448:MET:O	2.41	0.54
2:X:125:PRO:O	2:X:126:ASP:HB2	2.07	0.54
2:F:58:MET:CE	2:F:184:LEU:HD13	2.38	0.53
2:L:90:TYR:HE1	5:L:2023:HOH:O	1.89	0.53
1:S:229:SER:HB2	1:S:437:ALA:HB3	1.90	0.53
2:N:36:GLN:HE21	2:R:12:PHE:H	1.55	0.53
1:S:345:ARG:HG3	1:S:351:GLU:HG3	1.91	0.53
1:O:339:ILE:CD1	1:O:357:LEU:HG	2.35	0.53
2:N:87:GLU:HB2	5:N:2041:HOH:O	2.09	0.53
1:O:123:HIS:CB	5:O:2035:HOH:O	2.57	0.53
1:I:269:TRP:CZ2	1:I:444:HIS:HE1	2.27	0.53
2:L:116:ASN:HA	2:R:32:TYR:CD1	2.44	0.53
1:K:340:ARG:HD3	1:K:342:TRP:CH2	2.43	0.53
2:N:25:ASN:HD21	2:R:24:GLN:HG2	1.74	0.53
1:W:302:ALA:HB1	1:W:317:ARG:HD3	1.91	0.53
1:G:244:LEU:HG	2:H:94:ARG:HG2	1.91	0.53
2:D:24:GLN:HG2	2:F:25:ASN:HD21	1.74	0.53
2:J:56:TYR:HB3	2:J:84:GLU:HB2	1.91	0.53
1:U:246:GLY:HA3	1:U:286:ALA:O	2.09	0.53
1:U:238:THR:OG1	1:W:122:TYR:O	2.27	0.53
1:I:332:PHE:O	1:I:334:PRO:HD3	2.08	0.52
2:R:56:TYR:HB3	2:R:84:GLU:HB2	1.91	0.52
1:I:435:GLU:OE1	1:O:102:HIS:NE2	2.34	0.52
2:J:186:MET:HA	5:J:2006:HOH:O	2.10	0.52
2:D:10:LYS:HD2	1:K:254:SER:HB3	1.90	0.52
1:M:74:LEU:HD21	1:M:211:MET:HE1	1.91	0.52
1:Q:265:PHE:CZ	1:Q:267:ALA:HA	2.44	0.52
1:U:309:LEU:HD13	1:U:316:VAL:HG11	1.91	0.52
1:U:413:MET:CG	1:W:142:ALA:HB1	2.37	0.52
1:W:217:PRO:HG2	1:W:393:VAL:HG22	1.91	0.52
1:A:244:LEU:HD13	1:A:253:LEU:HG	1.91	0.52
1:E:334:PRO:O	1:E:337:ASN:OD1	2.27	0.52
1:K:36:ASP:O	1:K:39:ILE:HG12	2.10	0.52
1:Q:294:GLN:NE2	1:Q:298:GLU:HG3	2.23	0.52
1:Q:356:THR:HG21	1:Q:374:ASN:HB3	1.92	0.52
1:Q:255:GLN:O	1:Q:256:ALA:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:297:THR:O	1:O:317:ARG:HD2	2.09	0.52
2:D:55:HIS:HB2	5:D:2035:HOH:O	2.09	0.52
1:I:284:LEU:HD23	1:I:293:THR:HG23	1.90	0.52
1:U:118:PHE:HD2	5:U:2024:HOH:O	1.91	0.52
2:F:55:HIS:HB2	5:F:2115:HOH:O	2.09	0.52
1:O:296:TRP:CH2	1:O:334:PRO:O	2.63	0.52
1:O:70:THR:HA	5:O:2026:HOH:O	2.10	0.52
1:S:334:PRO:O	1:S:337:ASN:OD1	2.28	0.52
1:U:227:PHE:HD2	5:U:2094:HOH:O	1.92	0.52
1:I:365:GLU:CD	1:I:365:GLU:H	2.12	0.52
2:P:54:ILE:HA	2:P:168:ALA:O	2.10	0.52
1:Q:418:SER:HB3	1:Q:428:ASN:OD1	2.10	0.52
1:G:279:ASP:O	1:G:281:PRO:HD3	2.10	0.52
1:Q:287:VAL:HG12	1:Q:288:MET:HE3	1.92	0.52
2:F:58:MET:HE3	2:F:81:HIS:CD2	2.45	0.51
2:F:56:TYR:HB3	2:F:84:GLU:HB2	1.93	0.51
1:K:338:ASN:C	1:K:339:ILE:HD12	2.30	0.51
1:S:422:HIS:HD2	1:S:424:ASP:H	1.58	0.51
1:I:36:ASP:O	1:I:39:ILE:HG12	2.10	0.51
2:P:56:TYR:HB3	2:P:84:GLU:HB2	1.92	0.51
1:U:232:TYR:CE1	1:W:123:HIS:HB3	2.45	0.51
1:E:287:VAL:CG1	1:E:288:MET:HE3	2.36	0.51
2:F:54:ILE:HA	2:F:168:ALA:O	2.10	0.51
1:S:189:ASP:OD1	5:S:2044:HOH:O	2.18	0.51
1:A:164:ARG:HD2	1:A:178:VAL:HA	1.92	0.51
1:O:123:HIS:HB2	5:O:2035:HOH:O	2.10	0.51
1:W:215:VAL:HG22	1:W:351:GLU:HG2	1.92	0.51
1:O:56:ARG:NH2	1:O:448:MET:O	2.44	0.51
1:O:102:HIS:HB3	3:O:900:FES:S1	2.50	0.51
1:S:21:PRO:O	1:S:25:ARG:HG3	2.11	0.51
5:S:2110:HOH:O	1:U:97:LEU:HD22	2.11	0.51
1:K:302:ALA:HB1	1:K:317:ARG:HD3	1.92	0.51
1:Q:334:PRO:O	1:Q:337:ASN:OD1	2.29	0.51
1:C:274:SER:OG	1:C:322:GLN:NE2	2.36	0.51
2:X:140:ARG:HG3	2:X:141:LEU:HG	1.91	0.51
1:K:259:PRO:HB3	1:K:280:GLU:CG	2.39	0.51
2:L:58:MET:HE2	2:L:81:HIS:CB	2.41	0.51
1:W:339:ILE:HD13	1:W:357:LEU:HG	1.92	0.51
2:D:120:LYS:HE3	2:N:67:ARG:HH12	1.75	0.50
2:F:17:LYS:HZ1	2:F:121:GLU:H	1.59	0.50
1:G:257:GLN:O	1:G:259:PRO:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:TYR:CG	2:H:116:ASN:HA	2.46	0.50
1:U:61:LEU:HD11	1:U:174:ALA:HB2	1.92	0.50
1:M:334:PRO:O	1:M:337:ASN:OD1	2.28	0.50
1:O:215:VAL:O	2:P:182:ASN:HA	2.11	0.50
1:Q:215:VAL:O	2:R:182:ASN:HA	2.11	0.50
1:S:287:VAL:HG12	1:S:288:MET:CE	2.41	0.50
1:E:299:GLY:O	1:E:303:GLU:HG3	2.10	0.50
2:F:58:MET:HE1	2:F:184:LEU:CD1	2.41	0.50
1:A:18:ASN:CG	1:A:19:TRP:H	2.15	0.50
1:K:339:ILE:HD13	1:K:357:LEU:HG	1.93	0.50
1:O:340:ARG:HD3	1:O:342:TRP:CH2	2.46	0.50
1:W:337:ASN:HB3	1:W:357:LEU:O	2.11	0.50
1:E:340:ARG:NH1	1:E:385:GLU:OE2	2.42	0.50
1:W:422:HIS:HB3	1:W:425:PHE:O	2.12	0.50
1:A:169:LYS:HE3	1:A:199:ASP:CG	2.32	0.50
2:D:7:HIS:CD2	2:D:7:HIS:N	2.79	0.50
1:I:107:ILE:HG22	1:I:118:PHE:HB3	1.94	0.50
1:K:444:HIS:O	1:K:445:TRP:C	2.50	0.50
1:K:139:GLU:HA	1:K:143:PHE:HD1	1.77	0.50
1:M:164:ARG:HD2	1:M:178:VAL:HA	1.93	0.50
2:N:111:ARG:HB2	2:R:175:ASP:OD2	2.12	0.49
1:Q:317:ARG:HB2	5:Q:2062:HOH:O	2.12	0.49
1:U:222:PHE:CZ	1:U:395:ILE:HG21	2.47	0.49
2:H:169:LYS:HE3	5:H:2110:HOH:O	2.12	0.49
1:I:226:GLN:HA	1:I:230:ASP:HB3	1.93	0.49
2:F:58:MET:HE3	2:F:81:HIS:HB2	1.92	0.49
2:F:135:ILE:HG13	2:H:113:LEU:HD22	1.95	0.49
1:I:339:ILE:HD13	1:I:357:LEU:HG	1.94	0.49
1:U:216:ILE:HD12	1:U:350:ILE:HD11	1.94	0.49
2:X:56:TYR:HB3	2:X:84:GLU:HB2	1.94	0.49
1:K:265:PHE:CZ	1:K:267:ALA:HA	2.48	0.49
1:W:410:ASN:HD21	1:W:412:GLN:HB2	1.77	0.49
1:C:195:ASP:HB3	1:C:309:LEU:HD21	1.93	0.49
2:D:120:LYS:HE2	5:D:2083:HOH:O	2.11	0.49
1:G:44:SER:O	1:G:48:LEU:HD13	2.13	0.49
1:C:339:ILE:HD13	1:C:357:LEU:HG	1.95	0.49
1:O:197:MET:HB2	1:O:334:PRO:HB3	1.95	0.49
1:Q:339:ILE:HD13	1:Q:357:LEU:HG	1.95	0.49
1:S:269:TRP:CZ2	1:S:444:HIS:HE1	2.31	0.49
2:D:135:ILE:HG13	2:F:113:LEU:HD22	1.92	0.49
1:I:131:GLY:O	1:I:160:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:376:ARG:HB2	5:I:2074:HOH:O	2.13	0.49
1:I:403:LYS:HD2	1:O:161:LEU:HD21	1.95	0.49
1:S:259:PRO:HB3	1:S:280:GLU:CG	2.37	0.49
1:S:82:PRO:HB2	1:S:98:ASN:HB3	1.94	0.49
2:X:29:GLN:O	2:X:33:ARG:HG3	2.13	0.49
1:K:340:ARG:HH12	1:K:385:GLU:CD	2.16	0.49
1:Q:339:ILE:CD1	1:Q:357:LEU:HG	2.43	0.49
1:G:169:LYS:HD3	1:G:199:ASP:HB2	1.95	0.49
2:H:55:HIS:HB2	5:H:2041:HOH:O	2.12	0.49
1:K:410:ASN:ND2	1:K:412:GLN:H	2.09	0.49
2:N:49:LEU:HD21	2:N:163:LEU:HD13	1.94	0.49
1:W:61:LEU:HB3	1:W:76:THR:HG21	1.94	0.49
1:I:417:ARG:HB3	5:I:2083:HOH:O	2.13	0.48
1:U:269:TRP:CD2	1:U:459:PRO:HG3	2.48	0.48
1:W:218:CYS:SG	1:W:392:TRP:HB3	2.53	0.48
1:W:412:GLN:O	1:W:415:LEU:HB2	2.13	0.48
1:A:65:SER:CB	1:A:206:VAL:HG23	2.43	0.48
1:A:259:PRO:HB3	1:A:280:GLU:HG3	1.94	0.48
1:E:259:PRO:HB3	1:E:280:GLU:HB3	1.93	0.48
2:D:113:LEU:HD22	2:H:135:ILE:HG13	1.95	0.48
1:K:27:LEU:HD13	1:K:39:ILE:HG22	1.95	0.48
1:O:193:TYR:CE2	1:O:276:TRP:CH2	3.01	0.48
1:O:209:GLY:HA3	2:P:78:ASP:OD1	2.12	0.48
2:P:162:ASN:ND2	2:P:162:ASN:H	2.10	0.48
2:H:56:TYR:HB3	2:H:84:GLU:HB2	1.96	0.48
1:I:215:VAL:O	2:J:182:ASN:HA	2.14	0.48
1:K:199:ASP:HB3	1:K:309:LEU:HD21	1.95	0.48
1:M:332:PHE:HB3	1:M:339:ILE:HG23	1.96	0.48
1:W:340:ARG:HD3	1:W:342:TRP:CH2	2.48	0.48
1:A:265:PHE:CZ	1:A:267:ALA:HA	2.49	0.48
1:A:287:VAL:HG12	1:A:288:MET:HE2	1.94	0.48
1:K:422:HIS:HD2	1:K:424:ASP:H	1.61	0.48
1:W:448:MET:HA	1:W:457:LEU:HD11	1.95	0.48
2:H:10:LYS:HD2	1:S:254:SER:CB	2.41	0.48
2:J:125:PRO:O	2:J:126:ASP:HB2	2.14	0.48
2:L:36:GLN:HE21	2:N:12:PHE:H	1.61	0.48
1:S:123:HIS:HA	5:W:2055:HOH:O	2.14	0.48
1:W:267:ALA:N	5:W:2059:HOH:O	2.46	0.48
1:W:381:GLY:O	2:X:92:ARG:NH1	2.46	0.48
1:G:212:GLN:HE21	1:G:212:GLN:HB2	1.55	0.48
1:G:356:THR:HG23	2:H:79:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:407:GLN:HB3	1:Q:101:ARG:NH2	2.29	0.48
2:T:22:GLU:CD	2:T:22:GLU:H	2.17	0.48
2:V:32:TYR:CD1	2:X:116:ASN:HA	2.48	0.48
2:D:58:MET:HE2	2:D:81:HIS:HB2	1.95	0.48
1:G:287:VAL:CG1	1:G:288:MET:HE2	2.30	0.48
1:O:226:GLN:HA	1:O:230:ASP:HB3	1.96	0.48
1:M:32:LYS:O	1:M:412:GLN:HG2	2.14	0.48
2:L:36:GLN:NE2	2:N:12:PHE:H	2.12	0.48
1:O:269:TRP:CD2	1:O:459:PRO:HG3	2.49	0.48
1:W:333:LEU:HB3	1:W:336:MET:HG3	1.95	0.48
1:K:143:PHE:HA	5:K:2035:HOH:O	2.12	0.47
1:O:120:CYS:SG	5:O:2036:HOH:O	2.61	0.47
1:S:164:ARG:HD2	1:S:178:VAL:HA	1.95	0.47
1:S:213:LYS:HA	1:S:352:VAL:O	2.14	0.47
1:E:36:ASP:O	1:E:39:ILE:HG12	2.14	0.47
1:E:303:GLU:HG2	1:E:317:ARG:NH1	2.30	0.47
2:J:6:PRO:HG3	5:J:2016:HOH:O	2.14	0.47
2:L:90:TYR:CE1	5:L:2023:HOH:O	2.55	0.47
2:T:24:GLN:HG2	2:X:25:ASN:HD21	1.78	0.47
1:Q:195:ASP:CB	1:Q:309:LEU:HD21	2.44	0.47
1:Q:73:PHE:HA	1:Q:85:MET:O	2.14	0.47
1:S:435:GLU:OE1	1:U:102:HIS:NE2	2.48	0.47
1:K:51:GLU:OE2	1:K:52:ARG:NH1	2.48	0.47
1:Q:287:VAL:HG12	1:Q:288:MET:HE2	1.96	0.47
1:Q:356:THR:HG21	1:Q:374:ASN:CG	2.34	0.47
1:E:25:ARG:HD3	5:E:2002:HOH:O	2.13	0.47
1:I:239:HIS:HE1	1:I:384:PHE:O	1.98	0.47
2:L:54:ILE:HA	2:L:168:ALA:O	2.15	0.47
2:N:25:ASN:ND2	5:N:2010:HOH:O	2.46	0.47
2:N:25:ASN:ND2	5:N:2012:HOH:O	2.43	0.47
1:O:195:ASP:HB3	1:O:309:LEU:HD21	1.96	0.47
1:O:76:THR:OG1	1:O:77:TYR:N	2.46	0.47
3:S:900:FES:S2	5:S:2029:HOH:O	2.61	0.47
1:U:208:ILE:HA	5:U:2069:HOH:O	2.13	0.47
1:U:218:CYS:CB	1:U:392:TRP:HB3	2.45	0.47
1:W:339:ILE:N	1:W:339:ILE:HD12	2.30	0.47
1:M:177:ASP:OD2	1:M:454:TRP:NE1	2.47	0.47
1:U:164:ARG:HD2	1:U:178:VAL:HA	1.97	0.47
1:A:107:ILE:HG22	1:A:118:PHE:HB3	1.97	0.47
1:C:212:GLN:HB2	1:C:212:GLN:HE21	1.54	0.47
1:I:57:SER:HB3	1:I:328:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:230:ASP:OD1	1:M:233:HIS:N	2.47	0.47
1:A:185:THR:HG22	1:A:459:PRO:HG2	1.96	0.47
1:I:228:CYS:HB2	1:I:325:THR:HB	1.96	0.47
1:M:131:GLY:O	1:M:160:PRO:HD2	2.14	0.47
1:M:303:GLU:O	1:M:307:GLN:HB2	2.14	0.47
1:A:189:ASP:O	1:A:192:PRO:HD2	2.15	0.47
1:E:339:ILE:N	1:E:339:ILE:HD12	2.29	0.47
1:G:410:ASN:ND2	1:G:412:GLN:H	2.13	0.47
1:S:217:PRO:HG2	1:S:393:VAL:HG22	1.97	0.47
1:W:181:PRO:HA	5:W:2044:HOH:O	2.15	0.47
1:I:56:ARG:NH2	1:I:448:MET:O	2.45	0.46
1:M:126:ALA:HB3	1:M:135:ASN:HB3	1.97	0.46
2:N:143:ARG:NH2	1:Q:349:GLU:OE2	2.48	0.46
1:S:332:PHE:CB	1:S:339:ILE:HG13	2.45	0.46
2:V:131:ASN:ND2	5:V:2031:HOH:O	2.48	0.46
1:E:448:MET:HA	1:E:457:LEU:HD11	1.97	0.46
1:O:322:GLN:HB3	1:O:334:PRO:HD2	1.97	0.46
1:M:346:GLY:O	5:M:2066:HOH:O	2.20	0.46
1:O:340:ARG:HA	1:O:353:TRP:O	2.15	0.46
2:N:113:LEU:HD21	2:R:113:LEU:HD23	1.98	0.46
1:S:64:GLU:HB3	1:S:87:ARG:HH22	1.80	0.46
1:S:394:GLU:HB2	1:U:105:MET:SD	2.55	0.46
1:E:123:HIS:HB2	3:E:900:FES:S2	2.55	0.46
1:G:255:GLN:O	1:G:256:ALA:C	2.54	0.46
1:K:78:MET:O	1:K:81:ASP:HB2	2.15	0.46
1:M:123:HIS:HB2	3:M:900:FES:S2	2.55	0.46
1:O:373:HIS:HD2	1:O:376:ARG:HH21	1.62	0.46
1:Q:359:ASP:HB2	1:Q:362:ALA:HB2	1.98	0.46
1:S:214:TRP:HE1	1:S:216:ILE:HD11	1.81	0.46
1:G:413:MET:HB2	1:G:435:GLU:OE2	2.15	0.46
1:I:255:GLN:O	1:I:256:ALA:C	2.53	0.46
2:L:116:ASN:HA	2:R:32:TYR:CG	2.51	0.46
1:W:233:HIS:HA	5:W:2055:HOH:O	2.16	0.46
1:Q:257:GLN:HG3	1:Q:258:ILE:N	2.30	0.46
1:Q:48:LEU:HD12	5:Q:2013:HOH:O	2.15	0.46
2:X:58:MET:HB3	2:X:82:PHE:HB2	1.97	0.46
1:M:338:ASN:HD22	1:M:356:THR:HG22	1.80	0.46
1:W:269:TRP:CD1	1:W:459:PRO:HA	2.51	0.46
2:F:113:LEU:HD23	2:H:113:LEU:CD2	2.45	0.46
1:W:169:LYS:HD3	1:W:199:ASP:HB2	1.97	0.46
2:B:22:GLU:O	2:B:26:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:GLU:OE1	1:E:167:THR:HG21	2.15	0.46
1:E:263:ASN:HB2	1:E:276:TRP:CZ2	2.51	0.46
1:G:373:HIS:CD2	1:G:376:ARG:HE	2.34	0.46
2:L:56:TYR:HB3	2:L:84:GLU:HB2	1.98	0.46
1:M:199:ASP:HB3	1:M:309:LEU:HD21	1.98	0.46
1:S:391:ASN:O	1:S:395:ILE:HG13	2.16	0.46
2:T:37:LEU:HD23	2:V:11:THR:HG21	1.98	0.46
1:E:356:THR:HG21	1:E:374:ASN:CB	2.46	0.46
1:I:244:LEU:HD13	1:I:253:LEU:HG	1.97	0.45
1:K:315:PRO:HB2	1:K:318:ARG:HD3	1.98	0.45
2:N:61:ARG:NH2	5:N:2025:HOH:O	2.48	0.45
1:S:448:MET:HA	1:S:457:LEU:HD11	1.98	0.45
1:W:413:MET:HG2	1:W:434:ALA:HA	1.98	0.45
2:X:110:THR:HG22	2:X:138:ARG:HG2	1.97	0.45
1:I:269:TRP:CD2	1:I:459:PRO:HG3	2.51	0.45
1:K:349:GLU:OE2	2:R:143:ARG:NH2	2.42	0.45
1:O:410:ASN:ND2	1:O:412:GLN:H	2.13	0.45
1:I:22:GLU:HG3	1:I:25:ARG:NH2	2.31	0.45
2:J:32:TYR:CD1	2:P:116:ASN:HA	2.51	0.45
1:Q:422:HIS:HD2	1:Q:424:ASP:H	1.65	0.45
1:U:370:TYR:O	1:U:374:ASN:HB2	2.15	0.45
2:T:32:TYR:CD1	2:V:116:ASN:HA	2.52	0.45
1:M:326:ILE:HB	1:M:330:CYS:HB3	1.97	0.45
2:N:67:ARG:HE	2:N:67:ARG:CA	2.14	0.45
2:X:136:LEU:HB3	2:X:148:PHE:HD1	1.82	0.45
1:A:368:GLU:O	1:A:372:ARG:HG3	2.17	0.45
1:I:395:ILE:O	1:I:399:LEU:HG	2.16	0.45
1:W:262:GLY:C	1:W:432:VAL:HB	2.35	0.45
1:E:340:ARG:HH21	1:E:378:PHE:HB3	1.81	0.45
1:I:223:ALA:HA	1:I:392:TRP:CZ2	2.51	0.45
1:M:359:ASP:HB2	1:M:362:ALA:HB2	1.97	0.45
2:N:15:PRO:HD3	2:N:120:LYS:HG3	1.98	0.45
2:N:58:MET:HE2	2:N:81:HIS:HB2	1.99	0.45
1:U:262:GLY:HA2	1:U:278:VAL:HG23	1.98	0.45
2:D:33:ARG:HD3	5:D:2015:HOH:O	2.16	0.45
1:K:419:GLN:HE21	1:K:421:GLY:H	1.65	0.45
1:M:69:GLU:O	1:M:87:ARG:HB3	2.17	0.45
1:O:321:GLY:HA2	1:O:336:MET:HE1	1.99	0.45
1:Q:195:ASP:HB3	1:Q:309:LEU:HD21	1.97	0.45
2:D:175:ASP:OD2	2:F:111:ARG:HB2	2.16	0.45
1:S:191:ARG:N	1:S:192:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:2056:HOH:O	2:T:52:LYS:CD	2.56	0.45
1:W:24:ILE:HA	1:W:27:LEU:HD12	1.99	0.45
1:K:332:PHE:HB3	1:K:339:ILE:HG13	1.98	0.45
1:M:213:LYS:HG2	1:M:353:TRP:CD1	2.51	0.45
1:Q:57:SER:HB3	1:Q:328:PRO:HD3	1.97	0.45
1:S:262:GLY:HA2	1:S:278:VAL:HG23	1.98	0.45
1:C:244:LEU:HD13	1:C:253:LEU:HG	1.99	0.44
1:C:413:MET:HG2	1:C:434:ALA:HA	1.99	0.44
2:D:116:ASN:HA	2:F:32:TYR:CD1	2.52	0.44
1:Q:422:HIS:CD2	1:Q:424:ASP:H	2.35	0.44
1:S:259:PRO:HB2	1:S:277:TYR:CE2	2.52	0.44
1:C:262:GLY:HA2	1:C:278:VAL:HG23	1.99	0.44
1:G:340:ARG:HD3	1:G:342:TRP:CH2	2.52	0.44
1:C:22:GLU:HG3	1:C:25:ARG:HH22	1.82	0.44
2:F:58:MET:CE	2:F:184:LEU:CD1	2.96	0.44
1:M:373:HIS:HD2	1:M:376:ARG:HE	1.65	0.44
1:Q:356:THR:HG23	2:R:79:LEU:HD11	1.99	0.44
1:C:419:GLN:HE22	1:O:162:GLN:HG3	1.83	0.44
1:S:183:LEU:O	1:S:186:TYR:HB3	2.17	0.44
5:H:2055:HOH:O	2:T:52:LYS:HD2	2.17	0.44
1:I:167:THR:HA	1:I:171:LEU:O	2.18	0.44
2:P:37:LEU:HD11	2:P:163:LEU:HD11	1.99	0.44
1:S:27:LEU:HD13	1:S:39:ILE:HG22	2.00	0.44
1:W:85:MET:HA	1:W:95:VAL:HG22	1.99	0.44
1:I:48:LEU:HD12	1:I:52:ARG:HG3	1.99	0.44
1:K:73:PHE:HA	1:K:85:MET:O	2.17	0.44
1:M:21:PRO:O	1:M:25:ARG:HG3	2.17	0.44
1:O:278:VAL:HA	1:O:318:ARG:O	2.17	0.44
1:S:143:PHE:HB3	1:S:153:PHE:HB3	1.99	0.44
1:S:287:VAL:HG12	1:S:288:MET:HE3	1.98	0.44
3:S:900:FES:S1	5:S:2028:HOH:O	2.62	0.44
2:T:125:PRO:O	2:T:126:ASP:HB2	2.18	0.44
1:G:196:VAL:O	1:G:200:ARG:HD2	2.17	0.44
1:G:389:GLY:O	1:G:393:VAL:HG23	2.17	0.44
1:I:270:GLY:O	1:I:327:PHE:HB3	2.17	0.44
1:O:119:THR:HA	5:O:2037:HOH:O	2.17	0.44
1:U:218:CYS:HB3	1:U:392:TRP:HB3	2.00	0.44
2:H:17:LYS:H	2:V:67:ARG:NH1	2.16	0.44
2:F:17:LYS:NZ	2:F:121:GLU:H	2.16	0.44
2:J:122:THR:HG22	2:J:129:GLU:HG3	1.99	0.44
1:S:193:TYR:CE2	1:S:276:TRP:CH2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:309:LEU:HD12	1:W:316:VAL:HG11	1.99	0.44
1:K:340:ARG:NH1	1:K:385:GLU:OE1	2.47	0.44
1:C:217:PRO:HD2	1:C:393:VAL:HG22	2.00	0.43
2:D:116:ASN:HA	2:F:32:TYR:CG	2.53	0.43
1:I:233:HIS:HB3	1:O:123:HIS:CD2	2.52	0.43
1:K:42:ASP:HB3	1:K:45:LEU:HB2	2.00	0.43
2:N:131:ASN:ND2	5:N:2055:HOH:O	2.51	0.43
2:P:136:LEU:HB3	2:P:148:PHE:HB2	2.00	0.43
1:W:42:ASP:HB3	1:W:45:LEU:HB2	1.99	0.43
1:M:246:GLY:O	5:M:2058:HOH:O	2.21	0.43
1:S:356:THR:HG23	2:T:79:LEU:HD11	2.00	0.43
1:C:336:MET:HG2	1:C:336:MET:H	1.55	0.43
1:I:413:MET:HG2	1:I:434:ALA:HA	2.00	0.43
1:K:19:TRP:HB3	1:K:24:ILE:HD11	1.98	0.43
1:S:100:CYS:SG	1:S:127:TYR:OH	2.77	0.43
2:T:128:PHE:HZ	2:T:158:ARG:NH1	2.15	0.43
2:V:67:ARG:HE	2:V:67:ARG:HA	1.84	0.43
1:A:64:GLU:OE1	1:A:167:THR:HG21	2.17	0.43
2:D:54:ILE:HA	2:D:168:ALA:O	2.19	0.43
2:F:17:LYS:HD3	2:F:17:LYS:N	2.34	0.43
1:G:185:THR:HG22	1:G:459:PRO:HG2	1.99	0.43
2:J:55:HIS:NE2	2:J:83:ASP:OD2	2.43	0.43
1:K:167:THR:HA	1:K:171:LEU:O	2.18	0.43
1:K:211:MET:HE1	1:K:353:TRP:CE3	2.54	0.43
1:Q:376:ARG:HA	2:R:92:ARG:NH2	2.33	0.43
1:U:229:SER:HB3	1:U:438:ALA:HB2	1.99	0.43
1:U:266:ARG:HB2	1:U:437:ALA:HA	2.00	0.43
2:X:58:MET:HE3	2:X:174:LEU:HD22	1.99	0.43
2:B:169:LYS:CE	5:E:2167:HOH:O	2.52	0.43
1:M:336:MET:HG2	1:M:336:MET:H	1.66	0.43
1:A:167:THR:CG2	5:A:2013:HOH:O	2.66	0.43
1:E:259:PRO:HB2	1:E:277:TYR:CD2	2.53	0.43
1:S:103:ARG:HA	1:W:409:LEU:HD13	2.01	0.43
1:S:73:PHE:CE1	1:S:108:CYS:SG	3.12	0.43
1:W:68:PRO:HD2	1:W:72:ASP:OD2	2.19	0.43
1:A:302:ALA:HB1	1:A:317:ARG:HD3	2.00	0.43
2:J:102:TRP:O	1:O:109:ARG:NH2	2.51	0.43
1:I:392:TRP:HA	1:I:395:ILE:HD12	2.00	0.43
1:K:336:MET:HG2	1:K:336:MET:H	1.54	0.43
1:K:211:MET:CE	1:K:353:TRP:CE3	3.02	0.43
1:O:332:PHE:HD1	1:O:334:PRO:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:38:ARG:HA	1:U:405:LYS:HD2	2.01	0.43
1:U:86:VAL:HG11	1:U:96:PHE:HE2	1.83	0.43
2:T:111:ARG:HB2	2:V:175:ASP:OD2	2.19	0.43
2:V:38:LEU:HD22	2:V:187:PHE:HB2	2.00	0.43
1:E:259:PRO:HB2	1:E:277:TYR:CE2	2.54	0.43
1:E:298:GLU:HG3	5:E:2136:HOH:O	2.19	0.43
1:E:311:HIS:HE1	5:E:2101:HOH:O	2.01	0.43
1:G:336:MET:H	1:G:336:MET:HG2	1.53	0.43
2:L:32:TYR:CG	2:N:116:ASN:HA	2.54	0.43
1:Q:212:GLN:HE21	1:Q:354:ALA:HB3	1.82	0.43
1:W:68:PRO:HA	1:W:87:ARG:HH21	1.84	0.43
1:A:448:MET:HA	1:A:457:LEU:HD11	2.01	0.43
2:B:186:MET:HA	5:B:2122:HOH:O	2.17	0.43
2:J:36:GLN:NE2	2:P:12:PHE:H	2.16	0.43
1:K:244:LEU:HG	2:L:94:ARG:HG2	2.01	0.43
1:W:164:ARG:O	1:W:174:ALA:HA	2.19	0.43
1:G:373:HIS:HD2	1:G:376:ARG:HE	1.67	0.42
1:K:123:HIS:HB3	1:Q:232:TYR:CE1	2.54	0.42
1:S:336:MET:H	1:S:336:MET:HG2	1.64	0.42
2:T:26:GLU:OE1	2:T:158:ARG:NH2	2.52	0.42
1:W:257:GLN:O	1:W:259:PRO:HD3	2.19	0.42
1:E:390:GLU:OE2	1:E:390:GLU:HA	2.19	0.42
1:I:227:PHE:CZ	1:I:340:ARG:HD2	2.53	0.42
2:J:49:LEU:HD21	2:J:163:LEU:HD13	2.00	0.42
1:K:104:GLY:N	5:K:2024:HOH:O	2.52	0.42
1:O:368:GLU:OE2	1:O:368:GLU:HA	2.19	0.42
1:S:124:GLY:N	5:S:2029:HOH:O	2.51	0.42
2:D:25:ASN:HD21	2:H:24:GLN:HG2	1.85	0.42
1:E:336:MET:H	1:E:336:MET:HG2	1.60	0.42
2:F:55:HIS:HB3	2:F:169:LYS:HD3	2.01	0.42
1:K:333:LEU:HB2	1:K:336:MET:HG3	2.00	0.42
2:L:58:MET:HE2	2:L:81:HIS:HB3	2.01	0.42
1:O:287:VAL:HG12	1:O:288:MET:HE2	2.01	0.42
1:K:142:ALA:CB	1:Q:413:MET:HG3	2.40	0.42
1:G:356:THR:HG21	1:G:374:ASN:CB	2.49	0.42
1:I:230:ASP:O	1:I:233:HIS:CE1	2.73	0.42
1:K:76:THR:OG1	1:K:77:TYR:N	2.52	0.42
1:M:212:GLN:HB2	1:M:212:GLN:HE21	1.61	0.42
1:S:104:GLY:N	5:S:2021:HOH:O	2.49	0.42
1:W:226:GLN:HA	1:W:230:ASP:HB3	2.00	0.42
1:W:276:TRP:HB3	1:W:322:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:ILE:HA	1:E:259:PRO:HD3	1.92	0.42
2:J:54:ILE:HA	2:J:168:ALA:O	2.19	0.42
2:P:49:LEU:HD21	2:P:163:LEU:HD13	2.00	0.42
1:U:284:LEU:HD23	1:U:293:THR:HG23	2.02	0.42
2:B:6:PRO:O	2:B:7:HIS:C	2.57	0.42
1:O:288:MET:SD	1:O:336:MET:HB3	2.60	0.42
1:I:164:ARG:O	1:I:174:ALA:HA	2.19	0.42
1:U:292:VAL:HG22	1:U:369:GLU:HB3	2.02	0.42
2:B:58:MET:CE	2:B:81:HIS:CD2	3.02	0.42
1:K:123:HIS:HB2	3:K:900:FES:S2	2.60	0.42
1:Q:24:ILE:HA	1:Q:27:LEU:HD12	2.02	0.42
1:A:359:ASP:HB2	1:A:362:ALA:HB2	2.02	0.42
2:D:108:SER:HB3	2:D:138:ARG:HD3	2.02	0.42
2:H:51:ASP:OD2	2:H:157:ARG:NH1	2.53	0.42
2:H:169:LYS:HG2	5:H:2110:HOH:O	2.20	0.42
1:I:105:MET:HB3	1:I:120:CYS:SG	2.60	0.42
1:U:288:MET:HE2	1:U:288:MET:HA	2.02	0.42
1:W:123:HIS:O	1:W:137:PRO:HG2	2.20	0.42
1:W:334:PRO:HA	5:W:2067:HOH:O	2.20	0.42
2:L:125:PRO:O	2:L:126:ASP:HB2	2.20	0.42
1:S:36:ASP:O	1:S:39:ILE:HG12	2.19	0.42
1:S:266:ARG:NH1	1:S:436:GLU:OE1	2.52	0.42
1:U:86:VAL:CG1	1:U:96:PHE:HE2	2.33	0.42
2:V:31:TYR:HB3	2:V:114:VAL:HG11	2.02	0.42
1:W:349:GLU:HG2	1:W:350:ILE:N	2.34	0.42
1:A:258:ILE:HA	1:A:259:PRO:HD3	1.70	0.41
1:G:277:TYR:HD1	1:G:283:SER:HG	1.67	0.41
1:I:230:ASP:O	1:I:233:HIS:ND1	2.53	0.41
1:U:200:ARG:CG	5:U:2065:HOH:O	2.64	0.41
1:E:212:GLN:HE21	1:E:212:GLN:HB2	1.56	0.41
1:E:251:MET:HG3	1:E:255:GLN:HE21	1.83	0.41
1:E:262:GLY:C	1:E:432:VAL:HB	2.41	0.41
2:N:58:MET:HE3	2:N:81:HIS:CD2	2.55	0.41
1:U:51:GLU:OE2	1:U:52:ARG:NH1	2.53	0.41
1:E:68:PRO:HD2	1:E:72:ASP:OD2	2.20	0.41
1:I:226:GLN:HA	1:I:230:ASP:CB	2.51	0.41
1:I:76:THR:OG1	1:I:77:TYR:N	2.51	0.41
1:O:136:VAL:O	1:O:139:GLU:HB2	2.20	0.41
1:O:270:GLY:O	1:O:327:PHE:HB3	2.20	0.41
2:V:56:TYR:HB3	2:V:84:GLU:HB2	2.02	0.41
1:S:76:THR:OG1	1:S:77:TYR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:153:PHE:HE2	1:U:155:LYS:HG2	1.84	0.41
1:W:359:ASP:HB2	1:W:362:ALA:HB2	2.03	0.41
1:W:57:SER:HB3	1:W:328:PRO:HD3	2.03	0.41
2:F:17:LYS:HD3	2:F:17:LYS:H	1.85	0.41
1:G:431:TYR:CE1	1:G:432:VAL:HG12	2.55	0.41
1:M:244:LEU:HD11	2:N:94:ARG:HG2	2.02	0.41
1:W:389:GLY:O	1:W:393:VAL:HG23	2.20	0.41
2:X:145:VAL:HB	5:X:2030:HOH:O	2.20	0.41
2:D:32:TYR:CD1	2:H:116:ASN:HA	2.56	0.41
1:E:262:GLY:HA2	1:E:278:VAL:HG23	2.03	0.41
1:M:403:LYS:HE3	1:Q:176:TRP:HB3	2.02	0.41
1:K:339:ILE:HD12	1:K:339:ILE:N	2.35	0.41
2:L:11:THR:HG23	2:R:36:GLN:HB3	2.02	0.41
2:N:36:GLN:NE2	2:R:12:PHE:H	2.16	0.41
2:R:29:GLN:O	2:R:33:ARG:HG3	2.21	0.41
2:T:116:ASN:HA	2:X:32:TYR:CG	2.56	0.41
2:V:53:ASP:OD1	2:V:53:ASP:N	2.48	0.41
1:G:376:ARG:HA	2:H:92:ARG:NH2	2.36	0.41
2:H:55:HIS:HB3	2:H:169:LYS:HE2	2.02	0.41
1:I:208:ILE:HD12	1:I:356:THR:OG1	2.21	0.41
1:K:52:ARG:HB3	1:K:448:MET:O	2.20	0.41
1:Q:248:PRO:HA	1:Q:249:PRO:HD3	1.95	0.41
1:S:136:VAL:O	1:S:139:GLU:HB2	2.21	0.41
1:S:355:PHE:HE1	1:S:357:LEU:HD21	1.86	0.41
1:W:248:PRO:HA	1:W:249:PRO:HD3	1.98	0.41
1:A:269:TRP:CZ2	1:A:444:HIS:HE1	2.39	0.41
2:B:52:LYS:NZ	5:B:2041:HOH:O	2.53	0.41
1:I:422:HIS:CD2	1:I:423:PRO:HD2	2.55	0.41
1:M:356:THR:HG21	1:M:374:ASN:CB	2.51	0.41
2:N:113:LEU:CD2	2:R:113:LEU:HD23	2.50	0.41
1:S:365:GLU:CD	1:S:365:GLU:H	2.24	0.41
1:S:52:ARG:NH2	1:S:452:PRO:HB3	2.36	0.41
1:U:314:MET:HA	1:U:315:PRO:HD3	1.96	0.41
1:C:65:SER:O	1:C:68:PRO:HD3	2.21	0.41
1:E:164:ARG:HB2	1:E:175:ASN:O	2.20	0.41
2:P:126:ASP:HB3	2:P:158:ARG:HB2	2.03	0.41
2:J:36:GLN:HE21	2:P:12:PHE:H	1.68	0.41
1:Q:280:GLU:HB2	5:Q:2054:HOH:O	2.19	0.41
1:S:120:CYS:HB3	5:S:2029:HOH:O	2.20	0.41
1:S:123:HIS:HB3	1:W:232:TYR:CE1	2.56	0.41
1:A:36:ASP:HA	1:A:37:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:HIS:CE1	2:D:57:PHE:HB2	2.56	0.41
2:F:121:GLU:HB3	5:F:2090:HOH:O	2.20	0.41
1:G:164:ARG:HD2	1:G:178:VAL:HA	2.03	0.41
1:K:259:PRO:HB2	1:K:277:TYR:CE2	2.55	0.41
1:K:185:THR:HG22	1:K:459:PRO:HG2	2.02	0.41
1:K:81:ASP:OD1	1:Q:401:GLY:HA3	2.21	0.41
1:M:136:VAL:O	1:M:139:GLU:HB2	2.20	0.41
2:N:155:VAL:HB	2:N:169:LYS:HB2	2.02	0.41
1:O:42:ASP:HB3	1:O:45:LEU:HD12	2.03	0.41
2:B:169:LYS:HG2	5:E:2167:HOH:O	2.21	0.40
1:E:267:ALA:HB2	1:E:272:HIS:HB2	2.03	0.40
1:U:220:TRP:HA	1:U:350:ILE:HG21	2.01	0.40
1:U:255:GLN:O	1:U:256:ALA:C	2.58	0.40
1:C:359:ASP:HB2	1:C:362:ALA:HB2	2.02	0.40
1:G:29:ASP:OD1	1:G:32:LYS:HD2	2.21	0.40
1:I:410:ASN:HB3	1:O:102:HIS:HA	2.02	0.40
1:Q:333:LEU:O	1:Q:337:ASN:N	2.53	0.40
1:A:270:GLY:O	1:A:327:PHE:HB3	2.21	0.40
1:G:229:SER:CB	1:G:438:ALA:HB2	2.51	0.40
2:J:124:THR:HB	2:J:127:THR:HB	2.02	0.40
1:Q:322:GLN:HG2	1:Q:323:HIS:N	2.37	0.40
1:U:292:VAL:CG2	1:U:369:GLU:HB3	2.51	0.40
1:W:229:SER:HB3	1:W:438:ALA:HB2	2.02	0.40
2:B:54:ILE:HA	2:B:168:ALA:O	2.21	0.40
1:M:373:HIS:CD2	1:M:376:ARG:HE	2.39	0.40
1:U:208:ILE:HD11	1:U:358:VAL:HG13	2.03	0.40
2:D:106:PRO:HA	2:D:107:PRO:HD3	1.89	0.40
1:E:105:MET:HB3	1:E:120:CYS:SG	2.62	0.40
2:T:158:ARG:NH1	5:T:2059:HOH:O	2.54	0.40
1:U:335:ALA:HB2	5:U:2091:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/459 (94%)	417 (97%)	12 (3%)	0	100	100
1	C	429/459 (94%)	410 (96%)	19 (4%)	0	100	100
1	E	429/459 (94%)	413 (96%)	15 (4%)	1 (0%)	47	55
1	G	429/459 (94%)	407 (95%)	22 (5%)	0	100	100
1	I	429/459 (94%)	414 (96%)	14 (3%)	1 (0%)	47	55
1	K	429/459 (94%)	407 (95%)	21 (5%)	1 (0%)	47	55
1	M	429/459 (94%)	402 (94%)	26 (6%)	1 (0%)	47	55
1	O	429/459 (94%)	407 (95%)	20 (5%)	2 (0%)	29	31
1	Q	429/459 (94%)	405 (94%)	23 (5%)	1 (0%)	47	55
1	S	429/459 (94%)	412 (96%)	15 (4%)	2 (0%)	29	31
1	U	429/459 (94%)	401 (94%)	24 (6%)	4 (1%)	17	16
1	W	429/459 (94%)	396 (92%)	33 (8%)	0	100	100
2	B	181/188 (96%)	172 (95%)	9 (5%)	0	100	100
2	D	181/188 (96%)	174 (96%)	7 (4%)	0	100	100
2	F	181/188 (96%)	174 (96%)	7 (4%)	0	100	100
2	H	181/188 (96%)	174 (96%)	7 (4%)	0	100	100
2	J	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	25	26
2	L	181/188 (96%)	171 (94%)	10 (6%)	0	100	100
2	N	179/188 (95%)	173 (97%)	6 (3%)	0	100	100
2	P	181/188 (96%)	170 (94%)	9 (5%)	2 (1%)	14	12
2	R	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
2	T	179/188 (95%)	172 (96%)	6 (3%)	1 (1%)	25	26
2	V	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
2	X	179/188 (95%)	168 (94%)	11 (6%)	0	100	100
All	All	7310/7764 (94%)	6959 (95%)	334 (5%)	17 (0%)	47	55

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	8	PHE
2	P	8	PHE
1	Q	256	ALA

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Mol	Chain	Res	Type
1	M	253	LEU
1	K	445	TRP
2	P	74	SER
1	S	321	GLY
1	U	279	ASP
1	U	428	ASN
2	T	141	LEU
1	U	280	GLU
1	U	290	PRO
1	S	142	ALA
1	E	248	PRO
1	O	334	PRO
1	I	328	PRO
1	O	328	PRO

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	350/372 (94%)	340 (97%)	10 (3%)	42	54
1	C	350/372 (94%)	338 (97%)	12 (3%)	37	47
1	E	350/372 (94%)	335 (96%)	15 (4%)	29	36
1	G	350/372 (94%)	336 (96%)	14 (4%)	31	40
1	I	350/372 (94%)	339 (97%)	11 (3%)	40	51
1	K	350/372 (94%)	336 (96%)	14 (4%)	31	40
1	M	350/372 (94%)	340 (97%)	10 (3%)	42	54
1	O	350/372 (94%)	340 (97%)	10 (3%)	42	54
1	Q	350/372 (94%)	340 (97%)	10 (3%)	42	54
1	S	350/372 (94%)	340 (97%)	10 (3%)	42	54
1	U	350/372 (94%)	336 (96%)	14 (4%)	31	40
1	W	350/372 (94%)	342 (98%)	8 (2%)	50	63
2	B	162/167 (97%)	157 (97%)	5 (3%)	40	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	162/167 (97%)	154 (95%)	8 (5%)	25	31
2	F	162/167 (97%)	155 (96%)	7 (4%)	29	36
2	H	162/167 (97%)	155 (96%)	7 (4%)	29	36
2	J	162/167 (97%)	159 (98%)	3 (2%)	57	71
2	L	162/167 (97%)	157 (97%)	5 (3%)	40	51
2	N	160/167 (96%)	154 (96%)	6 (4%)	33	42
2	P	162/167 (97%)	156 (96%)	6 (4%)	34	43
2	R	160/167 (96%)	155 (97%)	5 (3%)	40	51
2	T	160/167 (96%)	155 (97%)	5 (3%)	40	51
2	V	160/167 (96%)	156 (98%)	4 (2%)	47	60
2	X	160/167 (96%)	153 (96%)	7 (4%)	28	35
All	All	6134/6468 (95%)	5928 (97%)	206 (3%)	37	47

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	VAL
1	A	94	LYS
1	A	103	ARG
1	A	122	TYR
1	A	258	ILE
1	A	280	GLU
1	A	336	MET
1	A	340	ARG
1	A	410	ASN
1	A	457	LEU
2	B	10	LYS
2	B	94	ARG
2	B	95	LYS
2	B	140	ARG
2	B	179	LEU
1	C	103	ARG
1	C	122	TYR
1	C	250	GLU
1	C	255	GLN
1	C	280	GLU
1	C	309	LEU
1	C	336	MET

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Mol	Chain	Res	Type
1	C	410	ASN
1	C	415	LEU
1	C	419	GLN
1	C	452	PRO
1	C	457	LEU
2	D	10	LYS
2	D	16	SER
2	D	94	ARG
2	D	131	ASN
2	D	140	ARG
2	D	143	ARG
2	D	160	ASP
2	D	179	LEU
1	E	48	LEU
1	E	103	ARG
1	E	122	TYR
1	E	252	ASP
1	E	261	LYS
1	E	280	GLU
1	E	307	GLN
1	E	336	MET
1	E	340	ARG
1	E	356	THR
1	E	410	ASN
1	E	415	LEU
1	E	419	GLN
1	E	453	SER
1	E	457	LEU
2	F	11	THR
2	F	16	SER
2	F	17	LYS
2	F	94	ARG
2	F	131	ASN
2	F	143	ARG
2	F	179	LEU
1	G	86	VAL
1	G	103	ARG
1	G	122	TYR
1	G	167	THR
1	G	212	GLN
1	G	250	GLU
1	G	261	LYS

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Mol	Chain	Res	Type
1	G	265	PHE
1	G	307	GLN
1	G	336	MET
1	G	340	ARG
1	G	410	ASN
1	G	419	GLN
1	G	457	LEU
2	H	10	LYS
2	H	14	TRP
2	H	16	SER
2	H	44	GLU
2	H	51	ASP
2	H	94	ARG
2	H	143	ARG
1	I	48	LEU
1	I	86	VAL
1	I	103	ARG
1	I	122	TYR
1	I	258	ILE
1	I	320	VAL
1	I	330	CYS
1	I	336	MET
1	I	410	ASN
1	I	419	GLN
1	I	457	LEU
2	J	44	GLU
2	J	140	ARG
2	J	179	LEU
1	K	48	LEU
1	K	86	VAL
1	K	100	CYS
1	K	103	ARG
1	K	122	TYR
1	K	254	SER
1	K	265	PHE
1	K	336	MET
1	K	356	THR
1	K	410	ASN
1	K	419	GLN
1	K	453	SER
1	K	457	LEU
1	K	458	LYS

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Mol	Chain	Res	Type
2	L	10	LYS
2	L	44	GLU
2	L	94	ARG
2	L	140	ARG
2	L	179	LEU
1	M	48	LEU
1	M	86	VAL
1	M	94	LYS
1	M	103	ARG
1	M	122	TYR
1	M	211	MET
1	M	252	ASP
1	M	280	GLU
1	M	336	MET
1	M	457	LEU
2	N	10	LYS
2	N	67	ARG
2	N	140	ARG
2	N	160	ASP
2	N	162	ASN
2	N	179	LEU
1	O	48	LEU
1	O	122	TYR
1	O	185	THR
1	O	212	GLN
1	O	217	PRO
1	O	307	GLN
1	O	336	MET
1	O	410	ASN
1	O	413	MET
1	O	457	LEU
2	P	7	HIS
2	P	10	LYS
2	P	44	GLU
2	P	116	ASN
2	P	140	ARG
2	P	162	ASN
1	Q	90	ASP
1	Q	103	ARG
1	Q	122	TYR
1	Q	280	GLU
1	Q	336	MET

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Mol	Chain	Res	Type
1	Q	340	ARG
1	Q	410	ASN
1	Q	419	GLN
1	Q	456	THR
1	Q	457	LEU
2	R	10	LYS
2	R	16	SER
2	R	140	ARG
2	R	143	ARG
2	R	179	LEU
1	S	94	LYS
1	S	103	ARG
1	S	122	TYR
1	S	307	GLN
1	S	336	MET
1	S	340	ARG
1	S	356	THR
1	S	419	GLN
1	S	453	SER
1	S	457	LEU
2	T	10	LYS
2	T	94	ARG
2	T	140	ARG
2	T	143	ARG
2	T	179	LEU
1	U	48	LEU
1	U	86	VAL
1	U	103	ARG
1	U	122	TYR
1	U	206	VAL
1	U	211	MET
1	U	212	GLN
1	U	226	GLN
1	U	255	GLN
1	U	320	VAL
1	U	336	MET
1	U	387	ASP
1	U	410	ASN
1	U	457	LEU
2	V	67	ARG
2	V	94	ARG
2	V	162	ASN

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Mol	Chain	Res	Type
2	V	179	LEU
1	W	122	TYR
1	W	182	ASP
1	W	255	GLN
1	W	328	PRO
1	W	336	MET
1	W	340	ARG
1	W	410	ASN
1	W	457	LEU
2	X	10	LYS
2	X	44	GLU
2	X	61	ARG
2	X	94	ARG
2	X	136	LEU
2	X	140	ARG
2	X	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	179	GLN
1	A	212	GLN
1	A	263	ASN
1	A	410	ASN
1	A	419	GLN
1	A	422	HIS
1	A	444	HIS
2	B	25	ASN
2	B	131	ASN
1	C	212	GLN
1	C	391	ASN
1	C	410	ASN
1	C	419	GLN
1	C	422	HIS
1	C	444	HIS
2	D	7	HIS
2	D	25	ASN
2	D	40	HIS
2	D	131	ASN
1	E	212	GLN
1	E	255	GLN

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Mol	Chain	Res	Type
1	E	263	ASN
1	E	311	HIS
1	E	373	HIS
1	E	391	ASN
1	E	410	ASN
1	E	419	GLN
1	E	422	HIS
1	E	444	HIS
2	F	25	ASN
2	F	40	HIS
2	F	77	GLN
2	F	131	ASN
1	G	212	GLN
1	G	373	HIS
1	G	391	ASN
1	G	410	ASN
1	G	419	GLN
1	G	422	HIS
1	G	444	HIS
2	H	40	HIS
2	H	131	ASN
1	I	179	GLN
1	I	212	GLN
1	I	263	ASN
1	I	373	HIS
1	I	391	ASN
1	I	410	ASN
1	I	419	GLN
1	I	422	HIS
1	I	444	HIS
2	J	25	ASN
2	J	36	GLN
2	J	131	ASN
1	K	212	GLN
1	K	226	GLN
1	K	307	GLN
1	K	391	ASN
1	K	410	ASN
1	K	419	GLN
1	K	422	HIS
2	L	25	ASN
2	L	36	GLN

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Mol	Chain	Res	Type
2	L	131	ASN
1	M	179	GLN
1	M	212	GLN
1	M	255	GLN
1	M	307	GLN
1	M	373	HIS
1	M	410	ASN
1	M	422	HIS
1	M	444	HIS
2	N	25	ASN
2	N	36	GLN
2	N	131	ASN
2	N	162	ASN
1	O	212	GLN
1	O	373	HIS
1	O	410	ASN
1	O	422	HIS
1	O	444	HIS
2	P	131	ASN
2	P	162	ASN
1	Q	212	GLN
1	Q	391	ASN
1	Q	410	ASN
1	Q	419	GLN
1	Q	422	HIS
1	Q	444	HIS
2	R	25	ASN
2	R	36	GLN
2	R	131	ASN
1	S	179	GLN
1	S	212	GLN
1	S	255	GLN
1	S	391	ASN
1	S	410	ASN
1	S	422	HIS
1	S	444	HIS
2	T	25	ASN
2	T	36	GLN
2	T	131	ASN
1	U	212	GLN
1	U	233	HIS
1	U	263	ASN

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Mol	Chain	Res	Type
1	U	373	HIS
1	U	386	GLN
1	U	410	ASN
1	U	419	GLN
1	U	428	ASN
1	U	444	HIS
2	V	25	ASN
2	V	36	GLN
2	V	131	ASN
2	V	162	ASN
1	W	135	ASN
1	W	212	GLN
1	W	307	GLN
1	W	391	ASN
1	W	410	ASN
1	W	422	HIS
2	X	25	ASN
2	X	36	GLN
2	X	81	HIS
2	X	131	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	$\# Z > 2$
3	FES	G	900	1	0,4,4	0.00	-	-		
3	FES	M	900	1	0,4,4	0.00	-	-		
3	FES	C	900	1	0,4,4	0.00	-	-		
3	FES	E	900	1	0,4,4	0.00	-	-		
3	FES	Q	900	1	0,4,4	0.00	-	-		
3	FES	W	900	1,5	0,4,4	0.00	-	-		
3	FES	S	900	1,5	0,4,4	0.00	-	-		
3	FES	I	900	1	0,4,4	0.00	-	-		
3	FES	O	900	1,5	0,4,4	0.00	-	-		
3	FES	U	900	1	0,4,4	0.00	-	-		
3	FES	K	900	1,5	0,4,4	0.00	-	-		
3	FES	A	900	1	0,4,4	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	G	900	1	-	-	0/1/1/1
3	FES	M	900	1	-	-	0/1/1/1
3	FES	C	900	1	-	-	0/1/1/1
3	FES	E	900	1	-	-	0/1/1/1
3	FES	Q	900	1	-	-	0/1/1/1
3	FES	W	900	1,5	-	-	0/1/1/1
3	FES	S	900	1,5	-	-	0/1/1/1
3	FES	I	900	1	-	-	0/1/1/1
3	FES	O	900	1,5	-	-	0/1/1/1
3	FES	U	900	1	-	-	0/1/1/1
3	FES	K	900	1,5	-	-	0/1/1/1
3	FES	A	900	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	900	FES	1	0
3	M	900	FES	1	0
3	C	900	FES	1	0
3	E	900	FES	1	0
3	W	900	FES	2	0
3	S	900	FES	4	0
3	O	900	FES	3	0
3	U	900	FES	1	0
3	K	900	FES	2	0
3	A	900	FES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	433/459 (94%)	-0.46	4 (0%) 84 83	-7, 10, 35, 51	18 (4%)
1	C	433/459 (94%)	-0.01	9 (2%) 63 61	3, 29, 56, 66	18 (4%)
1	E	433/459 (94%)	-0.46	7 (1%) 72 70	-11, 7, 33, 47	18 (4%)
1	G	433/459 (94%)	-0.17	13 (3%) 50 48	-3, 17, 42, 60	18 (4%)
1	I	433/459 (94%)	0.52	43 (9%) 7 6	7, 50, 89, 101	18 (4%)
1	K	433/459 (94%)	0.03	17 (3%) 39 37	12, 29, 54, 99	18 (4%)
1	M	433/459 (94%)	0.63	52 (12%) 4 3	17, 47, 83, 92	18 (4%)
1	O	433/459 (94%)	0.48	28 (6%) 18 17	20, 49, 71, 100	18 (4%)
1	Q	433/459 (94%)	1.00	62 (14%) 2 2	37, 64, 92, 108	18 (4%)
1	S	433/459 (94%)	0.64	46 (10%) 6 5	15, 48, 80, 113	18 (4%)
1	U	433/459 (94%)	2.11	192 (44%) 0 0	43, 88, 126, 135	18 (4%)
1	W	433/459 (94%)	2.83	280 (64%) 0 0	71, 111, 142, 155	18 (4%)
2	B	183/188 (97%)	-0.62	2 (1%) 80 79	-12, -2, 16, 28	4 (2%)
2	D	183/188 (97%)	-0.61	2 (1%) 80 79	-12, 2, 28, 40	4 (2%)
2	F	183/188 (97%)	-0.61	1 (0%) 91 90	-16, -5, 19, 32	4 (2%)
2	H	183/188 (97%)	-0.53	4 (2%) 62 59	-15, -4, 33, 48	4 (2%)
2	J	183/188 (97%)	-0.02	8 (4%) 34 32	1, 22, 47, 58	4 (2%)
2	L	183/188 (97%)	-0.46	5 (2%) 54 52	3, 12, 33, 52	4 (2%)
2	N	181/188 (96%)	-0.16	4 (2%) 62 59	8, 25, 40, 46	4 (2%)
2	P	183/188 (97%)	-0.16	10 (5%) 25 24	-11, 12, 45, 67	4 (2%)
2	R	181/188 (96%)	-0.41	3 (1%) 70 68	7, 22, 41, 53	4 (2%)
2	T	181/188 (96%)	-0.34	2 (1%) 80 79	5, 20, 49, 75	4 (2%)
2	V	181/188 (96%)	0.51	9 (4%) 28 27	25, 50, 81, 99	4 (2%)
2	X	181/188 (96%)	1.04	30 (16%) 1 1	42, 69, 103, 117	4 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7382/7764 (95%)	0.36	833 (11%) 5 4	-16, 33, 105, 155	264 (3%)

All (833) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	256	ALA	8.0
1	U	421	GLY	7.9
1	W	429	VAL	7.7
1	U	321	GLY	7.6
1	W	333	LEU	7.6
1	U	259	PRO	7.5
1	U	273	GLY	7.4
1	W	332	PHE	7.3
1	W	227	PHE	7.0
1	W	105	MET	6.9
1	W	207	ALA	6.9
1	U	260	THR	6.9
1	W	153	PHE	6.8
1	U	301	ALA	6.8
1	U	332	PHE	6.7
1	W	193	TYR	6.7
1	W	339	ILE	6.7
1	W	419	GLN	6.6
1	U	416	GLY	6.6
1	Q	456	THR	6.6
1	W	113	GLY	6.5
1	W	317	ARG	6.4
1	U	324	MET	6.4
1	U	330	CYS	6.4
1	U	105	MET	6.3
1	U	437	ALA	6.3
1	W	442	TYR	6.2
1	W	334	PRO	6.2
1	U	322	GLN	6.2
1	W	228	CYS	6.2
1	U	378	PHE	6.1
1	U	228	CYS	6.1
1	U	227	PHE	6.1
1	W	355	PHE	6.1
1	U	326	ILE	6.0
2	X	8	PHE	6.0
1	W	296	TRP	5.9

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Mol	Chain	Res	Type	RSRZ
1	E	256	ALA	5.9
1	W	341	ILE	5.9
1	W	322	GLN	5.8
1	W	337	ASN	5.8
1	W	253	LEU	5.7
1	U	323	HIS	5.7
1	W	431	TYR	5.7
1	W	100	CYS	5.7
2	N	8	PHE	5.7
1	W	384	PHE	5.7
1	W	103	ARG	5.7
1	W	335	ALA	5.6
1	U	224	ALA	5.6
1	W	331	SER	5.6
1	U	253	LEU	5.6
1	W	273	GLY	5.5
1	U	274	SER	5.5
1	W	109	ARG	5.5
2	J	6	PRO	5.5
1	U	415	LEU	5.5
2	J	8	PHE	5.5
1	U	289	GLY	5.5
1	W	285	LEU	5.5
1	M	257	GLN	5.4
1	W	194	MET	5.4
1	W	154	ASP	5.4
1	W	338	ASN	5.4
1	W	183	LEU	5.4
1	W	261	LYS	5.4
1	U	35	LEU	5.4
1	W	324	MET	5.4
1	U	438	ALA	5.3
1	U	339	ILE	5.3
1	W	143	PHE	5.3
1	W	425	PHE	5.3
1	W	122	TYR	5.3
1	W	258	ILE	5.3
1	W	107	ILE	5.3
1	M	261	LYS	5.2
1	W	420	THR	5.2
1	W	86	VAL	5.2
1	W	357	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	U	409	LEU	5.1
1	S	122	TYR	5.1
1	O	105	MET	5.1
1	U	325	THR	5.1
2	X	77	GLN	5.1
1	Q	455	ALA	5.1
1	W	197	MET	5.1
1	W	74	LEU	5.1
1	W	354	ALA	5.0
1	U	333	LEU	5.0
1	W	198	LEU	5.0
1	U	364	ALA	5.0
1	W	356	THR	5.0
2	J	160	ASP	5.0
1	U	334	PRO	5.0
1	W	58	TRP	5.0
2	L	6	PRO	4.9
1	U	320	VAL	4.9
1	U	456	THR	4.9
1	W	325	THR	4.9
1	S	105	MET	4.9
1	W	156	ALA	4.9
1	U	406	SER	4.9
1	Q	257	GLN	4.9
1	W	200	ARG	4.8
1	M	18	ASN	4.8
1	W	320	VAL	4.8
1	W	430	GLY	4.8
1	W	203	ALA	4.8
1	U	275	GLY	4.8
1	U	337	ASN	4.8
1	W	257	GLN	4.8
1	W	414	GLY	4.8
1	U	331	SER	4.8
1	W	106	ARG	4.8
1	W	409	LEU	4.8
1	W	104	GLY	4.8
1	U	178	VAL	4.8
1	U	257	GLN	4.7
1	S	109	ARG	4.7
1	W	93	ILE	4.7
1	W	118	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	W	160	PRO	4.7
1	Q	258	ILE	4.7
1	W	224	ALA	4.7
1	W	336	MET	4.6
1	W	316	VAL	4.6
2	X	58	MET	4.6
1	W	268	ALA	4.6
1	W	226	GLN	4.6
1	M	256	ALA	4.5
1	U	32	LYS	4.5
1	W	410	ASN	4.5
1	G	257	GLN	4.5
2	P	16	SER	4.5
1	W	76	THR	4.5
1	W	311	HIS	4.5
1	W	330	CYS	4.5
1	W	84	VAL	4.5
2	H	14	TRP	4.5
2	J	162	ASN	4.5
1	W	59	LEU	4.5
1	W	125	TRP	4.5
1	W	176	TRP	4.5
1	W	375	ILE	4.5
1	Q	190	ALA	4.4
1	W	97	LEU	4.4
1	U	277	TYR	4.4
1	S	107	ILE	4.4
1	U	40	TYR	4.4
1	U	314	MET	4.4
1	U	258	ILE	4.4
1	U	197	MET	4.4
1	U	231	MET	4.4
1	M	254	SER	4.4
1	W	124	GLY	4.4
1	M	258	ILE	4.4
1	M	313	GLY	4.3
2	X	71	LEU	4.3
1	W	95	VAL	4.3
1	Q	22	GLU	4.3
1	W	294	GLN	4.3
1	W	459	PRO	4.3
1	W	99	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	S	89	LYS	4.3
1	W	374	ASN	4.3
1	W	309	LEU	4.3
1	U	296	TRP	4.3
1	W	48	LEU	4.3
1	W	212	GLN	4.2
1	W	142	ALA	4.2
1	W	270	GLY	4.2
1	W	378	PHE	4.2
1	W	274	SER	4.2
1	K	153	PHE	4.2
1	U	229	SER	4.2
1	W	353	TRP	4.2
1	U	341	ILE	4.2
1	W	186	TYR	4.2
1	I	18	ASN	4.2
1	U	271	GLY	4.1
1	O	109	ARG	4.1
1	W	256	ALA	4.1
1	I	260	THR	4.1
1	W	423	PRO	4.1
1	W	340	ARG	4.1
1	W	61	LEU	4.1
1	W	123	HIS	4.1
1	W	206	VAL	4.1
1	W	326	ILE	4.1
1	W	275	GLY	4.1
1	W	250	GLU	4.0
1	M	310	GLY	4.0
1	W	60	LEU	4.0
1	U	335	ALA	4.0
1	U	315	PRO	4.0
1	M	421	GLY	4.0
1	U	18	ASN	4.0
1	K	455	ALA	4.0
1	U	256	ALA	4.0
1	U	425	PHE	4.0
1	Q	260	THR	4.0
2	R	8	PHE	4.0
1	W	108	CYS	4.0
1	W	238	THR	4.0
1	U	28	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	W	120	CYS	3.9
1	U	263	ASN	3.9
1	W	286	ALA	3.9
1	W	438	ALA	3.9
1	U	327	PHE	3.9
1	C	18	ASN	3.9
1	Q	105	MET	3.9
2	X	76	ASP	3.9
1	W	370	TYR	3.9
1	I	256	ALA	3.9
1	M	260	THR	3.8
1	W	456	THR	3.8
1	U	264	GLN	3.8
1	W	158	TRP	3.8
2	P	7	HIS	3.8
1	U	20	THR	3.8
1	W	177	ASP	3.8
1	M	19	TRP	3.8
1	U	58	TRP	3.8
1	U	287	VAL	3.8
1	W	75	ALA	3.8
1	O	70	THR	3.8
1	W	161	LEU	3.8
1	W	83	VAL	3.8
2	D	14	TRP	3.8
1	W	255	GLN	3.8
1	Q	109	ARG	3.8
1	S	103	ARG	3.8
1	U	329	THR	3.8
1	M	423	PRO	3.8
1	M	282	GLY	3.8
1	U	39	ILE	3.7
1	K	109	ARG	3.7
1	U	393	VAL	3.7
1	U	419	GLN	3.7
1	W	440	GLY	3.7
1	W	323	HIS	3.7
1	Q	253	LEU	3.7
1	W	321	GLY	3.7
1	W	91	LYS	3.7
1	O	143	PHE	3.7
1	U	442	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	W	287	VAL	3.7
1	W	319	MET	3.7
1	U	452	PRO	3.7
1	S	416	GLY	3.7
1	W	98	ASN	3.7
1	W	31	GLU	3.7
1	Q	335	ALA	3.7
1	W	89	LYS	3.7
1	U	384	PHE	3.7
1	C	258	ILE	3.7
1	W	452	PRO	3.6
1	E	257	GLN	3.6
1	W	327	PHE	3.6
1	W	314	MET	3.6
1	M	253	LEU	3.6
1	W	110	SER	3.6
1	W	209	GLY	3.6
1	Q	35	LEU	3.6
1	U	269	TRP	3.6
1	U	457	LEU	3.6
1	W	18	ASN	3.6
1	W	132	LYS	3.6
1	U	311	HIS	3.6
1	U	19	TRP	3.6
1	M	324	MET	3.6
1	U	288	MET	3.6
1	W	230	ASP	3.6
1	U	392	TRP	3.6
1	M	332	PHE	3.5
1	U	223	ALA	3.5
1	S	140	LYS	3.5
1	U	230	ASP	3.5
1	Q	143	PHE	3.5
1	W	129	ILE	3.5
1	I	20	THR	3.5
1	U	234	ALA	3.5
1	U	316	VAL	3.5
1	U	423	PRO	3.5
1	W	217	PRO	3.5
1	W	358	VAL	3.5
1	W	301	ALA	3.5
1	W	241	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	W	67	VAL	3.5
1	U	276	TRP	3.5
1	U	355	PHE	3.5
1	U	22	GLU	3.5
1	W	66	HIS	3.5
1	W	85	MET	3.4
1	U	357	LEU	3.4
2	X	113	LEU	3.4
2	X	10	LYS	3.4
1	S	104	GLY	3.4
1	W	231	MET	3.4
1	Q	203	ALA	3.4
2	L	67	ARG	3.4
1	W	288	MET	3.4
2	J	7	HIS	3.4
1	E	254	SER	3.4
1	I	333	LEU	3.4
1	K	138	PHE	3.4
1	U	215	VAL	3.4
1	U	292	VAL	3.4
1	W	116	LYS	3.4
1	W	40	TYR	3.4
1	U	363	PRO	3.4
1	W	73	PHE	3.4
1	C	259	PRO	3.4
1	M	271	GLY	3.4
1	S	121	SER	3.4
2	V	16	SER	3.4
1	U	27	LEU	3.4
2	T	8	PHE	3.4
1	U	417	ARG	3.3
1	G	258	ILE	3.3
1	S	311	HIS	3.3
2	X	67	ARG	3.3
1	U	312	THR	3.3
1	W	377	ASN	3.3
1	W	411	ALA	3.3
1	U	297	THR	3.3
1	U	420	THR	3.3
1	U	455	ALA	3.3
2	X	160	ASP	3.3
1	W	448	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	W	94	LYS	3.3
1	M	311	HIS	3.3
1	S	137	PRO	3.3
1	W	329	THR	3.3
1	U	23	ALA	3.3
1	W	202	PRO	3.3
2	H	6	PRO	3.3
1	Q	251	MET	3.3
1	W	102	HIS	3.3
1	G	259	PRO	3.3
2	V	188	PHE	3.2
1	W	213	LYS	3.2
1	W	432	VAL	3.2
1	W	416	GLY	3.2
1	U	443	HIS	3.2
1	S	332	PHE	3.2
1	I	257	GLN	3.2
1	I	253	LEU	3.2
1	U	441	MET	3.2
1	U	391	ASN	3.2
1	W	445	TRP	3.2
1	O	261	LYS	3.2
1	Q	254	SER	3.2
1	S	23	ALA	3.2
1	W	305	ALA	3.2
1	U	104	GLY	3.2
1	S	155	LYS	3.2
1	W	136	VAL	3.2
1	M	306	GLU	3.2
1	U	340	ARG	3.2
1	W	211	MET	3.2
1	W	372	ARG	3.2
1	Q	339	ILE	3.1
1	U	272	HIS	3.1
1	W	392	TRP	3.1
1	U	338	ASN	3.1
1	G	261	LYS	3.1
1	U	358	VAL	3.1
1	O	416	GLY	3.1
1	I	423	PRO	3.1
1	W	310	GLY	3.1
1	U	233	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
2	V	113	LEU	3.1
1	O	18	ASN	3.1
1	G	153	PHE	3.1
1	S	455	ALA	3.1
1	W	376	ARG	3.1
1	G	254	SER	3.1
1	M	105	MET	3.1
1	W	251	MET	3.1
2	X	79	LEU	3.1
1	W	39	ILE	3.1
1	M	227	PHE	3.1
1	U	265	PHE	3.1
1	U	84	VAL	3.1
1	U	59	LEU	3.1
1	U	60	LEU	3.1
1	W	34	LEU	3.1
1	O	156	ALA	3.1
2	X	117	VAL	3.0
1	C	257	GLN	3.0
1	U	232	TYR	3.0
1	I	19	TRP	3.0
1	Q	281	PRO	3.0
2	P	6	PRO	3.0
1	W	291	LYS	3.0
1	I	410	ASN	3.0
1	U	62	GLY	3.0
1	U	336	MET	3.0
1	E	261	LYS	3.0
1	S	156	ALA	3.0
2	L	8	PHE	3.0
1	K	134	VAL	3.0
1	W	82	PRO	3.0
1	U	240	LEU	3.0
1	W	415	LEU	3.0
1	W	422	HIS	3.0
1	O	364	ALA	3.0
1	U	434	ALA	3.0
1	I	332	PHE	3.0
1	U	74	LEU	3.0
1	Q	422	HIS	3.0
1	U	109	ARG	3.0
1	W	437	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	U	194	MET	3.0
1	U	25	ARG	3.0
1	K	256	ALA	3.0
1	Q	375	ILE	3.0
1	W	165	VAL	3.0
1	Q	410	ASN	3.0
1	W	386	GLN	2.9
1	U	107	ILE	2.9
1	W	208	ILE	2.9
1	M	323	HIS	2.9
1	W	210	GLY	2.9
1	W	280	GLU	2.9
2	X	102	TRP	2.9
1	I	336	MET	2.9
1	W	205	THR	2.9
2	V	160	ASP	2.9
1	W	254	SER	2.9
2	X	133	ALA	2.9
1	U	373	HIS	2.9
1	U	318	ARG	2.9
2	T	67	ARG	2.9
1	Q	255	GLN	2.9
1	U	411	ALA	2.9
1	W	155	LYS	2.9
1	K	311	HIS	2.9
1	U	328	PRO	2.9
1	W	64	GLU	2.9
1	W	281	PRO	2.9
2	H	160	ASP	2.9
1	U	375	ILE	2.9
1	I	227	PHE	2.9
1	K	453	SER	2.9
1	K	310	GLY	2.9
1	U	448	MET	2.9
1	Q	334	PRO	2.9
1	M	339	ILE	2.8
1	M	419	GLN	2.8
1	U	284	LEU	2.8
1	W	302	ALA	2.8
1	W	19	TRP	2.8
1	W	276	TRP	2.8
1	W	140	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	103	ARG	2.8
1	O	115	ALA	2.8
1	S	108	CYS	2.8
1	K	423	PRO	2.8
1	U	226	GLN	2.8
1	W	178	VAL	2.8
1	U	305	ALA	2.8
1	I	259	PRO	2.8
1	Q	259	PRO	2.8
1	U	309	LEU	2.8
1	W	307	GLN	2.8
1	Q	337	ASN	2.8
1	I	312	THR	2.8
1	I	318	ARG	2.8
1	W	225	GLU	2.8
1	U	307	GLN	2.8
1	W	96	PHE	2.8
1	O	335	ALA	2.8
1	W	192	PRO	2.8
2	X	162	ASN	2.8
1	W	382	GLY	2.8
1	W	252	ASP	2.8
1	W	395	ILE	2.8
2	X	188	PHE	2.8
1	W	112	ALA	2.8
1	Q	252	ASP	2.8
1	Q	333	LEU	2.8
1	S	324	MET	2.8
1	U	221	LYS	2.8
1	W	199	ASP	2.7
1	W	393	VAL	2.7
1	M	331	SER	2.7
1	M	333	LEU	2.7
1	W	171	LEU	2.7
1	S	102	HIS	2.7
2	X	66	ILE	2.7
1	U	290	PRO	2.7
1	S	256	ALA	2.7
1	C	179	GLN	2.7
1	W	134	VAL	2.7
1	K	105	MET	2.7
1	M	456	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	W	70	THR	2.7
1	U	454	TRP	2.7
2	N	160	ASP	2.7
1	U	395	ILE	2.7
1	M	202	PRO	2.7
1	W	390	GLU	2.7
1	W	308	ARG	2.7
1	Q	324	MET	2.7
1	U	176	TRP	2.7
1	W	260	THR	2.7
1	Q	430	GLY	2.7
2	X	115	SER	2.7
1	U	267	ALA	2.7
1	U	83	VAL	2.7
1	W	35	LEU	2.7
1	K	273	GLY	2.7
1	W	57	SER	2.7
1	I	455	ALA	2.7
1	U	90	ASP	2.7
1	W	298	GLU	2.7
1	W	367	LYS	2.7
1	M	327	PHE	2.7
1	U	97	LEU	2.7
1	W	229	SER	2.6
1	W	32	LYS	2.6
1	U	203	ALA	2.6
1	M	325	THR	2.6
1	M	321	GLY	2.6
1	Q	198	LEU	2.6
1	Q	332	PHE	2.6
1	U	222	PHE	2.6
1	W	399	LEU	2.6
1	W	441	MET	2.6
1	M	22	GLU	2.6
1	W	418	SER	2.6
1	S	90	ASP	2.6
1	U	424	ASP	2.6
1	W	81	ASP	2.6
1	W	259	PRO	2.6
1	W	391	ASN	2.6
2	F	14	TRP	2.6
1	Q	224	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	U	196	VAL	2.6
1	W	54	PHE	2.6
1	W	265	PHE	2.6
1	W	283	SER	2.6
1	W	220	TRP	2.6
1	U	261	LYS	2.6
1	U	183	LEU	2.6
1	U	370	TYR	2.6
1	W	127	TYR	2.6
1	W	352	VAL	2.6
2	X	114	VAL	2.6
1	O	123	HIS	2.6
1	I	339	ILE	2.6
1	O	158	TRP	2.6
1	W	342	TRP	2.6
1	G	18	ASN	2.6
1	O	110	SER	2.6
2	P	162	ASN	2.6
1	W	68	PRO	2.6
1	W	78	MET	2.6
1	W	413	MET	2.6
2	X	82	PHE	2.6
1	S	38	ARG	2.6
1	Q	302	ALA	2.6
1	W	30	GLN	2.6
1	Q	182	ASP	2.6
1	O	310	GLY	2.6
1	U	440	GLY	2.6
2	X	69	GLY	2.6
1	M	20	THR	2.5
1	S	325	THR	2.5
1	W	101	ARG	2.5
2	B	6	PRO	2.5
1	W	262	GLY	2.5
1	W	271	GLY	2.5
1	M	455	ALA	2.5
1	U	418	SER	2.5
1	W	363	PRO	2.5
1	W	279	ASP	2.5
1	W	222	PHE	2.5
1	O	120	CYS	2.5
1	K	135	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	122	TYR	2.5
1	Q	193	TYR	2.5
1	U	193	TYR	2.5
1	S	339	ILE	2.5
1	U	167	THR	2.5
1	U	294	GLN	2.5
1	W	249	PRO	2.5
1	W	240	LEU	2.5
1	C	254	SER	2.5
1	M	228	CYS	2.5
1	U	110	SER	2.5
1	U	404	ALA	2.5
1	U	225	GLU	2.5
1	W	121	SER	2.5
2	X	44	GLU	2.5
1	U	179	GLN	2.5
1	W	167	THR	2.5
1	W	315	PRO	2.5
1	S	83	VAL	2.5
1	W	435	GLU	2.5
1	K	89	LYS	2.5
1	S	117	ALA	2.5
2	V	32	TYR	2.5
1	U	185	THR	2.5
1	A	258	ILE	2.5
1	I	197	MET	2.5
1	S	118	PHE	2.5
1	U	388	ASP	2.5
1	U	432	VAL	2.5
2	P	74	SER	2.5
1	W	52	ARG	2.5
2	B	7	HIS	2.5
1	A	105	MET	2.4
1	I	229	SER	2.4
1	U	379	SER	2.4
1	U	38	ARG	2.4
1	W	436	GLU	2.4
1	Q	341	ILE	2.4
1	G	252	ASP	2.4
1	U	171	LEU	2.4
1	M	437	ALA	2.4
2	H	162	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	U	181	PRO	2.4
1	W	272	HIS	2.4
1	W	297	THR	2.4
1	Q	365	GLU	2.4
1	S	258	ILE	2.4
1	U	439	ARG	2.4
1	I	283	SER	2.4
1	W	284	LEU	2.4
1	I	273	GLY	2.4
1	Q	58	TRP	2.4
1	U	445	TRP	2.4
1	U	453	SER	2.4
1	A	419	GLN	2.4
1	M	415	LEU	2.4
1	E	22	GLU	2.4
1	Q	197	MET	2.4
1	I	311	HIS	2.4
1	W	190	ALA	2.4
1	C	261	LYS	2.4
2	P	8	PHE	2.4
1	U	283	SER	2.4
1	U	402	TYR	2.4
1	U	450	SER	2.4
1	O	198	LEU	2.4
1	G	251	MET	2.4
1	I	324	MET	2.4
1	M	305	ALA	2.4
1	I	254	SER	2.4
1	W	214	TRP	2.4
1	M	416	GLY	2.4
1	W	235	GLY	2.4
1	W	361	ASP	2.4
2	L	7	HIS	2.4
1	Q	21	PRO	2.4
1	U	302	ALA	2.4
1	U	280	GLU	2.4
1	S	228	CYS	2.4
1	W	221	LYS	2.3
1	W	164	ARG	2.3
1	W	387	ASP	2.3
1	M	224	ALA	2.3
1	M	259	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	W	21	PRO	2.3
1	W	328	PRO	2.3
1	I	416	GLY	2.3
1	W	346	GLY	2.3
1	O	334	PRO	2.3
1	S	334	PRO	2.3
1	Q	156	ALA	2.3
1	U	34	LEU	2.3
1	W	364	ALA	2.3
1	W	65	SER	2.3
2	N	16	SER	2.3
1	U	173	PHE	2.3
1	U	444	HIS	2.3
1	S	100	CYS	2.3
1	U	61	LEU	2.3
1	U	168	TYR	2.3
1	U	186	TYR	2.3
1	W	50	LEU	2.3
1	W	117	ALA	2.3
1	W	223	ALA	2.3
2	X	90	TYR	2.3
2	X	134	PHE	2.3
1	M	179	GLN	2.3
1	Q	415	LEU	2.3
1	I	274	SER	2.3
1	W	295	TYR	2.3
1	U	413	MET	2.3
1	I	255	GLN	2.3
1	W	421	GLY	2.3
1	M	335	ALA	2.3
1	O	457	LEU	2.3
1	W	433	TYR	2.3
1	Q	104	GLY	2.3
1	U	31	GLU	2.3
1	U	353	TRP	2.3
1	O	21	PRO	2.3
1	O	423	PRO	2.3
1	M	322	GLN	2.3
1	Q	331	SER	2.3
1	U	190	ALA	2.3
2	V	133	ALA	2.3
1	Q	325	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	457	LEU	2.2
1	M	431	TYR	2.2
2	X	32	TYR	2.2
1	W	263	ASN	2.2
1	G	138	PHE	2.2
1	Q	192	PRO	2.2
2	X	125	PRO	2.2
1	M	229	SER	2.2
1	I	326	ILE	2.2
2	X	87	GLU	2.2
1	S	275	GLY	2.2
1	U	70	THR	2.2
2	P	67	ARG	2.2
1	M	197	MET	2.2
1	Q	336	MET	2.2
2	X	31	TYR	2.2
1	K	91	LYS	2.2
1	M	32	LYS	2.2
1	Q	185	THR	2.2
1	S	310	GLY	2.2
1	U	354	ALA	2.2
2	J	123	ALA	2.2
2	V	35	ALA	2.2
1	I	419	GLN	2.2
1	O	100	CYS	2.2
1	Q	229	SER	2.2
2	N	9	PHE	2.2
1	U	381	GLY	2.2
1	O	456	THR	2.2
1	U	205	THR	2.2
2	R	160	ASP	2.2
1	I	35	LEU	2.2
1	I	32	LYS	2.2
1	O	259	PRO	2.2
1	U	77	TYR	2.2
1	W	290	PRO	2.2
1	M	178	VAL	2.2
2	L	16	SER	2.2
1	I	421	GLY	2.2
1	I	424	ASP	2.2
1	Q	153	PHE	2.2
1	W	239	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	W	380	ALA	2.2
2	X	172	ILE	2.2
1	E	251	MET	2.2
1	W	137	PRO	2.2
1	U	33	GLY	2.2
1	W	62	GLY	2.2
1	W	242	GLY	2.2
2	P	160	ASP	2.2
1	K	143	PHE	2.2
1	Q	227	PHE	2.2
1	S	257	GLN	2.2
1	C	311	HIS	2.2
2	R	67	ARG	2.2
1	I	322	GLN	2.2
1	I	437	ALA	2.1
1	M	411	ALA	2.1
1	O	455	ALA	2.1
1	W	234	ALA	2.1
1	S	120	CYS	2.1
1	W	187	LEU	2.1
1	W	195	ASP	2.1
1	Q	283	SER	2.1
1	S	255	GLN	2.1
1	I	337	ASN	2.1
2	J	67	ARG	2.1
1	A	256	ALA	2.1
1	W	119	THR	2.1
1	I	33	GLY	2.1
1	U	103	ARG	2.1
1	K	454	TRP	2.1
1	W	277	TYR	2.1
1	Q	222	PHE	2.1
1	W	424	ASP	2.1
1	I	418	SER	2.1
1	Q	275	GLY	2.1
1	S	139	GLU	2.1
1	W	426	PRO	2.1
1	M	286	ALA	2.1
1	S	312	THR	2.1
1	U	295	TYR	2.1
1	S	227	PHE	2.1
1	I	323	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	420	THR	2.1
1	E	18	ASN	2.1
1	Q	438	ALA	2.1
2	V	162	ASN	2.1
1	W	427	GLY	2.1
1	W	300	PRO	2.1
1	C	424	ASP	2.1
2	D	160	ASP	2.1
1	G	105	MET	2.1
1	I	420	THR	2.1
2	J	17	LYS	2.1
2	P	10	LYS	2.1
2	X	122	THR	2.1
1	S	41	ALA	2.1
2	P	18	ALA	2.1
1	I	432	VAL	2.1
1	S	21	PRO	2.1
1	Q	69	GLU	2.0
1	S	326	ILE	2.0
1	Q	140	LYS	2.0
1	S	260	THR	2.0
1	Q	273	GLY	2.0
1	O	422	HIS	2.0
1	S	417	ARG	2.0
2	V	58	MET	2.0
2	X	70	GLU	2.0
1	U	255	GLN	2.0
1	U	282	GLY	2.0
1	U	414	GLY	2.0
1	W	55	GLY	2.0
1	U	268	ALA	2.0
1	W	179	GLN	2.0
1	S	106	ARG	2.0
1	Q	186	TYR	2.0
1	I	228	CYS	2.0
1	Q	409	LEU	2.0
1	U	285	LEU	2.0
1	Q	322	GLN	2.0
1	U	446	MET	2.0
1	G	420	THR	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FE2	U	901	1/1	0.84	0.27	67,67,67,67	0
3	FES	W	900	4/4	0.91	0.10	65,67,68,69	0
3	FES	S	900	4/4	0.93	0.09	48,48,50,50	0
3	FES	O	900	4/4	0.94	0.06	41,42,43,43	0
4	FE2	Q	901	1/1	0.94	0.08	45,45,45,45	0
4	FE2	I	901	1/1	0.95	0.13	48,48,48,48	0
3	FES	U	900	4/4	0.96	0.07	21,23,23,27	0
3	FES	K	900	4/4	0.96	0.06	32,33,34,35	0
3	FES	G	900	4/4	0.97	0.10	25,26,26,27	0
4	FE2	W	901	1/1	0.97	0.08	57,57,57,57	0
3	FES	A	900	4/4	0.97	0.09	19,20,22,22	0
3	FES	Q	900	4/4	0.97	0.07	31,32,37,37	0
4	FE2	O	901	1/1	0.97	0.15	32,32,32,32	0
4	FE2	S	901	1/1	0.97	0.10	26,26,26,26	0
3	FES	E	900	4/4	0.98	0.10	13,13,14,15	0
4	FE2	M	901	1/1	0.98	0.08	37,37,37,37	0
3	FES	M	900	4/4	0.98	0.09	21,21,21,21	0
3	FES	I	900	4/4	0.98	0.10	14,15,15,17	0
3	FES	C	900	4/4	0.99	0.10	17,18,19,19	0
4	FE2	K	901	1/1	0.99	0.14	19,19,19,19	0
4	FE2	A	901	1/1	0.99	0.14	13,13,13,13	0
4	FE2	C	901	1/1	0.99	0.14	29,29,29,29	0
4	FE2	E	901	1/1	0.99	0.12	20,20,20,20	0
4	FE2	G	901	1/1	0.99	0.14	14,14,14,14	0

6.5 Other polymers

There are no such residues in this entry.