



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:52 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

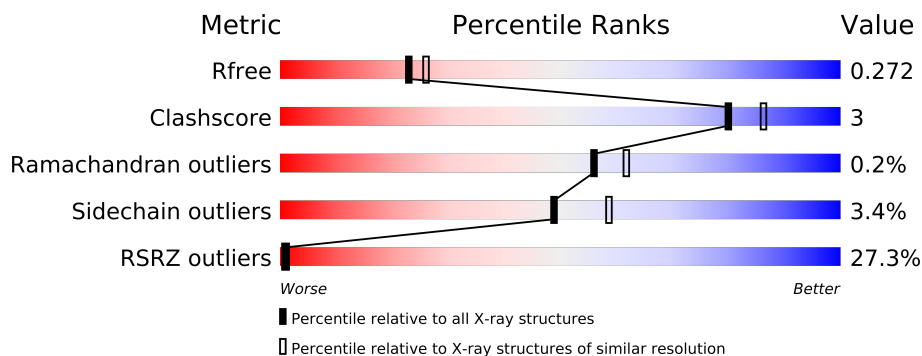
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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.












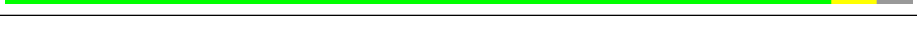
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	459	
1	C	459	
1	E	459	
1	G	459	
1	I	459	
1	K	459	
1	M	459	
1	O	459	
1	Q	459	
1	S	459	
1	U	459	
1	W	459	
2	B	188	
2	D	188	

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Mol	Chain	Length	Quality of chain
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	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 61911 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

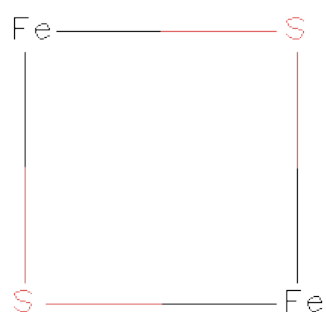
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	D	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	F	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	H	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	J	183	Total	C	N	O	S	0	0	0
			1524	968	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: Fe_2S_2).



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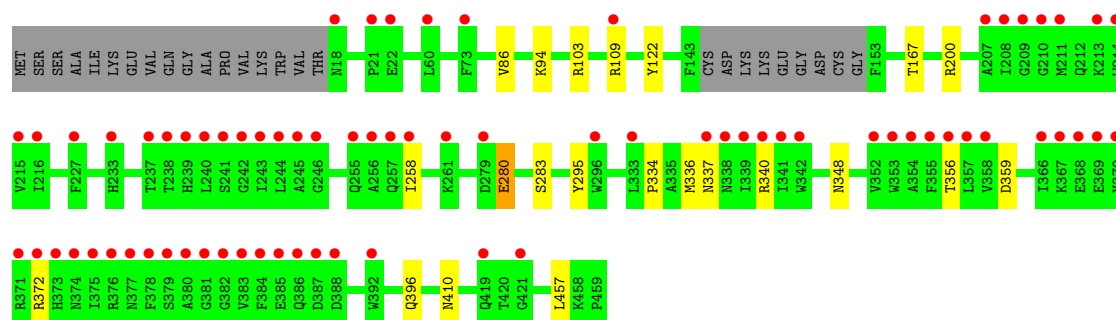
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	37	Total	O	0	0
			37	37		

3 Residue-property plots

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

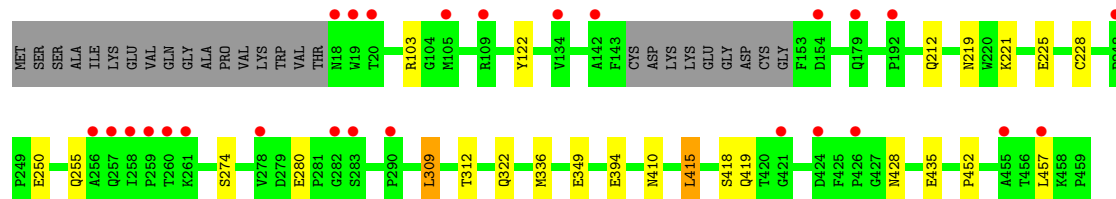
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain A: 



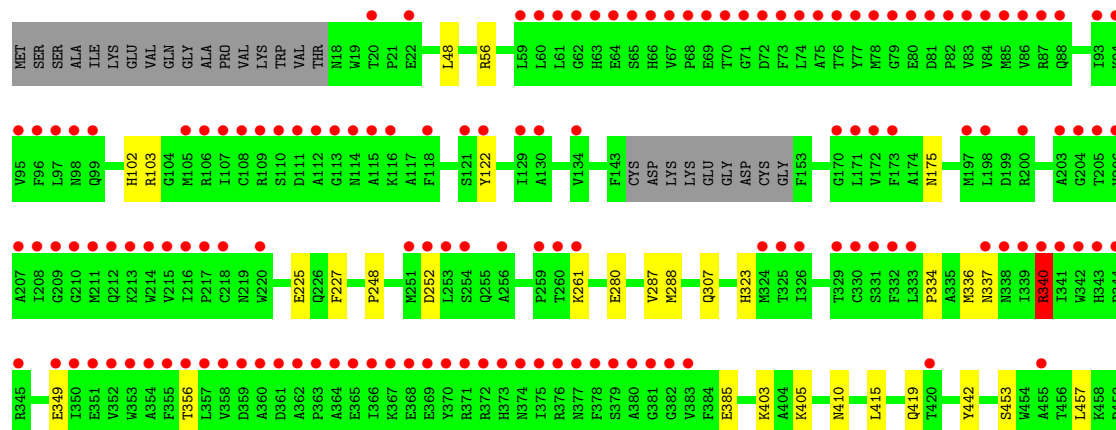
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain C: 



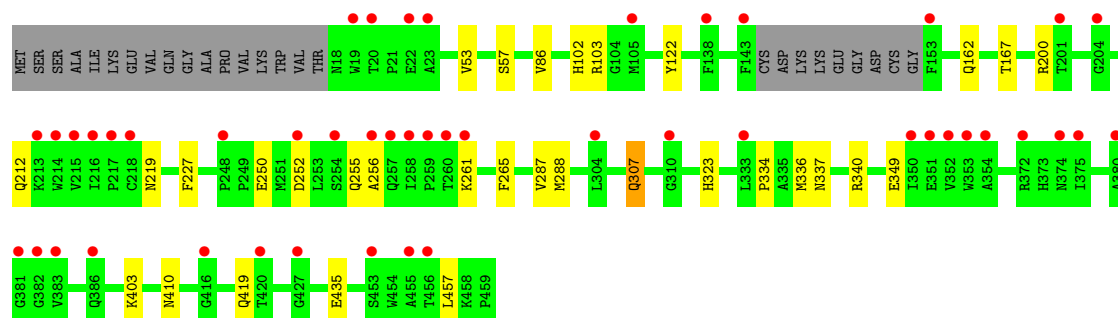
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain E: 



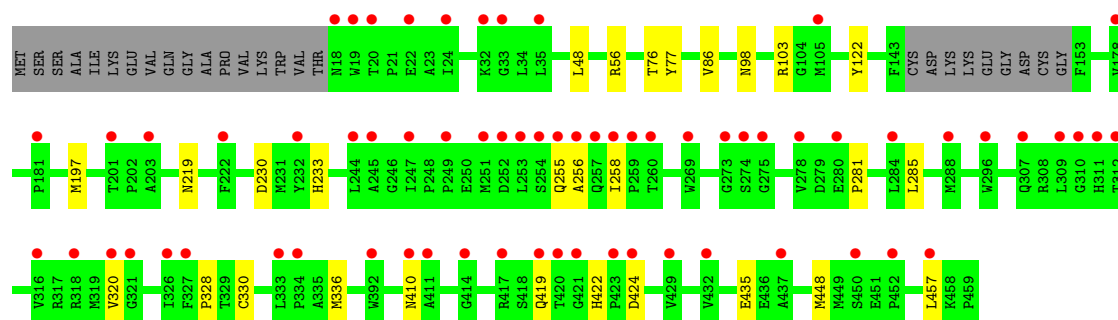
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain G:



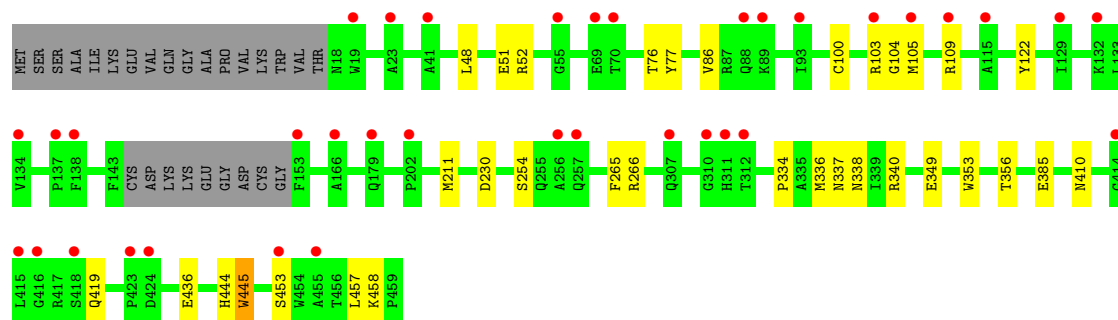
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain I:



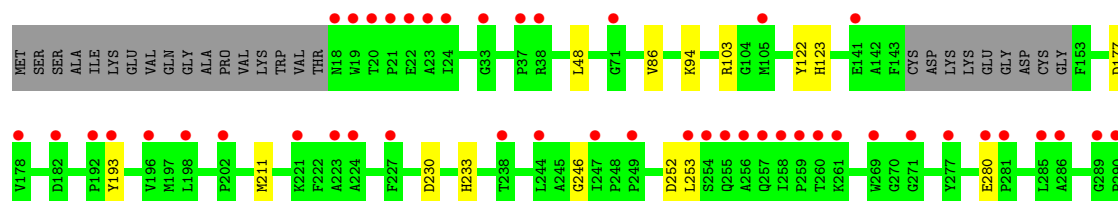
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

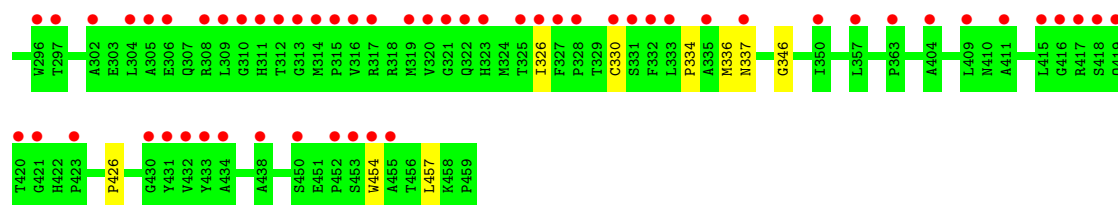
Chain K:



- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

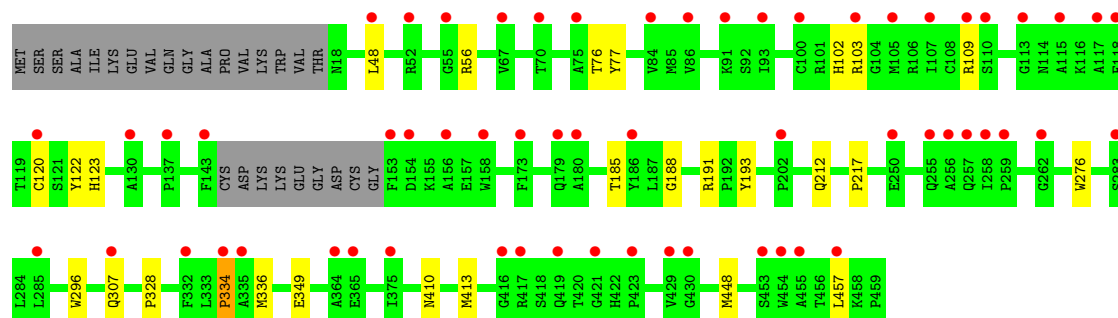
Chain M:





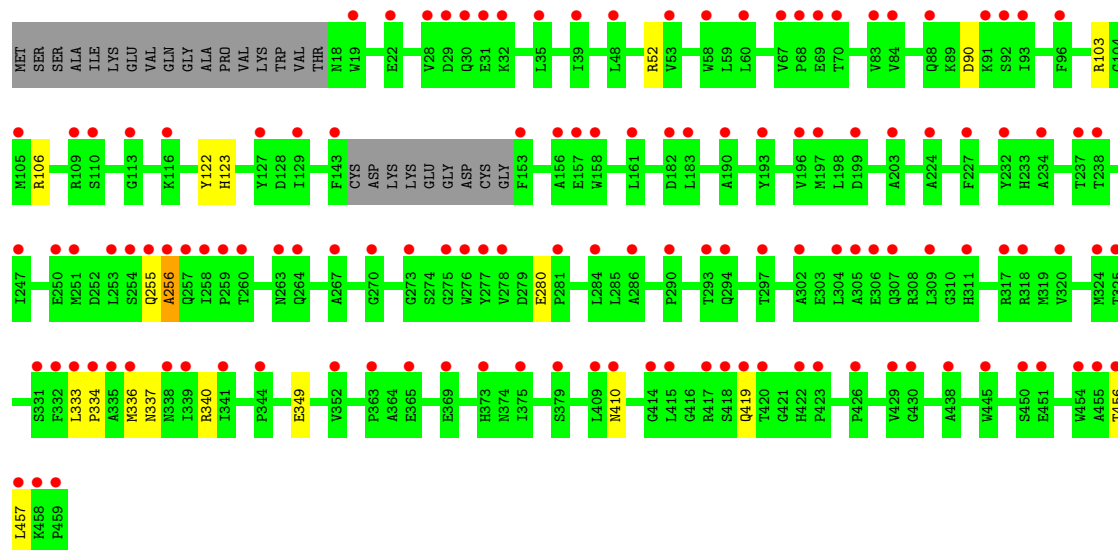
● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain O:



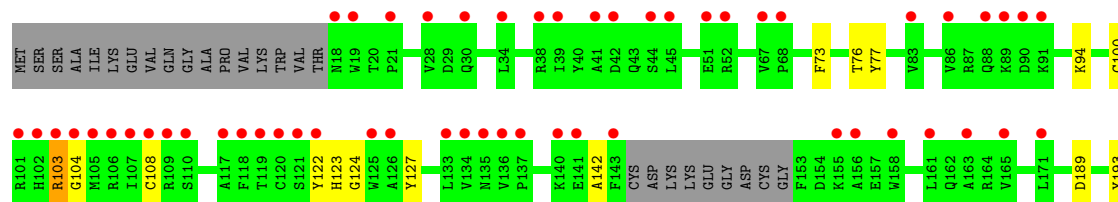
● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

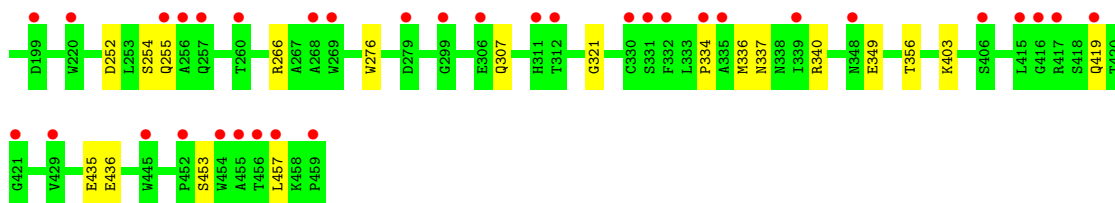
Chain Q:



● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

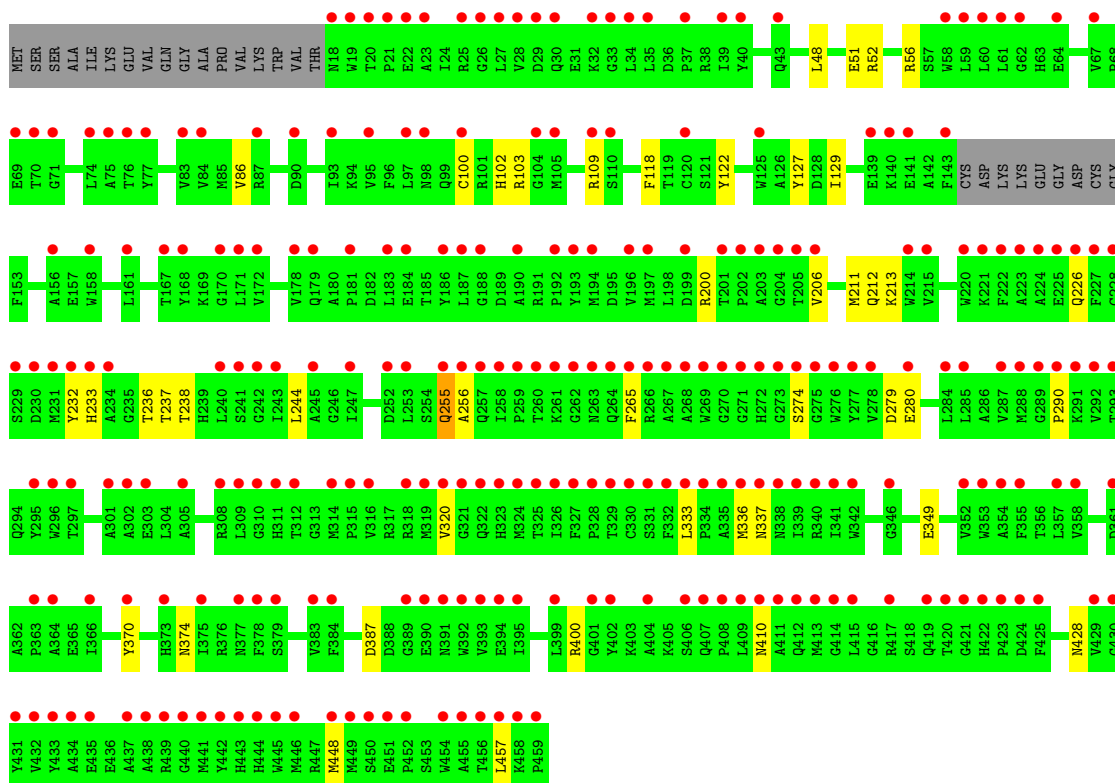
Chain S:





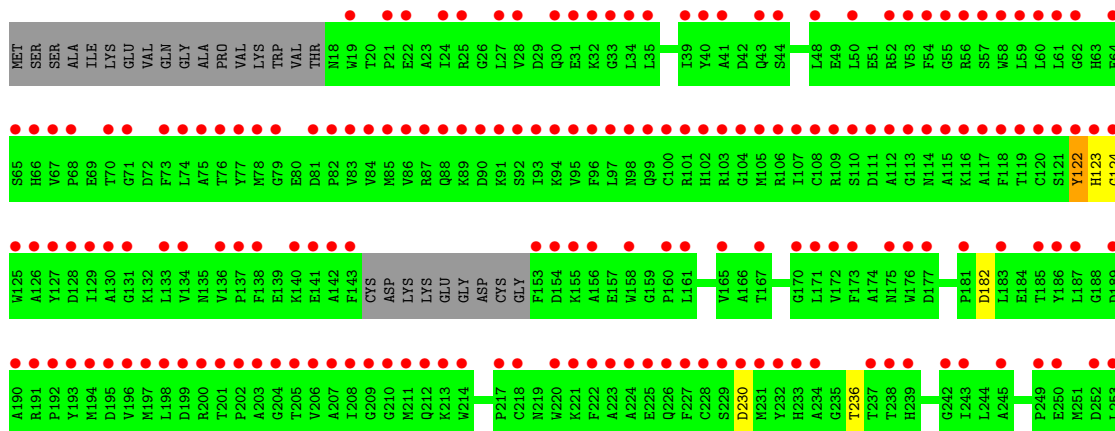
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

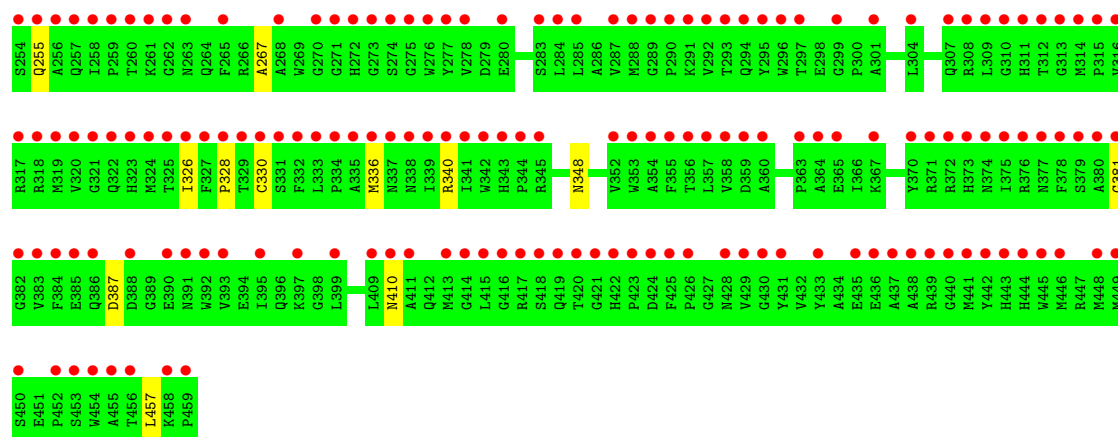
Chain U: 



- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

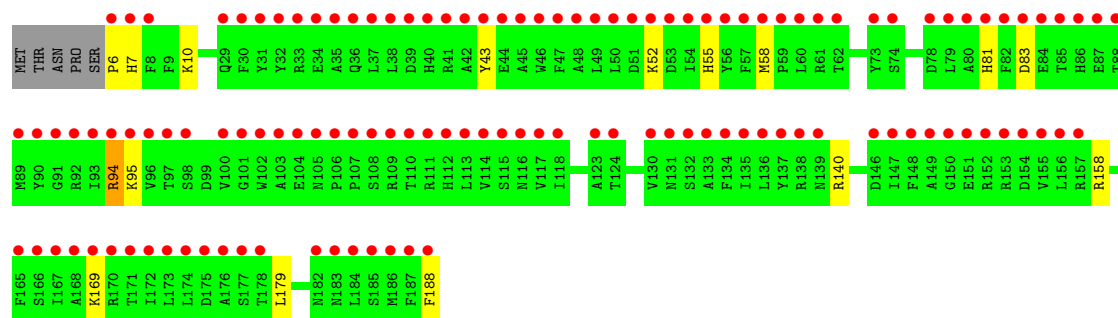
Chain W:





• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain B:



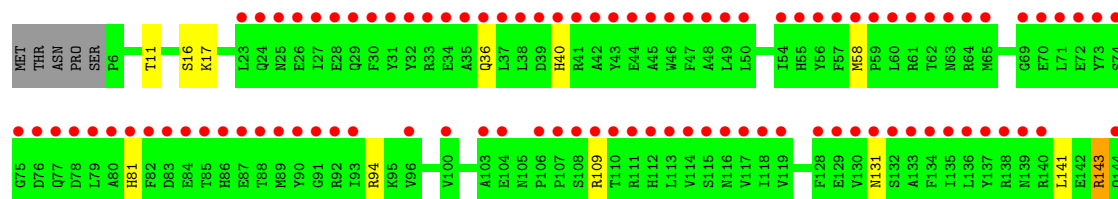
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

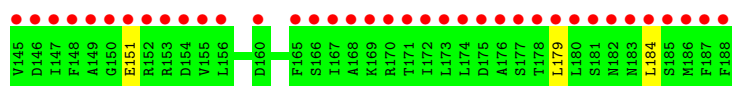
Chain D:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

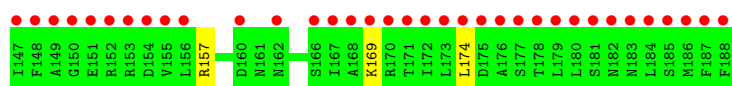
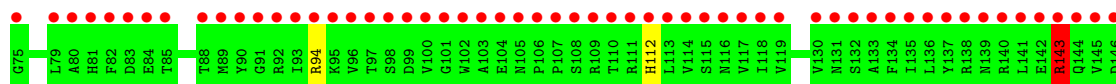
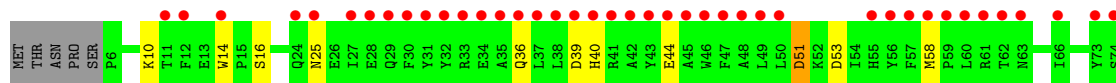
Chain F:





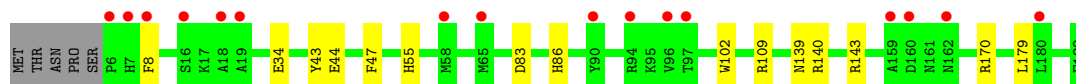
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain H:



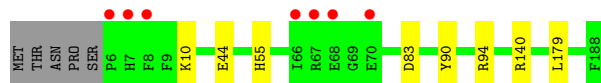
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain J:



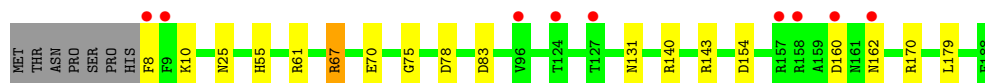
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain L:



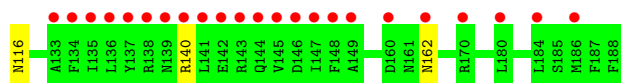
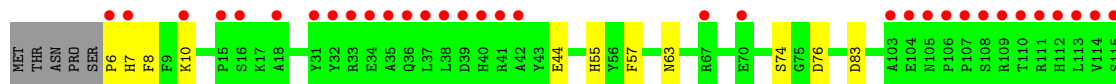
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain N:



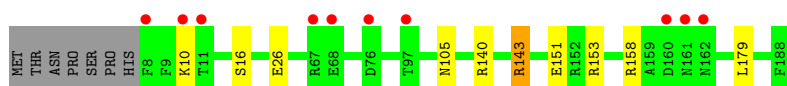
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain P:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain R:



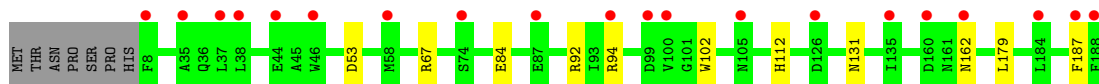
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain T:



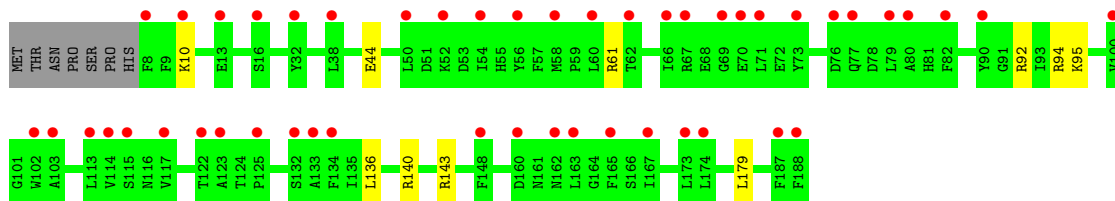
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain V:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain X:



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	17050 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 20.7	EDS
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
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 339687 reflections	Xtriage
F_o, F_c correlation	0.83	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3427	0	0	10	0
1	C	3427	0	0	9	0
1	E	3427	0	0	10	0
1	G	3427	0	0	14	0
1	I	3427	0	0	11	0
1	K	3427	0	0	13	0
1	M	3427	0	0	9	0
1	O	3427	0	0	12	0
1	Q	3427	0	0	7	0
1	S	3427	0	0	16	0
1	U	3427	0	0	21	0
1	W	3427	0	0	10	0
2	B	1524	0	0	10	0
2	D	1524	0	0	7	0
2	F	1524	0	0	7	0
2	H	1524	0	0	11	0
2	J	1524	0	0	8	0
2	L	1524	0	0	2	0
2	N	1507	0	0	10	0
2	P	1524	0	14	4	0
2	R	1507	0	0	4	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	38	0	0	0	0
5	Q	90	0	0	2	0
5	R	89	0	0	0	0
5	S	116	0	0	9	0
5	T	69	0	0	1	0
5	U	115	0	0	7	0
5	V	45	0	0	1	0
5	W	89	0	0	4	0
5	X	37	0	0	1	0
All	All	61911	0	14	199	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (199) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:188:PHE:C	5:B:2106:HOH:O	2.03	0.97
1:I:197:MET:SD	5:I:2068:HOH:O	2.27	0.92
3:O:900:FES:S2	5:O:2036:HOH:O	2.28	0.90
2:D:55:HIS:NE2	2:D:83:ASP:OD2	2.07	0.87
1:S:103:ARG:CB	5:S:2028:HOH:O	2.26	0.83
1:A:372:ARG:NH1	5:A:2156:HOH:O	2.13	0.81
2:B:158:ARG:NE	5:B:2101:HOH:O	2.16	0.79
1:A:356:THR:CB	5:A:2142:HOH:O	2.34	0.75
1:U:233:HIS:CE1	5:U:2073:HOH:O	2.39	0.74
1:S:255:GLN:OE1	5:S:2066:HOH:O	2.06	0.74
2:H:36:GLN:NE2	5:H:2026:HOH:O	2.21	0.73
3:K:900:FES:S1	5:K:2024:HOH:O	2.47	0.72
1:W:123:HIS:N	3:W:900:FES:S2	2.64	0.70
1:O:123:HIS:N	5:O:2035:HOH:O	2.25	0.70
1:G:287:VAL:CG1	1:G:288:MET:CE	2.70	0.70
1:A:334:PRO:O	1:A:337:ASN:OD1	2.10	0.69
2:X:143:ARG:O	5:X:2029:HOH:O	2.10	0.69
3:S:900:FES:S1	5:S:2021:HOH:O	2.51	0.69
1:C:435:GLU:OE1	1:G:102:HIS:NE2	2.26	0.69
1:K:334:PRO:O	1:K:337:ASN:OD1	2.11	0.68
2:H:53:ASP:OD2	2:H:157:ARG:NH2	2.31	0.64
2:H:25:ASN:ND2	5:H:2012:HOH:O	2.31	0.64
2:P:55:HIS:NE2	2:P:83:ASP:OD2	2.30	0.64
2:R:26:GLU:OE1	2:R:158:ARG:NH2	2.31	0.63
1:A:356:THR:OG1	5:A:2142:HOH:O	2.15	0.63
1:G:307:GLN:NE2	5:G:2122:HOH:O	2.31	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:43:TYR:OH	5:B:2034:HOH:O	2.15	0.62
1:U:400:ARG:NH2	5:U:2103:HOH:O	2.34	0.61
2:H:169:LYS:CE	5:H:2110:HOH:O	2.49	0.61
1:W:124:GLY:N	5:W:2027:HOH:O	2.34	0.60
1:I:435:GLU:OE1	1:O:102:HIS:NE2	2.34	0.60
1:O:103:ARG:N	3:O:900:FES:S1	2.75	0.60
2:H:169:LYS:NZ	5:H:2111:HOH:O	2.34	0.59
1:W:348:ASN:ND2	5:W:2070:HOH:O	2.34	0.59
2:D:143:ARG:NH2	1:G:349:GLU:OE2	2.36	0.59
2:B:55:HIS:NE2	2:B:83:ASP:OD2	2.36	0.59
1:C:274:SER:OG	1:C:322:GLN:NE2	2.36	0.58
1:G:334:PRO:O	1:G:337:ASN:OD1	2.20	0.58
2:P:6:PRO:HG2	2:P:76:ASP:OD1	2.02	0.58
1:S:349:GLU:OE2	2:X:143:ARG:NH2	2.37	0.57
2:F:58:MET:CE	2:F:81:HIS:CB	2.82	0.57
2:B:169:LYS:CE	5:E:2167:HOH:O	2.52	0.57
2:F:36:GLN:NE2	5:F:2018:HOH:O	2.38	0.56
1:G:200:ARG:NH2	5:G:2082:HOH:O	2.38	0.56
5:A:2110:HOH:O	2:H:40:HIS:CD2	2.60	0.55
2:D:33:ARG:CZ	5:D:2100:HOH:O	2.55	0.55
2:D:51:ASP:OD2	2:D:166:SER:OG	2.24	0.54
1:U:56:ARG:NH2	1:U:448:MET:O	2.41	0.54
1:G:403:LYS:NZ	5:G:2164:HOH:O	2.41	0.53
2:H:58:MET:CE	2:H:174:LEU:CD2	2.85	0.53
5:H:2056:HOH:O	2:T:52:LYS:CD	2.56	0.53
1:O:123:HIS:CB	5:O:2035:HOH:O	2.57	0.53
1:K:349:GLU:OE2	2:R:143:ARG:NH2	2.42	0.53
1:U:238:THR:OG1	1:W:122:TYR:O	2.27	0.53
1:W:236:THR:OG1	5:W:2055:HOH:O	2.19	0.52
2:J:109:ARG:NH1	2:P:63:ASN:OD1	2.42	0.52
1:I:219:ASN:ND2	5:I:2052:HOH:O	2.42	0.52
1:E:334:PRO:O	1:E:337:ASN:OD1	2.27	0.52
2:N:25:ASN:ND2	5:N:2012:HOH:O	2.43	0.52
1:Q:255:GLN:O	1:Q:256:ALA:O	2.27	0.52
1:O:296:TRP:CH2	1:O:334:PRO:O	2.63	0.52
1:S:334:PRO:O	1:S:337:ASN:OD1	2.28	0.52
2:J:55:HIS:NE2	2:J:83:ASP:OD2	2.43	0.52
1:K:109:ARG:NH1	2:R:105:ASN:O	2.43	0.51
1:E:340:ARG:NH1	1:E:385:GLU:OE2	2.42	0.51
1:S:189:ASP:OD1	5:S:2044:HOH:O	2.18	0.51
1:O:56:ARG:NH2	1:O:448:MET:O	2.44	0.51
1:Q:334:PRO:O	1:Q:337:ASN:OD1	2.29	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:232:TYR:O	1:U:236:THR:OG1	2.29	0.51
1:M:334:PRO:O	1:M:337:ASN:OD1	2.28	0.50
2:D:7:HIS:CD2	2:D:7:HIS:N	2.79	0.50
1:K:444:HIS:O	1:K:445:TRP:C	2.50	0.50
1:C:349:GLU:OE2	2:F:143:ARG:NH2	2.45	0.50
1:W:387:ASP:OD1	2:X:95:LYS:NZ	2.45	0.49
1:I:56:ARG:NH2	1:I:448:MET:O	2.45	0.49
1:I:98:ASN:ND2	5:I:2022:HOH:O	2.44	0.49
1:A:200:ARG:NH2	5:A:2087:HOH:O	2.45	0.49
2:F:151:GLU:OE2	2:H:40:HIS:CE1	2.65	0.49
1:O:193:TYR:CE2	1:O:276:TRP:CH2	3.01	0.48
1:G:53:VAL:O	1:G:57:SER:OG	2.30	0.48
1:S:123:HIS:NE2	1:W:230:ASP:OD2	2.46	0.48
1:M:230:ASP:OD2	1:Q:123:HIS:NE2	2.46	0.48
1:W:381:GLY:O	2:X:92:ARG:NH1	2.46	0.48
1:W:267:ALA:N	5:W:2059:HOH:O	2.46	0.48
1:G:162:GLN:NE2	5:G:2065:HOH:O	2.45	0.48
1:O:76:THR:OG1	1:O:77:TYR:N	2.46	0.48
1:O:120:CYS:SG	5:O:2036:HOH:O	2.61	0.47
2:L:90:TYR:CE1	5:L:2023:HOH:O	2.55	0.47
1:G:227:PHE:O	1:G:323:HIS:ND1	2.47	0.47
1:S:435:GLU:OE1	1:U:102:HIS:NE2	2.48	0.47
1:K:340:ARG:NH1	1:K:385:GLU:OE1	2.47	0.47
1:K:51:GLU:OE2	1:K:52:ARG:NH1	2.48	0.47
3:S:900:FES:S2	5:S:2029:HOH:O	2.61	0.47
2:N:25:ASN:ND2	5:N:2010:HOH:O	2.46	0.47
1:M:230:ASP:OD1	1:M:233:HIS:N	2.47	0.47
1:O:188:GLY:O	1:O:191:ARG:NE	2.48	0.47
2:J:109:ARG:NE	2:J:139:ASN:OD1	2.48	0.47
1:M:177:ASP:OD2	1:M:454:TRP:NE1	2.47	0.47
1:Q:106:ARG:NH1	5:Q:2022:HOH:O	2.48	0.47
2:N:143:ARG:NH2	1:Q:349:GLU:OE2	2.48	0.46
2:V:131:ASN:ND2	5:V:2031:HOH:O	2.48	0.46
2:N:55:HIS:NE2	2:N:83:ASP:OD2	2.48	0.46
1:M:346:GLY:O	5:M:2066:HOH:O	2.20	0.46
1:G:255:GLN:O	1:G:256:ALA:C	2.54	0.46
1:A:295:TYR:OH	1:A:359:ASP:OD2	2.32	0.46
1:I:255:GLN:O	1:I:256:ALA:C	2.53	0.46
1:C:394:GLU:CG	5:G:2045:HOH:O	2.63	0.46
2:J:34:GLU:OE1	2:J:170:ARG:NH1	2.48	0.46
1:K:230:ASP:OD2	1:M:123:HIS:NE2	2.49	0.46
2:T:143:ARG:NH2	1:U:349:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:86:HIS:N	5:J:2027:HOH:O	2.48	0.46
2:N:61:ARG:NH2	5:N:2025:HOH:O	2.48	0.45
2:T:105:ASN:O	1:U:109:ARG:NH1	2.50	0.45
1:S:104:GLY:N	5:S:2021:HOH:O	2.49	0.45
1:U:200:ARG:CG	5:U:2065:HOH:O	2.64	0.45
1:U:129:ILE:N	5:U:2033:HOH:O	2.49	0.45
1:E:227:PHE:O	1:E:323:HIS:ND1	2.50	0.45
1:E:403:LYS:NZ	5:E:2191:HOH:O	2.49	0.45
1:E:405:LYS:NZ	5:E:2192:HOH:O	2.50	0.44
2:F:58:MET:CE	2:F:184:LEU:CD1	2.96	0.44
2:B:94:ARG:NH1	5:B:2069:HOH:O	2.50	0.44
1:U:213:LYS:NZ	5:U:2072:HOH:O	2.50	0.44
3:S:900:FES:S1	5:S:2028:HOH:O	2.62	0.44
2:V:53:ASP:N	2:V:53:ASP:OD1	2.48	0.44
1:C:309:LEU:O	1:C:312:THR:OG1	2.35	0.44
1:I:281:PRO:O	1:I:285:LEU:N	2.51	0.44
1:S:193:TYR:CE2	1:S:276:TRP:CH2	3.06	0.44
2:H:39:ASP:OD1	2:H:112:HIS:ND1	2.50	0.44
2:N:8:PHE:CE2	2:N:70:GLU:CB	3.01	0.44
1:I:76:THR:OG1	1:I:77:TYR:N	2.51	0.44
1:U:244:LEU:N	5:U:2075:HOH:O	2.50	0.44
1:C:212:GLN:NE2	5:C:2090:HOH:O	2.50	0.44
2:N:131:ASN:ND2	5:N:2055:HOH:O	2.51	0.43
1:S:252:ASP:OD1	1:S:254:SER:OG	2.36	0.43
1:E:102:HIS:NE2	1:G:435:GLU:OE1	2.51	0.43
1:M:246:GLY:O	5:M:2058:HOH:O	2.21	0.43
1:U:333:LEU:O	1:U:337:ASN:N	2.51	0.43
1:S:100:CYS:SG	1:S:127:TYR:OH	2.77	0.43
1:E:349:GLU:OE2	2:H:143:ARG:NH2	2.51	0.43
2:R:151:GLU:OE1	2:R:153:ARG:NE	2.52	0.43
1:K:266:ARG:NH1	1:K:436:GLU:OE1	2.52	0.43
1:K:105:MET:N	5:K:2024:HOH:O	2.51	0.43
1:K:338:ASN:OD1	1:K:340:ARG:NH2	2.52	0.43
1:S:73:PHE:CE1	1:S:108:CYS:SG	3.12	0.43
1:A:167:THR:CG2	5:A:2013:HOH:O	2.66	0.43
1:I:422:HIS:CD2	1:I:424:ASP:N	2.87	0.43
2:N:67:ARG:CA	2:N:67:ARG:NE	2.82	0.43
2:J:102:TRP:O	1:O:109:ARG:NH2	2.51	0.43
1:K:211:MET:CE	1:K:353:TRP:CE3	3.02	0.43
1:A:109:ARG:NE	5:A:2047:HOH:O	2.51	0.43
1:U:118:PHE:O	1:U:127:TYR:N	2.52	0.43
1:G:252:ASP:OD1	1:G:252:ASP:N	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:75:GLY:N	2:N:78:ASP:OD2	2.52	0.42
1:M:326:ILE:N	1:M:330:CYS:O	2.52	0.42
2:T:26:GLU:OE1	2:T:158:ARG:NH2	2.52	0.42
1:S:124:GLY:N	5:S:2029:HOH:O	2.51	0.42
1:K:104:GLY:N	5:K:2024:HOH:O	2.52	0.42
2:D:151:GLU:OE2	2:F:40:HIS:CE1	2.72	0.42
1:U:237:THR:O	2:V:102:TRP:NE1	2.52	0.42
2:J:43:TYR:O	2:J:47:PHE:N	2.53	0.42
1:K:76:THR:OG1	1:K:77:TYR:N	2.52	0.42
1:I:230:ASP:O	1:I:233:HIS:CE1	2.73	0.42
1:A:348:ASN:OD1	1:A:396:GLN:NE2	2.53	0.42
1:U:370:TYR:O	1:U:374:ASN:ND2	2.52	0.42
1:S:266:ARG:NH1	1:S:436:GLU:OE1	2.52	0.42
2:B:6:PRO:O	2:B:7:HIS:C	2.57	0.42
1:C:418:SER:CB	1:C:428:ASN:OD1	2.67	0.42
1:U:200:ARG:NH2	5:U:2066:HOH:O	2.53	0.42
2:B:58:MET:CE	2:B:81:HIS:CD2	3.02	0.42
2:H:51:ASP:OD2	2:H:157:ARG:NH1	2.53	0.42
2:B:58:MET:CE	2:B:81:HIS:CB	2.98	0.42
1:U:100:CYS:SG	1:U:127:TYR:OH	2.78	0.42
2:N:154:ASP:OD1	2:N:170:ARG:NH2	2.53	0.42
1:I:230:ASP:O	1:I:233:HIS:ND1	2.53	0.41
2:V:112:HIS:NE2	2:V:187:PHE:O	2.52	0.41
1:Q:333:LEU:O	1:Q:337:ASN:N	2.53	0.41
1:U:51:GLU:OE2	1:U:52:ARG:NH1	2.53	0.41
2:L:55:HIS:NE2	2:L:83:ASP:OD2	2.53	0.41
1:Q:52:ARG:NE	5:Q:2013:HOH:O	2.53	0.41
1:S:403:LYS:NZ	5:S:2109:HOH:O	2.54	0.41
1:S:76:THR:OG1	1:S:77:TYR:N	2.54	0.41
1:M:193:TYR:OH	1:M:426:PRO:O	2.38	0.41
2:P:6:PRO:HA	2:P:57:PHE:CE2	2.55	0.41
2:D:29:GLN:NE2	5:D:2013:HOH:O	2.54	0.41
2:B:52:LYS:NZ	5:B:2041:HOH:O	2.53	0.41
1:E:56:ARG:O	1:E:175:ASN:ND2	2.54	0.41
1:A:280:GLU:O	1:A:283:SER:OG	2.38	0.41
1:C:219:ASN:OD1	1:C:221:LYS:NZ	2.54	0.41
1:U:265:PHE:N	1:U:274:SER:O	2.54	0.41
1:C:225:GLU:O	1:C:228:CYS:N	2.54	0.41
1:U:255:GLN:O	1:U:256:ALA:C	2.58	0.40
1:E:287:VAL:CG1	1:E:288:MET:CE	2.99	0.40
2:V:84:GLU:OE1	2:V:92:ARG:NE	2.54	0.40
2:F:109:ARG:NH2	2:F:141:LEU:O	2.55	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:143:ARG:NH2	1:O:349:GLU:OE2	2.54	0.40
1:E:225:GLU:OE2	1:E:442:TYR:OH	2.40	0.40
2:T:158:ARG:NH1	5:T:2059:HOH:O	2.54	0.40
1:W:326:ILE:N	1:W:330:CYS:O	2.54	0.40
1:G:219:ASN:ND2	5:G:2091:HOH:O	2.54	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%)	56	62
1	G	429/459 (94%)	407 (95%)	22 (5%)	0	100	100
1	I	429/459 (94%)	414 (96%)	14 (3%)	1 (0%)	56	62
1	K	429/459 (94%)	407 (95%)	21 (5%)	1 (0%)	56	62
1	M	429/459 (94%)	402 (94%)	26 (6%)	1 (0%)	56	62
1	O	429/459 (94%)	407 (95%)	20 (5%)	2 (0%)	38	38
1	Q	429/459 (94%)	405 (94%)	23 (5%)	1 (0%)	56	62
1	S	429/459 (94%)	412 (96%)	15 (4%)	2 (0%)	38	38
1	U	429/459 (94%)	401 (94%)	24 (6%)	4 (1%)	25	21
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%)	33	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	21	16
2	R	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
2	T	179/188 (95%)	172 (96%)	6 (3%)	1 (1%)	33	32
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%)	56	62

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	8	PHE
2	P	8	PHE
1	Q	256	ALA
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%)	55	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	350/372 (94%)	338 (97%)	12 (3%)	49	59
1	E	350/372 (94%)	335 (96%)	15 (4%)	40	47
1	G	350/372 (94%)	336 (96%)	14 (4%)	42	51
1	I	350/372 (94%)	339 (97%)	11 (3%)	52	63
1	K	350/372 (94%)	336 (96%)	14 (4%)	42	51
1	M	350/372 (94%)	340 (97%)	10 (3%)	55	66
1	O	350/372 (94%)	340 (97%)	10 (3%)	55	66
1	Q	350/372 (94%)	340 (97%)	10 (3%)	55	66
1	S	350/372 (94%)	340 (97%)	10 (3%)	55	66
1	U	350/372 (94%)	336 (96%)	14 (4%)	42	51
1	W	350/372 (94%)	342 (98%)	8 (2%)	63	74
2	B	162/167 (97%)	157 (97%)	5 (3%)	52	63
2	D	162/167 (97%)	154 (95%)	8 (5%)	35	40
2	F	162/167 (97%)	155 (96%)	7 (4%)	40	47
2	H	162/167 (97%)	155 (96%)	7 (4%)	40	47
2	J	162/167 (97%)	159 (98%)	3 (2%)	69	81
2	L	162/167 (97%)	157 (97%)	5 (3%)	52	63
2	N	160/167 (96%)	154 (96%)	6 (4%)	44	53
2	P	162/167 (97%)	156 (96%)	6 (4%)	45	54
2	R	160/167 (96%)	155 (97%)	5 (3%)	52	63
2	T	160/167 (96%)	155 (97%)	5 (3%)	52	63
2	V	160/167 (96%)	156 (98%)	4 (2%)	60	71
2	X	160/167 (96%)	153 (96%)	7 (4%)	39	45
All	All	6134/6468 (95%)	5928 (97%)	206 (3%)	49	59

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 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	A	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	C	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	E	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	G	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	I	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	K	900	1,5	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	M	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	O	900	1,5	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	Q	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	S	900	1,5	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	U	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	W	900	1,5	0,4,4	0.00	-	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	A	900	1	-	0/0/4/4	0/0/1/1
3	FES	C	900	1	-	0/0/4/4	0/0/1/1
3	FES	E	900	1	-	0/0/4/4	0/0/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	G	900	1	-	0/0/4/4	0/0/1/1
3	FES	I	900	1	-	0/0/4/4	0/0/1/1
3	FES	K	900	1,5	-	0/0/4/4	0/0/1/1
3	FES	M	900	1	-	0/0/4/4	0/0/1/1
3	FES	O	900	1,5	-	0/0/4/4	0/0/1/1
3	FES	Q	900	1	-	0/0/4/4	0/0/1/1
3	FES	S	900	1,5	-	0/0/4/4	0/0/1/1
3	FES	U	900	1	-	0/0/4/4	0/0/1/1
3	FES	W	900	1,5	-	0/0/4/4	0/0/1/1

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	2.35	74 (17%) 2 2	-7, 10, 35, 51	18 (4%)
1	C	433/459 (94%)	0.46	26 (6%) 21 21	3, 29, 56, 66	18 (4%)
1	E	433/459 (94%)	5.48	143 (33%) 1 1	-11, 7, 33, 47	18 (4%)
1	G	433/459 (94%)	1.15	47 (10%) 6 6	-3, 17, 42, 60	18 (4%)
1	I	433/459 (94%)	0.95	67 (15%) 3 3	7, 50, 89, 101	18 (4%)
1	K	433/459 (94%)	0.55	36 (8%) 11 11	12, 29, 54, 99	18 (4%)
1	M	433/459 (94%)	1.25	102 (23%) 1 1	17, 47, 83, 92	18 (4%)
1	O	433/459 (94%)	0.88	60 (13%) 4 3	20, 49, 71, 100	18 (4%)
1	Q	433/459 (94%)	1.57	130 (30%) 1 1	37, 64, 92, 108	18 (4%)
1	S	433/459 (94%)	1.13	89 (20%) 1 1	15, 48, 80, 113	18 (4%)
1	U	433/459 (94%)	2.81	257 (59%) 0 0	43, 88, 126, 135	18 (4%)
1	W	433/459 (94%)	3.66	339 (78%) 0 0	71, 111, 142, 155	18 (4%)
2	B	183/188 (97%)	10.66	124 (67%) 0 0	-12, -2, 16, 28	4 (2%)
2	D	183/188 (97%)	7.43	88 (48%) 1 0	-12, 2, 28, 40	4 (2%)
2	F	183/188 (97%)	11.98	134 (73%) 0 0	-16, -5, 19, 32	4 (2%)
2	H	183/188 (97%)	11.64	133 (72%) 0 0	-15, -4, 33, 48	4 (2%)
2	J	183/188 (97%)	0.46	16 (8%) 10 10	1, 22, 47, 58	4 (2%)
2	L	183/188 (97%)	-0.03	7 (3%) 38 39	3, 12, 33, 52	4 (2%)
2	N	181/188 (96%)	0.30	9 (4%) 28 27	8, 25, 40, 46	4 (2%)
2	P	183/188 (97%)	5.57	56 (30%) 1 1	-11, 12, 45, 67	4 (2%)
2	R	181/188 (96%)	0.19	10 (5%) 24 24	7, 22, 41, 53	4 (2%)
2	T	181/188 (96%)	0.17	7 (3%) 37 38	5, 20, 49, 75	4 (2%)
2	V	181/188 (96%)	0.96	20 (11%) 6 6	25, 50, 81, 99	4 (2%)
2	X	181/188 (96%)	1.53	48 (26%) 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%)	2.56	2022 (27%) 1 1	-16, 33, 105, 155	264 (3%)

All (2022) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	PHE	41.3
1	E	325	THR	40.1
1	A	353	TRP	39.3
2	D	46	TRP	38.9
2	P	134	PHE	38.8
1	E	95	VAL	38.0
2	P	32	TYR	37.6
2	D	106	PRO	37.5
1	A	207	ALA	36.6
1	G	352	VAL	36.2
1	E	218	CYS	36.1
2	P	106	PRO	35.3
1	E	331	SER	35.1
2	P	114	VAL	35.0
1	E	332	PHE	34.4
2	P	103	ALA	33.9
2	P	38	LEU	33.8
1	E	342	TRP	33.4
1	E	198	LEU	33.4
1	E	96	PHE	32.8
2	H	168	ALA	32.8
1	E	59	LEU	32.5
1	E	97	LEU	32.1
2	F	119	VAL	31.1
1	E	344	PRO	31.0
1	E	98	ASN	30.9
2	P	135	ILE	30.8
1	A	256	ALA	30.7
2	F	130	VAL	30.4
1	G	353	TRP	30.3
1	E	115	ALA	30.1
2	D	43	TYR	30.1
1	E	83	VAL	30.0
2	H	79	LEU	29.9
1	E	78	MET	29.8
1	E	366	ILE	29.7
2	H	167	ILE	29.7

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Mol	Chain	Res	Type	RSRZ
2	F	88	THR	29.5
1	E	378	PHE	29.3
1	E	82	PRO	29.3
1	G	214	TRP	29.2
2	B	168	ALA	29.0
1	E	70	THR	29.0
1	E	370	TYR	28.9
2	B	114	VAL	28.9
2	B	113	LEU	28.9
2	H	102	TRP	28.5
1	E	99	GLN	28.4
1	G	375	ILE	28.4
2	B	31	TYR	28.3
1	E	107	ILE	28.3
2	D	31	TYR	28.2
1	A	338	ASN	28.2
1	A	354	ALA	28.1
1	E	108	CYS	28.1
2	B	110	THR	27.9
2	P	107	PRO	27.8
2	P	113	LEU	27.8
2	D	107	PRO	27.7
1	A	208	ILE	27.7
2	H	80	ALA	27.7
2	P	35	ALA	27.6
2	D	173	LEU	27.5
2	F	43	TYR	27.5
2	B	155	VAL	27.4
2	D	186	MET	27.3
2	D	174	LEU	27.3
2	H	49	LEU	27.1
2	P	33	ARG	27.0
2	D	184	LEU	26.9
1	E	173	PHE	26.9
1	G	216	ILE	26.8
1	G	215	VAL	26.8
2	B	130	VAL	26.6
2	P	105	ASN	26.6
2	B	108	SER	26.6
2	D	45	ALA	26.5
2	B	156	LEU	26.5
2	P	42	ALA	26.4

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Mol	Chain	Res	Type	RSRZ
1	E	79	GLY	26.4
2	D	37	LEU	26.3
1	E	84	VAL	26.2
2	D	118	ILE	26.1
2	P	148	PHE	26.1
2	P	142	GLU	26.0
2	D	176	ALA	26.0
1	E	382	GLY	25.9
2	P	37	LEU	25.8
1	E	105	MET	25.7
2	F	73	TYR	25.6
2	F	173	LEU	25.1
2	D	30	PHE	25.1
2	P	104	GLU	25.1
2	F	71	LEU	25.1
2	B	166	SER	25.0
2	H	42	ALA	25.0
2	B	42	ALA	24.9
2	H	118	ILE	24.9
2	F	155	VAL	24.8
2	H	155	VAL	24.8
2	F	128	PHE	24.8
2	B	49	LEU	24.8
2	F	118	ILE	24.8
2	H	107	PRO	24.7
2	B	167	ILE	24.7
1	A	209	GLY	24.7
1	A	215	VAL	24.6
2	F	171	THR	24.5
1	A	210	GLY	24.4
1	E	324	MET	24.4
1	E	373	HIS	24.3
2	F	85	THR	24.3
2	H	46	TRP	24.3
2	F	47	PHE	24.2
2	D	42	ALA	24.2
2	B	96	VAL	24.2
2	F	89	MET	24.2
2	D	38	LEU	24.2
1	E	217	PRO	24.1
2	H	73	TYR	24.1
1	E	364	ALA	24.1

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Mol	Chain	Res	Type	RSRZ
2	H	45	ALA	24.1
1	A	384	PHE	24.1
2	P	34	GLU	24.1
2	B	97	THR	24.0
2	H	47	PHE	24.0
1	E	350	ILE	23.9
2	P	136	LEU	23.9
2	F	46	TRP	23.9
2	B	35	ALA	23.9
2	H	57	PHE	23.8
1	E	60	LEU	23.7
2	B	50	LEU	23.7
2	B	98	SER	23.7
2	H	27	ILE	23.6
2	H	37	LEU	23.6
2	D	104	GLU	23.6
2	H	56	TYR	23.6
2	B	54	ILE	23.6
2	B	45	ALA	23.6
2	H	89	MET	23.6
2	B	30	PHE	23.4
2	H	40	HIS	23.4
1	G	382	GLY	23.4
2	F	108	SER	23.3
2	H	103	ALA	23.3
1	G	217	PRO	23.3
2	B	39	ASP	23.3
2	D	108	SER	23.2
2	B	101	GLY	23.2
2	B	79	LEU	23.2
2	H	83	ASP	23.2
1	E	172	VAL	23.1
1	E	71	GLY	23.1
1	A	214	TRP	23.1
1	A	378	PHE	23.0
2	F	48	ALA	23.0
1	E	86	VAL	23.0
2	P	141	LEU	23.0
1	E	114	ASN	22.9
1	G	350	ILE	22.9
2	B	93	ILE	22.7
2	B	48	ALA	22.6

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Mol	Chain	Res	Type	RSRZ
2	H	30	PHE	22.6
2	B	43	TYR	22.6
2	B	107	PRO	22.6
2	F	107	PRO	22.5
1	A	239	HIS	22.5
2	F	42	ALA	22.5
2	F	50	LEU	22.5
2	B	46	TRP	22.5
2	H	48	ALA	22.4
2	B	132	SER	22.4
2	F	154	ASP	22.4
2	P	147	ILE	22.4
1	A	240	LEU	22.4
2	H	106	PRO	22.3
2	D	117	VAL	22.3
2	F	117	VAL	22.2
2	B	38	LEU	22.2
2	P	140	ARG	22.2
1	E	358	VAL	22.2
2	H	100	VAL	22.2
2	B	37	LEU	22.1
2	H	96	VAL	22.1
1	A	370	TYR	22.1
2	F	56	TYR	22.1
2	P	40	HIS	22.0
2	P	108	SER	22.0
2	H	101	GLY	22.0
2	F	172	ILE	21.9
1	A	243	ILE	21.9
2	B	157	ARG	21.9
2	F	104	GLU	21.9
2	F	49	LEU	21.8
1	A	245	ALA	21.8
1	E	106	ARG	21.7
2	F	167	ILE	21.6
2	B	111	ARG	21.6
2	B	47	PHE	21.6
2	F	45	ALA	21.6
1	E	197	MET	21.4
1	E	77	TYR	21.2
1	A	242	GLY	21.2
1	E	61	LEU	21.2

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Mol	Chain	Res	Type	RSRZ
2	F	156	LEU	21.2
2	H	31	TYR	21.2
1	E	360	ALA	21.2
2	F	27	ILE	21.2
1	A	241	SER	21.1
1	E	122	TYR	21.1
2	H	97	THR	21.1
2	H	32	TYR	21.0
2	H	130	VAL	21.0
2	B	103	ALA	21.0
1	E	73	PHE	21.0
2	D	148	PHE	20.9
2	H	171	THR	20.9
2	F	187	PHE	20.9
2	H	178	THR	20.9
2	B	133	ALA	20.9
2	F	168	ALA	20.9
2	F	109	ARG	20.9
2	B	171	THR	20.9
2	H	141	LEU	20.9
2	H	117	VAL	20.8
2	H	82	PHE	20.8
2	H	62	THR	20.8
2	D	32	TYR	20.8
2	B	60	LEU	20.8
2	F	57	PHE	20.7
1	A	352	VAL	20.7
2	D	29	GLN	20.7
2	H	38	LEU	20.7
2	H	154	ASP	20.6
2	P	36	GLN	20.6
2	H	43	TYR	20.6
1	E	357	LEU	20.6
1	E	339	ILE	20.6
2	F	37	LEU	20.6
2	F	153	ARG	20.6
1	E	204	GLY	20.5
2	D	40	HIS	20.5
1	A	374	ASN	20.4
1	E	216	ILE	20.4
2	D	58	MET	20.3
2	H	74	SER	20.3

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Mol	Chain	Res	Type	RSRZ
1	E	205	THR	20.3
2	H	98	SER	20.3
2	F	139	ASN	20.2
2	H	60	LEU	20.2
1	E	68	PRO	20.2
1	E	85	MET	20.0
2	F	30	PHE	20.0
2	F	185	SER	20.0
2	F	38	LEU	20.0
1	A	373	HIS	19.9
2	D	35	ALA	19.9
2	D	145	VAL	19.9
1	E	338	ASN	19.8
2	F	103	ALA	19.8
2	P	112	HIS	19.8
2	F	32	TYR	19.8
1	E	110	SER	19.8
2	B	57	PHE	19.7
2	H	29	GLN	19.7
1	E	67	VAL	19.7
1	E	113	GLY	19.6
2	F	31	TYR	19.5
2	B	135	ILE	19.5
2	H	108	SER	19.5
2	H	93	ILE	19.5
2	D	41	ARG	19.5
2	F	145	VAL	19.4
2	F	54	ILE	19.4
1	E	374	ASN	19.4
1	E	341	ILE	19.4
2	H	110	THR	19.3
1	A	383	VAL	19.3
2	D	34	GLU	19.2
2	F	92	ARG	19.2
2	F	132	SER	19.1
2	H	35	ALA	19.1
2	B	55	HIS	19.0
2	F	82	PHE	19.0
2	F	29	GLN	19.0
1	E	76	THR	19.0
1	E	109	ARG	19.0
1	E	75	ALA	18.9

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Mol	Chain	Res	Type	RSRZ
2	H	41	ARG	18.9
2	B	86	HIS	18.9
1	G	381	GLY	18.9
1	A	387	ASP	18.8
2	D	110	THR	18.8
2	H	75	GLY	18.8
2	H	180	LEU	18.8
2	B	112	HIS	18.7
2	P	39	ASP	18.7
2	F	174	LEU	18.7
2	D	59	PRO	18.6
2	B	102	TRP	18.6
2	H	39	ASP	18.6
2	D	132	SER	18.5
2	F	166	SER	18.5
2	F	62	THR	18.5
2	B	56	TYR	18.4
2	P	110	THR	18.4
2	B	173	LEU	18.4
1	A	238	THR	18.4
1	A	375	ILE	18.3
1	E	381	GLY	18.3
2	F	91	GLY	18.3
1	A	213	LYS	18.3
2	H	187	PHE	18.2
1	E	375	ILE	18.1
2	B	88	THR	18.1
2	B	89	MET	18.1
2	F	58	MET	18.1
2	P	144	GLN	18.1
2	F	24	GLN	18.0
1	E	74	LEU	18.0
2	F	110	THR	18.0
1	E	112	ALA	18.0
2	F	182	ASN	18.0
2	F	184	LEU	18.0
2	B	80	ALA	18.0
2	H	59	PRO	17.9
1	E	343	HIS	17.9
2	B	91	GLY	17.9
2	D	144	GLN	17.8
2	F	186	MET	17.8

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Mol	Chain	Res	Type	RSRZ
2	B	85	THR	17.8
2	F	72	GLU	17.8
2	H	92	ARG	17.7
2	D	146	ASP	17.7
2	D	134	PHE	17.7
2	H	182	ASN	17.6
2	B	59	PRO	17.6
2	F	59	PRO	17.6
2	F	188	PHE	17.6
2	D	172	ILE	17.6
2	P	145	VAL	17.5
2	F	133	ALA	17.5
2	B	134	PHE	17.4
2	B	170	ARG	17.4
1	E	214	TRP	17.4
2	B	176	ALA	17.4
2	B	94	ARG	17.3
2	D	138	ARG	17.3
2	F	64	ARG	17.3
2	H	179	LEU	17.3
1	E	359	ASP	17.2
1	E	380	ALA	17.2
1	G	213	LYS	17.2
2	D	136	LEU	17.2
2	B	32	TYR	17.1
1	E	215	VAL	17.1
2	D	149	ALA	17.0
1	E	206	VAL	17.0
2	D	47	PHE	17.0
2	B	172	ILE	17.0
2	B	106	PRO	17.0
2	H	58	MET	16.9
1	E	352	VAL	16.9
2	P	143	ARG	16.9
2	F	137	TYR	16.8
2	F	75	GLY	16.8
2	B	165	PHE	16.8
2	D	81	HIS	16.7
2	H	91	GLY	16.7
2	B	100	VAL	16.7
1	A	371	ARG	16.6
2	H	183	ASN	16.6

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Mol	Chain	Res	Type	RSRZ
2	H	177	SER	16.6
2	P	137	TYR	16.6
2	H	184	LEU	16.6
2	F	63	ASN	16.6
2	D	39	ASP	16.5
2	H	81	HIS	16.5
2	D	147	ILE	16.5
2	F	170	ARG	16.5
1	E	379	SER	16.5
2	H	95	LYS	16.5
2	F	176	ALA	16.5
2	B	136	LEU	16.4
2	H	145	VAL	16.4
2	D	140	ARG	16.3
2	H	185	SER	16.3
2	H	28	GLU	16.3
2	F	74	SER	16.3
2	D	133	ALA	16.2
2	F	83	ASP	16.2
2	F	183	ASN	16.2
2	H	173	LEU	16.2
2	F	134	PHE	16.1
2	F	149	ALA	16.1
2	B	104	GLU	16.1
2	H	172	ILE	16.0
2	H	170	ARG	16.0
2	P	146	ASP	16.0
2	H	104	GLU	16.0
2	P	109	ARG	16.0
2	F	150	GLY	16.0
1	E	353	TRP	15.9
1	E	356	THR	15.9
1	A	377	ASN	15.9
2	D	139	ASN	15.9
2	F	152	ARG	15.8
2	H	176	ALA	15.8
2	H	137	TYR	15.8
2	F	61	ARG	15.8
2	H	186	MET	15.7
2	F	35	ALA	15.7
2	D	114	VAL	15.6
2	H	181	SER	15.6

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Mol	Chain	Res	Type	RSRZ
2	B	40	HIS	15.6
2	F	39	ASP	15.6
2	F	175	ASP	15.5
2	D	150	GLY	15.5
2	F	148	PHE	15.5
1	A	356	THR	15.4
2	D	112	HIS	15.4
2	B	138	ARG	15.4
2	B	58	MET	15.3
2	F	84	GLU	15.3
2	F	80	ALA	15.3
1	E	62	GLY	15.3
1	A	380	ALA	15.2
2	H	139	ASN	15.2
2	F	147	ILE	15.2
2	F	60	LEU	15.2
1	A	379	SER	15.1
2	B	82	PHE	15.1
2	B	74	SER	15.1
1	E	367	LYS	15.1
2	P	139	ASN	15.1
2	F	181	SER	15.1
2	P	138	ARG	15.0
2	F	138	ARG	15.0
2	H	140	ARG	15.0
1	G	218	CYS	15.0
2	H	109	ARG	15.0
1	E	362	ALA	14.9
2	D	137	TYR	14.9
2	H	132	SER	14.9
2	B	185	SER	14.9
2	B	117	VAL	14.8
2	F	114	VAL	14.7
2	H	114	VAL	14.7
2	F	136	LEU	14.7
1	E	207	ALA	14.7
2	B	83	ASP	14.7
1	E	63	HIS	14.7
2	B	34	GLU	14.7
2	F	116	ASN	14.7
2	B	174	LEU	14.6
2	F	178	THR	14.6

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Mol	Chain	Res	Type	RSRZ
1	E	355	PHE	14.5
2	H	188	PHE	14.5
1	A	386	GLN	14.5
2	H	34	GLU	14.4
2	F	146	ASP	14.4
2	F	179	LEU	14.3
2	H	144	GLN	14.3
1	E	65	SER	14.3
2	B	150	GLY	14.2
2	F	177	SER	14.2
1	E	208	ILE	14.2
1	E	111	ASP	14.1
2	B	186	MET	14.1
2	P	111	ARG	14.1
2	H	112	HIS	14.1
2	F	115	SER	14.1
2	H	174	LEU	14.0
2	B	95	LYS	14.0
2	B	188	PHE	14.0
2	F	93	ILE	14.0
2	D	109	ARG	13.9
2	B	81	HIS	13.9
2	F	144	GLN	13.9
2	F	79	LEU	13.9
1	E	371	ARG	13.9
1	A	339	ILE	13.9
2	D	115	SER	13.8
2	H	133	ALA	13.8
2	B	149	ALA	13.7
1	A	382	GLY	13.7
2	D	135	ILE	13.6
2	H	116	ASN	13.6
2	D	113	LEU	13.6
2	F	112	HIS	13.6
2	H	147	ILE	13.5
2	B	148	PHE	13.4
2	F	81	HIS	13.4
1	E	377	ASN	13.4
2	D	116	ASN	13.4
2	H	148	PHE	13.3
2	F	140	ARG	13.3
2	H	61	ARG	13.2

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Mol	Chain	Res	Type	RSRZ
2	B	183	ASN	13.2
2	F	135	ILE	13.2
2	B	184	LEU	13.2
2	H	136	LEU	13.1
2	H	146	ASP	13.1
2	H	111	ARG	13.1
2	F	77	GLN	13.0
2	F	34	GLU	13.0
2	H	113	LEU	12.9
2	H	138	ARG	12.9
2	H	135	ILE	12.8
1	A	381	GLY	12.8
2	D	185	SER	12.7
1	E	354	ALA	12.7
2	B	131	ASN	12.7
1	E	209	GLY	12.7
2	F	113	LEU	12.7
1	E	94	LYS	12.6
2	H	134	PHE	12.6
1	E	337	ASN	12.5
2	H	115	SER	12.5
2	F	165	PHE	12.4
2	F	111	ARG	12.4
1	E	66	HIS	12.4
1	E	363	PRO	12.4
2	H	149	ALA	12.3
2	B	146	ASP	12.3
1	E	121	SER	12.2
2	B	175	ASP	12.1
1	U	421	GLY	12.1
2	B	53	ASP	12.1
2	F	78	ASP	12.1
1	U	258	ILE	12.0
2	B	92	ARG	11.9
1	E	171	LEU	11.9
2	B	187	PHE	11.9
2	B	84	GLU	11.8
1	A	257	GLN	11.8
1	W	430	GLY	11.8
2	H	152	ARG	11.8
2	P	41	ARG	11.7
2	H	105	ASN	11.7

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Mol	Chain	Res	Type	RSRZ
2	D	152	ARG	11.7
1	E	351	GLU	11.7
2	B	41	ARG	11.5
2	F	86	HIS	11.4
2	B	109	ARG	11.3
2	B	147	ILE	11.3
2	H	175	ASP	11.3
2	H	150	GLY	11.3
1	A	296	TRP	11.3
2	D	105	ASN	11.3
1	U	406	SER	11.2
1	G	380	ALA	11.2
2	D	111	ARG	11.2
2	H	151	GLU	11.1
1	A	357	LEU	11.0
2	D	27	ILE	11.0
1	E	129	ILE	10.9
1	E	210	GLY	10.9
2	F	151	GLU	10.6
1	E	72	ASP	10.4
2	D	154	ASP	10.2
2	H	131	ASN	10.2
2	H	169	LYS	10.1
2	F	131	ASN	10.0
1	E	326	ILE	9.9
1	C	257	GLN	9.8
2	F	169	LYS	9.7
2	B	154	ASP	9.7
2	D	188	PHE	9.6
1	W	113	GLY	9.6
2	D	175	ASP	9.5
1	A	244	LEU	9.5
1	E	333	LEU	9.4
2	B	169	LYS	9.4
1	W	73	PHE	9.3
1	A	255	GLN	9.3
1	W	320	VAL	9.2
1	W	438	ALA	9.2
2	D	25	ASN	9.1
2	D	28	GLU	9.1
2	B	177	SER	9.0
1	W	112	ALA	9.0

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Mol	Chain	Res	Type	RSRZ
2	H	50	LEU	9.0
1	E	345	ARG	8.9
2	B	137	TYR	8.9
2	D	49	LEU	8.9
1	M	310	GLY	8.8
1	W	227	PHE	8.8
2	H	36	GLN	8.8
2	B	151	GLU	8.8
1	A	358	VAL	8.8
1	W	358	VAL	8.8
1	E	213	LYS	8.7
1	W	420	THR	8.6
1	E	349	GLU	8.6
1	E	220	TRP	8.5
1	W	326	ILE	8.4
2	B	178	THR	8.4
1	A	216	ILE	8.3
1	E	87	ARG	8.3
1	E	368	GLU	8.2
1	W	311	HIS	8.2
1	W	156	ALA	8.2
2	F	180	LEU	8.2
1	U	314	MET	8.2
1	W	93	ILE	8.0
1	U	35	LEU	8.0
1	W	268	ALA	8.0
1	W	335	ALA	7.9
1	U	321	GLY	7.9
1	W	334	PRO	7.9
1	U	457	LEU	7.9
1	W	332	PHE	7.9
1	W	452	PRO	7.9
2	D	33	ARG	7.9
2	P	149	ALA	7.8
1	U	378	PHE	7.8
2	J	6	PRO	7.8
1	W	256	ALA	7.8
1	U	273	GLY	7.7
1	W	296	TRP	7.7
1	W	105	MET	7.6
2	X	71	LEU	7.6
1	W	336	MET	7.6

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Mol	Chain	Res	Type	RSRZ
1	W	95	VAL	7.6
1	U	332	PHE	7.5
2	J	160	ASP	7.5
1	M	420	THR	7.5
1	U	269	TRP	7.5
1	U	438	ALA	7.4
1	M	257	GLN	7.4
2	D	103	ALA	7.4
2	H	99	ASP	7.3
1	W	143	PHE	7.3
1	W	109	ARG	7.2
1	W	363	PRO	7.1
1	W	294	GLN	7.1
1	W	456	THR	7.0
1	E	212	GLN	7.0
1	W	339	ILE	7.0
1	W	257	GLN	7.0
1	W	384	PHE	6.9
2	D	24	GLN	6.9
1	W	341	ILE	6.9
1	U	259	PRO	6.9
2	B	62	THR	6.8
2	X	79	LEU	6.8
2	H	166	SER	6.8
1	W	91	LYS	6.8
2	F	69	GLY	6.8
1	W	107	ILE	6.7
1	W	153	PHE	6.7
1	U	257	GLN	6.7
1	W	429	VAL	6.7
1	S	109	ARG	6.6
1	W	333	LEU	6.6
1	U	256	ALA	6.6
1	W	74	LEU	6.6
1	W	142	ALA	6.6
1	C	258	ILE	6.5
1	W	75	ALA	6.5
1	U	260	THR	6.5
1	I	256	ALA	6.5
2	B	36	GLN	6.5
1	W	337	ASN	6.5
1	W	209	GLY	6.5

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Mol	Chain	Res	Type	RSRZ
1	E	365	GLU	6.4
1	U	326	ILE	6.4
1	E	81	ASP	6.4
1	W	129	ILE	6.4
1	U	295	TYR	6.4
1	W	60	LEU	6.4
1	Q	267	ALA	6.4
1	W	97	LEU	6.3
1	W	228	CYS	6.3
1	W	317	ARG	6.2
2	F	33	ARG	6.2
1	W	231	MET	6.2
1	A	342	TRP	6.2
2	F	25	ASN	6.2
1	U	420	THR	6.2
1	M	261	LYS	6.2
1	Q	430	GLY	6.2
1	W	176	TRP	6.2
1	W	224	ALA	6.2
1	W	183	LEU	6.2
1	W	261	LYS	6.1
1	U	229	SER	6.1
1	U	322	GLN	6.1
2	X	77	GLN	6.1
2	T	8	PHE	6.1
1	U	18	ASN	6.1
1	M	258	ILE	6.1
1	W	167	THR	6.1
1	E	256	ALA	6.1
1	M	313	GLY	6.1
2	H	84	GLU	6.1
1	K	455	ALA	6.0
1	W	54	PHE	6.0
1	W	171	LEU	6.0
1	U	323	HIS	6.0
1	W	431	TYR	6.0
2	F	28	GLU	6.0
1	W	207	ALA	6.0
1	W	442	TYR	6.0
1	A	388	ASP	6.0
1	G	256	ALA	6.0
1	W	291	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
1	S	105	MET	6.0
1	W	103	ARG	6.0
1	W	338	ASN	6.0
1	E	170	GLY	6.0
1	W	127	TYR	6.0
1	U	424	ASP	5.9
2	B	153	ARG	5.9
2	D	82	PHE	5.9
2	H	25	ASN	5.9
1	U	105	MET	5.9
1	U	324	MET	5.9
1	G	351	GLU	5.9
1	U	27	LEU	5.9
1	W	285	LEU	5.8
1	W	330	CYS	5.8
1	W	314	MET	5.8
1	U	93	ILE	5.8
2	J	8	PHE	5.8
1	Q	143	PHE	5.8
2	P	115	SER	5.8
1	W	115	ALA	5.8
1	W	154	ASP	5.8
2	F	76	ASP	5.8
1	W	258	ILE	5.7
2	B	44	GLU	5.7
2	X	160	ASP	5.7
2	H	153	ARG	5.7
2	B	87	GLU	5.7
2	D	61	ARG	5.7
1	U	276	TRP	5.7
1	W	354	ALA	5.7
1	W	418	SER	5.7
1	W	301	ALA	5.7
1	W	160	PRO	5.6
1	U	301	ALA	5.6
1	U	433	TYR	5.6
1	U	409	LEU	5.6
1	U	275	GLY	5.6
1	E	376	ARG	5.6
1	I	257	GLN	5.6
1	W	253	LEU	5.6
1	W	299	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	372	ARG	5.6
1	W	297	THR	5.6
1	U	224	ALA	5.6
1	U	331	SER	5.6
1	W	413	MET	5.6
1	W	158	TRP	5.6
1	I	18	ASN	5.5
1	M	416	GLY	5.5
1	U	452	PRO	5.5
1	W	203	ALA	5.5
1	A	337	ASN	5.5
1	M	311	HIS	5.5
1	W	161	LEU	5.4
1	U	205	THR	5.4
1	W	321	GLY	5.4
1	W	322	GLN	5.4
2	F	55	HIS	5.4
1	U	267	ALA	5.4
1	W	100	CYS	5.4
1	U	290	PRO	5.4
1	W	217	PRO	5.4
1	U	215	VAL	5.4
2	B	115	SER	5.4
1	W	86	VAL	5.4
1	A	227	PHE	5.4
1	I	411	ALA	5.4
1	W	122	TYR	5.3
1	U	437	ALA	5.3
1	I	259	PRO	5.3
2	H	55	HIS	5.3
1	I	32	LYS	5.3
2	F	36	GLN	5.3
1	W	39	ILE	5.3
1	E	211	MET	5.3
2	H	63	ASN	5.3
1	W	383	VAL	5.2
1	W	210	GLY	5.2
1	W	252	ASP	5.2
1	Q	258	ILE	5.2
1	W	155	LYS	5.2
1	U	330	CYS	5.2
1	U	384	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	G	453	SER	5.2
1	A	258	ILE	5.2
1	W	104	GLY	5.2
1	M	20	THR	5.2
1	U	312	THR	5.2
1	W	120	CYS	5.2
1	I	312	THR	5.2
1	W	118	PHE	5.2
1	W	226	GLN	5.2
1	W	71	GLY	5.2
1	W	316	VAL	5.2
1	Q	257	GLN	5.2
1	W	67	VAL	5.1
1	W	205	THR	5.1
1	U	450	SER	5.1
1	W	212	GLN	5.1
1	W	288	MET	5.1
2	F	23	LEU	5.1
1	W	331	SER	5.1
1	W	276	TRP	5.1
2	V	188	PHE	5.1
1	U	284	LEU	5.1
2	D	187	PHE	5.1
1	W	293	THR	5.1
1	U	227	PHE	5.1
1	U	197	MET	5.1
1	U	333	LEU	5.1
1	W	198	LEU	5.1
1	A	372	ARG	5.0
1	W	130	ALA	5.0
1	G	383	VAL	5.0
1	W	329	THR	5.0
2	F	40	HIS	5.0
1	M	247	ILE	5.0
2	H	44	GLU	5.0
1	W	21	PRO	5.0
2	F	41	ARG	5.0
1	Q	68	PRO	5.0
1	W	340	ARG	5.0
1	W	323	HIS	5.0
1	W	357	LEU	5.0
1	W	108	CYS	5.0

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Mol	Chain	Res	Type	RSRZ
2	H	33	ARG	5.0
1	U	419	GLN	5.0
2	L	6	PRO	5.0
1	W	66	HIS	5.0
2	J	162	ASN	4.9
1	M	178	VAL	4.9
1	W	125	TRP	4.9
1	E	330	CYS	4.9
1	W	99	GLN	4.9
1	W	312	THR	4.9
1	W	325	THR	4.9
1	A	367	LYS	4.9
2	D	60	LEU	4.9
1	U	178	VAL	4.9
1	E	80	GLU	4.9
1	U	393	VAL	4.9
1	U	432	VAL	4.9
1	U	339	ILE	4.9
2	F	87	GLU	4.9
1	U	19	TRP	4.9
1	U	296	TRP	4.9
1	E	118	PHE	4.9
1	W	425	PHE	4.9
1	M	260	THR	4.9
1	W	310	GLY	4.9
1	W	370	TYR	4.8
1	W	313	GLY	4.8
1	G	354	ALA	4.8
1	Q	422	HIS	4.8
1	Q	307	GLN	4.8
1	K	179	GLN	4.8
1	W	445	TRP	4.8
1	O	48	LEU	4.8
1	W	61	LEU	4.8
1	U	241	SER	4.8
1	U	334	PRO	4.8
2	D	73	TYR	4.8
1	W	229	SER	4.8
1	U	425	PHE	4.7
1	W	423	PRO	4.7
1	Q	35	LEU	4.7
1	O	70	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	U	264	GLN	4.7
1	M	415	LEU	4.7
1	W	319	MET	4.7
2	B	51	ASP	4.7
1	Q	302	ALA	4.7
1	U	335	ALA	4.7
1	W	83	VAL	4.7
1	U	337	ASN	4.7
1	U	389	GLY	4.7
2	F	129	GLU	4.7
1	W	84	VAL	4.7
1	W	134	VAL	4.7
1	M	421	GLY	4.7
1	W	206	VAL	4.6
1	U	271	GLY	4.6
1	E	340	ARG	4.6
1	M	455	ALA	4.6
1	W	411	ALA	4.6
1	Q	281	PRO	4.6
2	D	151	GLU	4.6
1	U	228	CYS	4.6
1	A	211	MET	4.6
2	X	90	TYR	4.6
1	U	280	GLU	4.6
1	U	58	TRP	4.6
1	W	187	LEU	4.6
2	P	133	ALA	4.6
1	M	419	GLN	4.6
1	W	419	GLN	4.6
1	U	71	GLY	4.6
1	W	275	GLY	4.6
1	U	315	PRO	4.6
1	W	32	LYS	4.6
1	U	255	GLN	4.6
1	W	186	TYR	4.5
2	F	44	GLU	4.5
1	W	260	THR	4.5
2	P	7	HIS	4.5
1	U	370	TYR	4.5
2	B	90	TYR	4.5
2	B	105	ASN	4.5
1	S	44	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	U	253	LEU	4.5
2	H	156	LEU	4.5
2	F	26	GLU	4.5
1	I	105	MET	4.5
1	K	89	LYS	4.5
1	W	433	TYR	4.5
1	W	52	ARG	4.5
1	E	329	THR	4.4
1	U	226	GLN	4.4
1	W	356	THR	4.4
1	C	18	ASN	4.4
2	V	184	LEU	4.4
1	Q	278	VAL	4.4
2	D	153	ARG	4.4
1	U	434	ALA	4.4
1	C	261	LYS	4.4
1	G	257	GLN	4.4
2	D	36	GLN	4.4
1	U	203	ALA	4.4
1	W	355	PHE	4.4
1	O	109	ARG	4.4
1	W	309	LEU	4.4
1	G	261	LYS	4.4
1	I	247	ILE	4.4
2	X	122	THR	4.4
1	W	35	LEU	4.4
1	U	28	VAL	4.4
1	U	292	VAL	4.4
1	U	383	VAL	4.4
1	W	62	GLY	4.4
1	U	303	GLU	4.4
1	I	253	LEU	4.4
2	V	162	ASN	4.4
1	W	197	MET	4.4
1	W	318	ARG	4.4
1	U	363	PRO	4.3
1	U	274	SER	4.3
1	U	302	ALA	4.3
1	U	417	ARG	4.3
1	O	153	PHE	4.3
1	U	305	ALA	4.3
2	B	78	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	W	392	TRP	4.3
1	M	411	ALA	4.3
1	W	30	GLN	4.3
1	U	310	GLY	4.3
1	U	342	TRP	4.3
1	U	445	TRP	4.3
1	W	31	GLU	4.3
1	W	85	MET	4.2
2	R	160	ASP	4.2
1	G	259	PRO	4.2
1	U	29	ASP	4.2
1	W	390	GLU	4.2
1	S	102	HIS	4.2
1	W	211	MET	4.2
1	W	255	GLN	4.2
1	W	225	GLU	4.2
1	U	230	ASP	4.2
1	S	121	SER	4.2
1	I	311	HIS	4.2
1	U	161	LEU	4.2
1	W	324	MET	4.2
1	Q	39	ILE	4.2
1	U	407	GLN	4.2
1	Q	105	MET	4.2
1	W	194	MET	4.2
1	U	193	TYR	4.2
1	Q	335	ALA	4.2
1	W	82	PRO	4.2
2	P	186	MET	4.2
2	F	106	PRO	4.2
1	A	376	ARG	4.1
1	Q	332	PHE	4.1
1	S	118	PHE	4.1
1	U	443	HIS	4.1
1	U	329	THR	4.1
1	W	76	THR	4.1
1	W	48	LEU	4.1
1	Q	320	VAL	4.1
1	W	98	ASN	4.1
1	Q	22	GLU	4.1
1	U	355	PHE	4.1
1	U	272	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	W	374	ASN	4.1
1	C	424	ASP	4.1
1	S	104	GLY	4.1
1	U	186	TYR	4.1
1	W	353	TRP	4.1
2	B	152	ARG	4.1
1	W	386	GLN	4.1
1	I	260	THR	4.1
1	U	325	THR	4.1
1	G	386	GLN	4.1
1	W	441	MET	4.1
1	Q	334	PRO	4.1
1	K	256	ALA	4.1
1	W	437	ALA	4.1
2	X	125	PRO	4.0
1	U	60	LEU	4.0
1	W	409	LEU	4.0
1	W	364	ALA	4.0
1	W	193	TYR	4.0
1	M	19	TRP	4.0
1	A	246	GLY	4.0
1	U	391	ASN	4.0
1	W	90	ASP	4.0
1	W	414	GLY	4.0
1	Q	297	THR	4.0
1	S	103	ARG	4.0
1	A	368	GLU	4.0
1	G	455	ALA	4.0
1	U	318	ARG	4.0
1	U	320	VAL	4.0
1	W	377	ASN	4.0
1	U	415	LEU	4.0
1	W	328	PRO	4.0
1	U	341	ILE	4.0
1	O	105	MET	4.0
2	D	141	LEU	4.0
2	D	26	GLU	3.9
1	W	440	GLY	3.9
1	I	181	PRO	3.9
1	U	32	LYS	3.9
1	E	455	ALA	3.9
1	W	124	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	33	ARG	3.9
1	M	452	PRO	3.9
1	U	287	VAL	3.9
1	W	375	ILE	3.9
2	R	8	PHE	3.9
1	E	254	SER	3.9
2	T	180	LEU	3.9
1	M	312	THR	3.9
1	M	196	VAL	3.9
1	S	122	TYR	3.9
2	P	67	ARG	3.9
1	W	190	ALA	3.9
1	W	278	VAL	3.9
2	B	7	HIS	3.9
1	K	134	VAL	3.9
1	W	395	ILE	3.9
1	G	374	ASN	3.9
1	W	277	TYR	3.9
1	W	274	SER	3.8
1	I	269	TRP	3.8
1	M	281	PRO	3.8
1	Q	113	GLY	3.8
1	W	65	SER	3.8
1	C	105	MET	3.8
1	U	20	THR	3.8
1	W	59	LEU	3.8
2	F	96	VAL	3.8
1	U	336	MET	3.8
1	W	123	HIS	3.8
1	W	272	HIS	3.8
1	S	158	TRP	3.8
1	S	89	LYS	3.8
2	J	7	HIS	3.8
1	Q	256	ALA	3.8
1	W	196	VAL	3.8
1	I	310	GLY	3.7
2	N	9	PHE	3.7
1	Q	32	LYS	3.7
1	W	106	ARG	3.7
1	W	393	VAL	3.7
1	U	361	ASP	3.7
1	W	64	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	W	53	VAL	3.7
1	U	201	THR	3.7
1	W	273	GLY	3.7
1	Q	254	SER	3.7
1	S	41	ALA	3.7
1	U	25	ARG	3.7
1	W	96	PHE	3.7
1	U	439	ARG	3.7
1	U	252	ASP	3.7
1	U	411	ALA	3.7
1	C	19	TRP	3.7
1	A	18	ASN	3.7
2	H	94	ARG	3.7
1	I	254	SER	3.7
1	Q	19	TRP	3.7
1	Q	93	ILE	3.7
1	Q	255	GLN	3.7
1	W	200	ARG	3.7
1	U	327	PHE	3.7
1	W	89	LYS	3.7
1	W	367	LYS	3.6
2	D	167	ILE	3.6
1	W	416	GLY	3.6
1	M	423	PRO	3.6
1	O	417	ARG	3.6
1	S	119	THR	3.6
1	U	109	ARG	3.6
1	I	178	VAL	3.6
1	U	140	LYS	3.6
1	M	253	LEU	3.6
1	U	309	LEU	3.6
2	L	8	PHE	3.6
1	M	22	GLU	3.6
1	M	71	GLY	3.6
2	H	142	GLU	3.6
1	I	318	ARG	3.6
2	H	143	ARG	3.6
1	U	358	VAL	3.6
1	O	257	GLN	3.6
1	U	455	ALA	3.6
1	W	220	TRP	3.6
1	W	378	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	Q	247	ILE	3.6
2	B	118	ILE	3.6
1	U	357	LEU	3.6
1	W	58	TRP	3.6
1	I	20	THR	3.6
1	U	70	THR	3.6
1	W	119	THR	3.6
1	S	90	ASP	3.5
1	S	38	ARG	3.5
1	U	240	LEU	3.5
1	W	25	ARG	3.5
1	W	27	LEU	3.5
1	W	233	HIS	3.5
2	N	162	ASN	3.5
1	W	372	ARG	3.5
2	B	61	ARG	3.5
2	D	143	ARG	3.5
1	C	260	THR	3.5
1	W	270	GLY	3.5
2	P	160	ASP	3.5
1	K	311	HIS	3.5
1	W	254	SER	3.5
1	S	86	VAL	3.5
1	U	392	TRP	3.5
1	U	442	TYR	3.5
1	W	117	ALA	3.5
1	W	192	PRO	3.5
1	U	33	GLY	3.5
1	E	69	GLU	3.5
2	F	70	GLU	3.5
2	P	16	SER	3.5
2	X	58	MET	3.5
1	K	115	ALA	3.5
1	Q	58	TRP	3.5
1	Q	454	TRP	3.5
1	W	40	TYR	3.5
1	O	113	GLY	3.5
1	S	52	ARG	3.5
1	E	64	GLU	3.5
1	U	61	LEU	3.5
1	S	137	PRO	3.5
1	A	341	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	Q	161	LEU	3.4
1	Q	253	LEU	3.4
1	O	173	PHE	3.4
1	W	453	SER	3.4
1	Q	336	MET	3.4
1	W	287	VAL	3.4
1	U	277	TYR	3.4
1	W	295	TYR	3.4
1	W	454	TRP	3.4
1	G	254	SER	3.4
1	W	380	ALA	3.4
2	X	133	ALA	3.4
1	U	289	GLY	3.4
1	S	415	LEU	3.4
1	A	233	HIS	3.4
1	M	18	ASN	3.4
1	I	423	PRO	3.4
1	M	21	PRO	3.4
1	Q	293	THR	3.4
1	W	79	GLY	3.4
1	W	365	GLU	3.4
1	C	283	SER	3.4
1	U	395	ILE	3.4
1	E	369	GLU	3.4
1	W	435	GLU	3.4
1	U	194	MET	3.4
1	U	204	GLY	3.4
1	M	259	PRO	3.4
1	U	181	PRO	3.4
1	W	249	PRO	3.4
1	A	419	GLN	3.4
1	U	83	VAL	3.4
1	W	121	SER	3.4
1	W	250	GLU	3.4
1	Q	309	LEU	3.4
2	B	139	ASN	3.3
1	M	182	ASP	3.3
2	J	96	VAL	3.3
1	U	120	CYS	3.3
1	W	56	ARG	3.3
2	H	88	THR	3.3
2	B	73	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	35	LEU	3.3
2	B	8	PHE	3.3
2	X	52	LYS	3.3
1	M	23	ALA	3.3
1	O	154	ASP	3.3
1	Q	456	THR	3.3
1	W	136	VAL	3.3
1	S	155	LYS	3.3
1	U	39	ILE	3.3
1	G	143	PHE	3.3
1	M	227	PHE	3.3
1	W	388	ASP	3.3
1	C	179	GLN	3.3
1	Q	260	THR	3.3
1	U	263	ASN	3.3
2	P	31	TYR	3.3
1	Q	294	GLN	3.3
1	E	93	ILE	3.3
1	I	24	ILE	3.3
1	U	247	ILE	3.3
1	U	328	PRO	3.3
1	U	366	ILE	3.3
1	U	232	TYR	3.3
1	W	110	SER	3.3
2	X	16	SER	3.3
1	W	327	PHE	3.3
1	U	316	VAL	3.3
1	C	259	PRO	3.3
1	U	399	LEU	3.3
1	W	208	ILE	3.3
2	H	66	ILE	3.3
1	U	242	GLY	3.3
1	G	260	THR	3.2
1	M	432	VAL	3.2
1	U	353	TRP	3.2
1	U	408	PRO	3.2
1	U	311	HIS	3.2
1	E	200	ARG	3.2
2	X	67	ARG	3.2
1	E	130	ALA	3.2
1	U	364	ALA	3.2
2	V	99	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	330	CYS	3.2
1	W	102	HIS	3.2
1	Q	409	LEU	3.2
1	S	457	LEU	3.2
1	U	171	LEU	3.2
1	U	288	MET	3.2
1	K	416	GLY	3.2
1	W	421	GLY	3.2
1	K	23	ALA	3.2
2	X	8	PHE	3.2
1	S	91	LYS	3.2
1	M	450	SER	3.2
1	W	259	PRO	3.2
1	Q	182	ASP	3.2
1	U	187	LEU	3.2
1	U	75	ALA	3.2
2	X	80	ALA	3.2
1	U	225	GLU	3.2
1	W	70	THR	3.2
1	W	101	ARG	3.2
1	Q	28	VAL	3.2
1	U	285	LEU	3.2
1	Q	455	ALA	3.2
2	H	90	TYR	3.2
1	Q	373	HIS	3.2
1	W	140	LYS	3.2
1	U	188	GLY	3.2
1	U	390	GLU	3.2
1	I	244	LEU	3.2
1	M	285	LEU	3.2
1	M	256	ALA	3.2
1	Q	450	SER	3.2
1	W	213	LYS	3.2
1	S	68	PRO	3.2
1	I	275	GLY	3.2
1	O	67	VAL	3.2
1	U	262	GLY	3.2
1	U	429	VAL	3.2
1	U	375	ILE	3.1
2	X	66	ILE	3.1
1	C	256	ALA	3.1
1	O	156	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	O	256	ALA	3.1
1	S	256	ALA	3.1
1	U	221	LYS	3.1
2	V	35	ALA	3.1
1	M	453	SER	3.1
1	Q	459	PRO	3.1
1	W	202	PRO	3.1
1	I	419	GLN	3.1
1	U	30	GLN	3.1
1	S	332	PHE	3.1
1	U	222	PHE	3.1
2	X	82	PHE	3.1
1	O	454	TRP	3.1
1	M	224	ALA	3.1
1	M	254	SER	3.1
1	M	337	ASN	3.1
1	S	406	SER	3.1
2	B	123	ALA	3.1
1	M	37	PRO	3.1
1	W	222	PHE	3.1
1	W	385	GLU	3.1
1	O	120	CYS	3.1
1	I	417	ARG	3.1
1	M	314	MET	3.1
1	Q	415	LEU	3.1
1	Q	339	ILE	3.1
1	U	167	THR	3.1
1	U	456	THR	3.1
1	U	104	GLY	3.1
1	K	138	PHE	3.1
1	Q	417	ARG	3.1
1	W	195	ASP	3.1
1	W	230	ASP	3.1
2	B	52	LYS	3.1
1	Q	31	GLU	3.1
1	S	110	SER	3.1
1	I	420	THR	3.1
1	M	315	PRO	3.1
1	U	21	PRO	3.1
2	X	69	GLY	3.1
1	A	261	LYS	3.1
1	U	87	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	W	458	LYS	3.1
1	Q	53	VAL	3.1
1	Q	92	SER	3.1
1	S	445	TRP	3.1
1	U	441	MET	3.1
1	I	33	GLY	3.1
1	U	404	ALA	3.1
1	W	34	LEU	3.1
1	U	340	ARG	3.1
1	W	290	PRO	3.1
1	U	77	TYR	3.0
1	A	421	GLY	3.0
1	W	382	GLY	3.0
2	R	10	LYS	3.0
1	U	98	ASN	3.0
1	U	377	ASN	3.0
1	U	40	TYR	3.0
1	W	308	ARG	3.0
1	S	429	VAL	3.0
1	Q	259	PRO	3.0
1	W	237	THR	3.0
2	P	6	PRO	3.0
1	W	19	TRP	3.0
1	U	394	GLU	3.0
1	M	431	TYR	3.0
1	Q	275	GLY	3.0
1	M	309	LEU	3.0
1	W	284	LEU	3.0
1	S	417	ARG	3.0
1	W	436	GLU	3.0
2	X	102	TRP	3.0
1	O	453	SER	3.0
1	U	440	GLY	3.0
1	W	232	TYR	3.0
2	X	56	TYR	3.0
1	I	203	ALA	3.0
1	U	184	GLU	3.0
1	U	74	LEU	3.0
2	X	54	ILE	3.0
1	I	222	PHE	3.0
1	W	265	PHE	3.0
1	U	293	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	W	446	MET	3.0
1	W	189	ASP	3.0
1	A	340	ARG	3.0
1	W	422	HIS	2.9
1	W	449	MET	2.9
1	E	252	ASP	2.9
2	H	160	ASP	2.9
1	C	421	GLY	2.9
1	W	410	ASN	2.9
2	H	162	ASN	2.9
1	G	456	THR	2.9
1	S	163	ALA	2.9
1	M	357	LEU	2.9
1	I	273	GLY	2.9
1	W	87	ARG	2.9
1	S	18	ASN	2.9
1	G	153	PHE	2.9
1	I	22	GLU	2.9
1	W	141	GLU	2.9
1	W	343	HIS	2.9
2	X	70	GLU	2.9
2	H	14	TRP	2.9
1	M	335	ALA	2.9
2	R	67	ARG	2.9
1	M	332	PHE	2.9
2	X	165	PHE	2.9
1	A	109	ARG	2.9
1	O	179	GLN	2.9
1	S	140	LYS	2.9
1	W	450	SER	2.9
1	S	67	VAL	2.9
1	U	430	GLY	2.9
1	W	352	VAL	2.9
2	J	19	ALA	2.9
1	A	369	GLU	2.9
1	W	415	LEU	2.9
1	U	100	CYS	2.9
1	O	258	ILE	2.9
1	K	109	ARG	2.9
1	S	452	PRO	2.9
1	W	459	PRO	2.9
2	V	74	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	W	289	GLY	2.9
2	X	162	ASN	2.9
1	M	269	TRP	2.9
1	S	269	TRP	2.9
1	W	342	TRP	2.9
1	Q	48	LEU	2.9
1	W	191	ARG	2.9
1	O	262	GLY	2.9
1	U	270	GLY	2.9
1	W	448	MET	2.9
1	U	97	LEU	2.8
2	V	44	GLU	2.8
1	K	93	ILE	2.8
1	U	459	PRO	2.8
2	X	132	SER	2.8
1	Q	414	GLY	2.8
1	W	78	MET	2.8
2	D	48	ALA	2.8
1	U	84	VAL	2.8
1	K	415	LEU	2.8
1	K	423	PRO	2.8
1	U	338	ASN	2.8
1	O	143	PHE	2.8
1	Q	317	ARG	2.8
1	W	22	GLU	2.8
2	T	70	GLU	2.8
1	Q	438	ALA	2.8
2	F	65	MET	2.8
1	I	320	VAL	2.8
1	U	458	LYS	2.8
1	W	114	ASN	2.8
1	S	125	TRP	2.8
1	U	214	TRP	2.8
1	U	243	ILE	2.8
1	U	454	TRP	2.8
1	W	43	GLN	2.8
2	B	29	GLN	2.8
1	I	424	ASP	2.8
1	Q	224	ALA	2.8
1	Q	311	HIS	2.8
2	J	65	MET	2.8
1	U	141	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	W	439	ARG	2.8
1	U	431	TYR	2.8
2	X	32	TYR	2.8
1	Q	273	GLY	2.8
1	S	416	GLY	2.8
2	J	16	SER	2.8
2	R	76	ASP	2.8
1	Q	276	TRP	2.8
1	U	265	PHE	2.8
1	U	297	THR	2.8
2	L	7	HIS	2.8
1	G	23	ALA	2.8
1	O	117	ALA	2.8
2	P	162	ASN	2.8
1	C	426	PRO	2.8
1	K	132	LYS	2.8
1	W	204	GLY	2.8
1	O	158	TRP	2.8
1	Q	227	PHE	2.8
1	U	233	HIS	2.8
1	W	417	ARG	2.8
1	M	286	ALA	2.8
1	Q	458	LYS	2.8
2	V	160	ASP	2.8
1	I	432	VAL	2.8
1	K	202	PRO	2.8
1	M	271	GLY	2.8
1	Q	110	SER	2.8
1	U	110	SER	2.8
1	W	68	PRO	2.8
1	U	69	GLU	2.8
2	J	90	TYR	2.8
2	J	94	ARG	2.8
1	W	173	PHE	2.7
2	D	12	PHE	2.7
1	Q	286	ALA	2.7
2	X	76	ASP	2.7
1	S	299	GLY	2.7
1	M	244	LEU	2.7
1	S	161	LEU	2.7
1	M	322	GLN	2.7
1	Q	193	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	S	108	CYS	2.7
1	M	323	HIS	2.7
1	K	153	PHE	2.7
2	V	187	PHE	2.7
1	U	449	MET	2.7
1	K	55	GLY	2.7
1	W	283	SER	2.7
1	K	137	PRO	2.7
1	M	202	PRO	2.7
1	M	290	PRO	2.7
1	W	376	ARG	2.7
2	B	6	PRO	2.7
1	S	133	LEU	2.7
1	S	339	ILE	2.7
1	W	138	PHE	2.7
1	C	455	ALA	2.7
1	I	421	GLY	2.7
1	M	305	ALA	2.7
1	O	430	GLY	2.7
1	W	381	GLY	2.7
1	U	308	ARG	2.7
1	M	327	PHE	2.7
1	S	143	PHE	2.7
1	U	412	GLN	2.7
1	E	251	MET	2.7
1	O	423	PRO	2.7
1	Q	196	VAL	2.7
1	K	41	ALA	2.7
1	Q	156	ALA	2.7
1	Q	190	ALA	2.7
1	W	245	ALA	2.7
1	A	21	PRO	2.7
1	S	21	PRO	2.7
1	Q	116	LYS	2.7
2	X	50	LEU	2.7
1	C	20	THR	2.7
1	M	141	GLU	2.7
1	W	271	GLY	2.7
1	G	105	MET	2.7
1	U	261	LYS	2.7
1	Q	423	PRO	2.7
1	U	319	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	U	448	MET	2.7
2	X	148	PHE	2.7
1	W	111	ASP	2.7
1	O	103	ARG	2.7
1	U	59	LEU	2.6
1	W	201	THR	2.6
1	G	204	GLY	2.6
1	W	57	SER	2.6
1	W	94	LYS	2.6
1	M	326	ILE	2.6
1	U	402	TYR	2.6
1	Q	153	PHE	2.6
1	W	315	PRO	2.6
1	U	139	GLU	2.6
1	W	88	GLN	2.6
1	Q	429	VAL	2.6
1	S	45	LEU	2.6
1	Q	379	SER	2.6
2	T	67	ARG	2.6
1	W	307	GLN	2.6
1	A	73	PHE	2.6
1	G	138	PHE	2.6
1	O	130	ALA	2.6
1	W	223	ALA	2.6
1	A	237	THR	2.6
1	Q	318	ARG	2.6
1	E	383	VAL	2.6
1	I	410	ASN	2.6
1	M	297	THR	2.6
1	I	333	LEU	2.6
1	S	171	LEU	2.6
1	U	423	PRO	2.6
2	P	10	LYS	2.6
1	I	288	MET	2.6
1	O	250	GLU	2.6
1	K	453	SER	2.6
1	S	279	ASP	2.6
2	H	11	THR	2.6
1	S	134	VAL	2.6
1	I	326	ILE	2.6
1	M	192	PRO	2.6
1	U	37	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	19	TRP	2.6
1	Q	69	GLU	2.6
1	U	234	ALA	2.6
1	U	354	ALA	2.6
1	W	234	ALA	2.6
2	J	58	MET	2.6
1	M	33	GLY	2.6
2	R	161	ASN	2.6
1	S	136	VAL	2.6
2	N	96	VAL	2.6
2	X	114	VAL	2.6
1	I	452	PRO	2.6
1	U	245	ALA	2.6
1	I	307	GLN	2.6
1	K	88	GLN	2.6
1	M	289	GLY	2.6
1	Q	158	TRP	2.6
1	U	414	GLY	2.6
2	D	14	TRP	2.6
2	X	134	PHE	2.6
1	I	274	SER	2.6
1	Q	306	GLU	2.6
1	S	306	GLU	2.6
1	S	83	VAL	2.6
1	U	196	VAL	2.6
1	Q	29	ASP	2.5
1	U	410	ASN	2.5
1	O	455	ALA	2.5
1	Q	324	MET	2.5
1	W	242	GLY	2.5
1	M	433	TYR	2.5
1	O	283	SER	2.5
2	X	73	TYR	2.5
1	W	444	HIS	2.5
2	X	10	LYS	2.5
1	O	84	VAL	2.5
1	S	28	VAL	2.5
2	H	24	GLN	2.5
1	W	41	ALA	2.5
1	W	126	ALA	2.5
1	W	77	TYR	2.5
1	O	100	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	S	19	TRP	2.5
1	Q	333	LEU	2.5
1	U	352	VAL	2.5
1	W	304	LEU	2.5
1	U	22	GLU	2.5
1	I	414	GLY	2.5
1	M	430	GLY	2.5
1	U	170	GLY	2.5
1	U	401	GLY	2.5
1	E	203	ALA	2.5
1	S	335	ALA	2.5
1	W	221	LYS	2.5
2	H	12	PHE	2.5
1	Q	127	TYR	2.5
1	G	201	THR	2.5
1	Q	70	THR	2.5
1	S	88	GLN	2.5
1	W	81	ASP	2.5
1	W	263	ASN	2.5
1	W	424	ASP	2.5
1	I	334	PRO	2.5
1	M	328	PRO	2.5
1	O	457	LEU	2.5
1	W	33	GLY	2.5
1	I	258	ILE	2.5
1	K	129	ILE	2.5
1	O	255	GLN	2.5
1	S	311	HIS	2.5
1	U	451	GLU	2.5
1	S	260	THR	2.5
2	V	105	ASN	2.5
1	Q	91	LYS	2.5
1	I	296	TRP	2.5
1	W	170	GLY	2.5
1	W	262	GLY	2.5
2	X	60	LEU	2.5
1	U	373	HIS	2.5
1	G	258	ILE	2.5
1	K	424	ASP	2.5
1	Q	232	TYR	2.5
2	L	70	GLU	2.5
1	I	316	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	S	34	LEU	2.5
1	W	379	SER	2.5
1	M	404	ALA	2.5
2	X	123	ALA	2.5
1	U	413	MET	2.5
1	G	20	THR	2.4
1	G	420	THR	2.4
1	C	192	PRO	2.4
1	M	255	GLN	2.4
1	W	92	SER	2.4
1	U	278	VAL	2.4
1	S	348	ASN	2.4
1	W	391	ASN	2.4
1	U	190	ALA	2.4
1	C	290	PRO	2.4
1	M	193	TYR	2.4
1	G	252	ASP	2.4
1	U	199	ASP	2.4
1	U	422	HIS	2.4
2	N	160	ASP	2.4
1	G	304	LEU	2.4
1	M	198	LEU	2.4
1	U	183	LEU	2.4
1	W	28	VAL	2.4
2	X	163	LEU	2.4
1	C	142	ALA	2.4
1	U	23	ALA	2.4
1	W	360	ALA	2.4
1	U	231	MET	2.4
1	G	310	GLY	2.4
1	Q	420	THR	2.4
2	R	11	THR	2.4
1	M	363	PRO	2.4
1	S	106	ARG	2.4
1	S	459	PRO	2.4
2	F	160	ASP	2.4
1	Q	60	LEU	2.4
2	D	156	LEU	2.4
2	V	37	LEU	2.4
1	K	257	GLN	2.4
1	Q	30	GLN	2.4
1	U	43	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	U	446	MET	2.4
1	K	310	GLY	2.4
1	O	52	ARG	2.4
1	Q	129	ILE	2.4
1	C	248	PRO	2.4
1	U	202	PRO	2.4
2	T	76	ASP	2.4
1	O	186	TYR	2.4
1	Q	419	GLN	2.4
2	P	180	LEU	2.4
1	Q	83	VAL	2.4
1	W	292	VAL	2.4
2	H	119	VAL	2.4
1	U	62	GLY	2.4
2	L	68	GLU	2.4
2	X	167	ILE	2.4
1	Q	344	PRO	2.4
2	F	90	TYR	2.4
1	A	22	GLU	2.4
1	I	284	LEU	2.4
1	I	457	LEU	2.4
1	M	304	LEU	2.4
1	M	316	VAL	2.4
2	V	126	ASP	2.4
1	U	76	THR	2.4
2	N	124	THR	2.4
1	M	331	SER	2.4
1	W	137	PRO	2.4
1	W	443	HIS	2.4
1	M	296	TRP	2.4
1	M	417	ARG	2.4
1	Q	365	GLU	2.4
1	U	266	ARG	2.4
1	M	321	GLY	2.3
1	U	34	LEU	2.3
1	U	346	GLY	2.3
1	W	55	GLY	2.3
1	E	134	VAL	2.3
1	O	259	PRO	2.3
1	Q	290	PRO	2.3
1	Q	418	SER	2.3
1	O	107	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	375	ILE	2.3
1	U	64	GLU	2.3
2	X	188	PHE	2.3
1	O	419	GLN	2.3
1	O	429	VAL	2.3
1	S	120	CYS	2.3
1	U	95	VAL	2.3
1	W	455	ALA	2.3
1	K	70	THR	2.3
1	M	325	THR	2.3
1	Q	426	PRO	2.3
1	W	426	PRO	2.3
2	J	97	THR	2.3
1	E	88	GLN	2.3
1	E	253	LEU	2.3
1	Q	109	ARG	2.3
1	Q	304	LEU	2.3
2	L	67	ARG	2.3
1	C	134	VAL	2.3
1	U	172	VAL	2.3
2	J	159	ALA	2.3
2	X	62	THR	2.3
1	W	243	ILE	2.3
1	G	416	GLY	2.3
1	O	118	PHE	2.3
1	Q	263	ASN	2.3
1	K	103	ARG	2.3
1	U	220	TRP	2.3
1	Q	284	LEU	2.3
1	W	239	HIS	2.3
2	X	38	LEU	2.3
1	M	434	ALA	2.3
1	G	248	PRO	2.3
1	I	278	VAL	2.3
1	S	165	VAL	2.3
1	Q	197	MET	2.3
1	S	312	THR	2.3
1	S	334	PRO	2.3
2	X	13	GLU	2.3
1	O	93	ILE	2.3
1	U	291	LYS	2.3
1	W	116	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	308	ARG	2.3
2	V	8	PHE	2.3
1	I	232	TYR	2.3
1	O	75	ALA	2.3
1	S	454	TRP	2.3
2	R	97	THR	2.3
2	X	117	VAL	2.3
1	M	38	ARG	2.3
1	O	375	ILE	2.3
1	Q	270	GLY	2.3
2	V	87	GLU	2.3
1	C	154	ASP	2.3
1	S	42	ASP	2.3
1	W	177	ASP	2.3
1	E	20	THR	2.3
1	M	302	ALA	2.3
1	O	335	ALA	2.3
1	S	257	GLN	2.3
1	Q	325	THR	2.3
1	W	238	THR	2.3
2	P	15	PRO	2.3
2	X	174	LEU	2.3
2	V	94	ARG	2.2
1	K	19	TRP	2.2
1	S	220	TRP	2.2
1	S	135	ASN	2.2
1	U	26	GLY	2.2
1	W	131	GLY	2.2
1	G	22	GLU	2.2
1	O	365	GLU	2.2
1	S	107	ILE	2.2
2	P	70	GLU	2.2
2	R	68	GLU	2.2
1	W	397	LYS	2.2
1	I	255	GLN	2.2
2	X	115	SER	2.2
1	I	245	ALA	2.2
1	I	437	ALA	2.2
1	Q	238	THR	2.2
1	W	185	THR	2.2
2	J	180	LEU	2.2
2	P	18	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	W	172	VAL	2.2
1	W	214	TRP	2.2
1	M	24	ILE	2.2
1	O	307	GLN	2.2
1	Q	199	ASP	2.2
1	W	199	ASP	2.2
2	T	16	SER	2.2
1	O	202	PRO	2.2
1	E	261	LYS	2.2
1	W	428	ASN	2.2
1	C	457	LEU	2.2
1	Q	234	ALA	2.2
1	W	399	LEU	2.2
2	V	38	LEU	2.2
2	X	173	LEU	2.2
1	K	105	MET	2.2
1	O	86	VAL	2.2
2	V	58	MET	2.2
1	U	168	TYR	2.2
1	I	252	ASP	2.2
1	Q	264	GLN	2.2
1	M	317	ARG	2.2
2	N	157	ARG	2.2
2	N	158	ARG	2.2
2	P	170	ARG	2.2
1	U	435	GLU	2.2
2	D	131	ASN	2.2
1	I	201	THR	2.2
1	I	309	LEU	2.2
1	K	166	ALA	2.2
1	M	333	LEU	2.2
1	M	409	LEU	2.2
1	S	156	ALA	2.2
2	J	18	ALA	2.2
1	K	307	GLN	2.2
1	A	279	ASP	2.2
2	X	100	VAL	2.2
2	R	162	ASN	2.2
1	I	327	PHE	2.2
1	S	456	THR	2.2
1	C	109	ARG	2.2
1	G	372	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	203	ALA	2.2
1	S	268	ALA	2.2
1	S	455	ALA	2.2
1	U	179	GLN	2.2
1	A	385	GLU	2.2
1	I	429	VAL	2.2
1	S	330	CYS	2.2
1	U	444	HIS	2.2
1	S	331	SER	2.2
1	Q	410	ASN	2.2
2	V	135	ILE	2.2
1	I	19	TRP	2.2
1	G	427	GLY	2.2
1	U	192	PRO	2.2
1	S	199	ASP	2.2
2	N	127	THR	2.2
1	M	223	ALA	2.2
1	O	115	ALA	2.2
1	S	117	ALA	2.2
1	M	105	MET	2.2
1	K	418	SER	2.2
1	U	206	VAL	2.2
1	W	371	ARG	2.1
1	E	259	PRO	2.1
2	H	85	THR	2.1
1	O	285	LEU	2.1
2	V	100	VAL	2.1
1	C	282	GLY	2.1
1	M	350	ILE	2.1
1	S	39	ILE	2.1
1	W	359	ASP	2.1
1	E	420	THR	2.1
1	U	143	PHE	2.1
1	U	158	TRP	2.1
1	E	116	LYS	2.1
1	I	251	MET	2.1
1	Q	88	GLN	2.1
1	W	133	LEU	2.1
2	X	113	LEU	2.1
1	C	278	VAL	2.1
1	M	320	VAL	2.1
1	E	361	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	414	GLY	2.1
1	A	366	ILE	2.1
1	O	137	PRO	2.1
1	Q	451	GLU	2.1
1	S	51	GLU	2.1
1	S	141	GLU	2.1
2	X	187	PHE	2.1
1	S	126	ALA	2.1
1	U	223	ALA	2.1
1	A	392	TRP	2.1
1	O	416	GLY	2.1
1	Q	250	GLU	2.1
1	W	280	GLU	2.1
1	O	180	ALA	2.1
1	O	364	ALA	2.1
1	U	156	ALA	2.1
1	Q	251	MET	2.1
1	W	128	ASP	2.1
2	D	160	ASP	2.1
1	E	22	GLU	2.1
1	I	392	TRP	2.1
1	M	221	LYS	2.1
1	Q	352	VAL	2.1
1	S	255	GLN	2.1
1	Q	277	TYR	2.1
2	B	116	ASN	2.1
1	Q	341	ILE	2.1
1	I	450	SER	2.1
1	M	418	SER	2.1
1	Q	331	SER	2.1
1	U	379	SER	2.1
1	Q	157	GLU	2.1
1	Q	305	ALA	2.1
1	U	90	ASP	2.1
1	M	319	MET	2.1
1	Q	457	LEU	2.1
2	P	184	LEU	2.1
1	W	345	ARG	2.1
1	Q	67	VAL	2.1
1	W	165	VAL	2.1
1	W	181	PRO	2.1
1	W	344	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	W	24	ILE	2.1
2	B	124	THR	2.1
1	U	268	ALA	2.1
1	O	55	GLY	2.0
1	O	421	GLY	2.0
1	A	60	LEU	2.0
1	A	333	LEU	2.0
1	G	333	LEU	2.0
1	Q	183	LEU	2.0
1	M	249	PRO	2.0
1	M	280	GLU	2.0
1	O	334	PRO	2.0
1	W	175	ASN	2.0
2	B	182	ASN	2.0
1	Q	84	VAL	2.0
2	F	100	VAL	2.0
1	E	260	THR	2.0
1	M	277	TYR	2.0
1	S	101	ARG	2.0
1	I	321	GLY	2.0
1	Q	96	PHE	2.0
1	S	30	GLN	2.0
1	S	419	GLN	2.0
1	S	421	GLY	2.0
2	N	8	PHE	2.0
2	X	103	ALA	2.0
1	I	280	GLU	2.0
1	K	69	GLU	2.0
2	T	10	LYS	2.0
1	W	50	LEU	2.0
2	D	183	ASN	2.0
1	Q	363	PRO	2.0
1	W	218	CYS	2.0
1	O	110	SER	2.0
1	U	125	TRP	2.0
1	W	44	SER	2.0
1	K	312	THR	2.0
1	Q	237	THR	2.0
2	L	66	ILE	2.0
1	M	438	ALA	2.0
1	Q	369	GLU	2.0
1	O	332	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	Q	338	ASN	2.0
1	W	373	HIS	2.0
1	I	249	PRO	2.0
1	U	67	VAL	2.0
1	O	91	LYS	2.0
1	M	238	THR	2.0
1	M	306	GLU	2.0
1	M	454	TRP	2.0
1	Q	445	TRP	2.0
2	D	124	THR	2.0
2	V	46	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	FE2	G	901	1/1	0.11	-0.49	14,14,14,14	0
3	FES	E	900	4/4	0.05	-0.60	13,13,14,15	0
3	FES	I	900	4/4	0.07	-0.85	14,15,15,17	0
3	FES	C	900	4/4	0.07	-0.86	17,18,19,19	0
4	FE2	A	901	1/1	0.10	-1.01	13,13,13,13	0
3	FES	G	900	4/4	0.09	-1.47	25,26,26,27	0
4	FE2	O	901	1/1	0.09	-1.53	32,32,32,32	0
3	FES	A	900	4/4	0.07	-1.59	19,20,22,22	0
4	FE2	C	901	1/1	0.08	-1.68	29,29,29,29	0
4	FE2	U	901	1/1	0.19	-1.83	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	FE2	E	901	1/1	0.05	-2.00	20,20,20,20	0
3	FES	S	900	4/4	0.07	-2.13	48,48,50,50	0
3	FES	U	900	4/4	0.05	-2.40	21,23,23,27	0
3	FES	Q	900	4/4	0.07	-2.50	31,32,37,37	0
3	FES	M	900	4/4	0.06	-2.56	21,21,21,21	0
3	FES	K	900	4/4	0.04	-2.73	32,33,34,35	0
3	FES	O	900	4/4	0.07	-2.86	41,42,43,43	0
4	FE2	M	901	1/1	0.07	-3.10	37,37,37,37	0
4	FE2	W	901	1/1	0.06	-3.19	57,57,57,57	0
4	FE2	K	901	1/1	0.05	-3.20	19,19,19,19	0
3	FES	W	900	4/4	0.08	-4.00	65,67,68,69	0
4	FE2	S	901	1/1	0.03	-4.06	26,26,26,26	0
4	FE2	Q	901	1/1	0.04	-5.03	45,45,45,45	0
4	FE2	I	901	1/1	0.09	-6.42	48,48,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.