Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

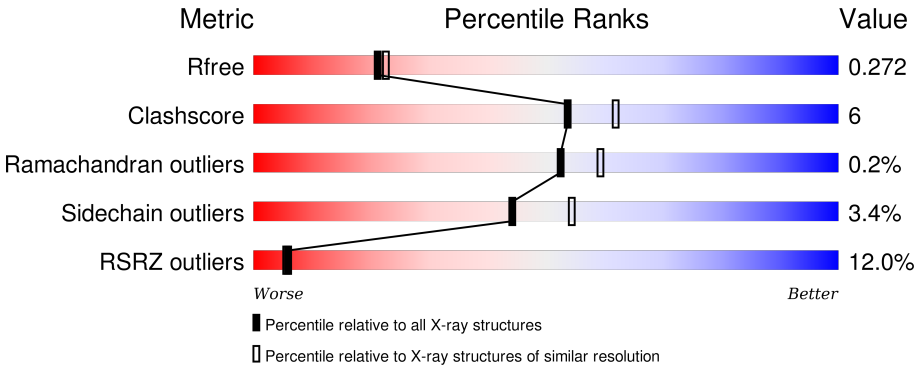
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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. 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 <=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	81% 13% • 6%
1	C	459	2% 83% 10% • 6%
1	E	459	2% 80% 14% • 6%
1	G	459	3% 80% 13% • 6%
1	I	459	10% 76% 18% • 6%

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Mol	Chain	Length	Quality of chain
1	K	459	4% 78% 14% 6%
1	M	459	12% 80% 14% 6%
1	O	459	6% 79% 14% 6%
1	Q	459	15% 78% 15% 6%
1	S	459	12% 75% 18% 6%
1	U	459	43% 74% 19% 6%
1	W	459	62% 76% 17% 6%
2	B	188	% 87% 10%
2	D	188	% 80% 16%
2	F	188	% 83% 14%
2	H	188	2% 85% 11%
2	J	188	4% 83% 14%
2	L	188	3% 86% 11%
2	N	188	2% 79% 16%
2	P	188	5% 83% 13%
2	R	188	2% 83% 13%
2	T	188	% 82% 14%
2	V	188	7% 85% 11%
2	X	188	19% 81% 14%

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	-
4	FE2	G	901	-	-	-	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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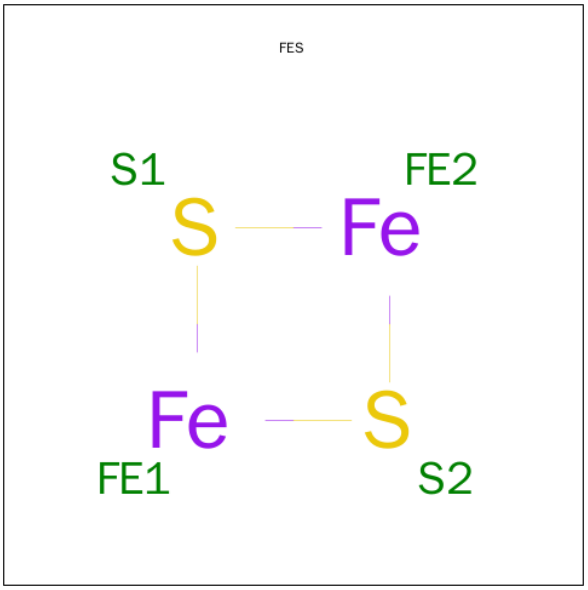
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	X	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: 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 Fe S 4 2 2	0	0
3	U	1	Total Fe S 4 2 2	0	0
3	W	1	Total Fe S 4 2 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 Fe 1 1	0	0
4	Q	1	Total Fe 1 1	0	0
4	K	1	Total Fe 1 1	0	0
4	E	1	Total Fe 1 1	0	0
4	I	1	Total Fe 1 1	0	0
4	C	1	Total Fe 1 1	0	0
4	W	1	Total Fe 1 1	0	0
4	A	1	Total Fe 1 1	0	0
4	U	1	Total Fe 1 1	0	0
4	O	1	Total Fe 1 1	0	0
4	S	1	Total Fe 1 1	0	0
4	M	1	Total Fe 1 1	0	0

- Molecule 5 is water.

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

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

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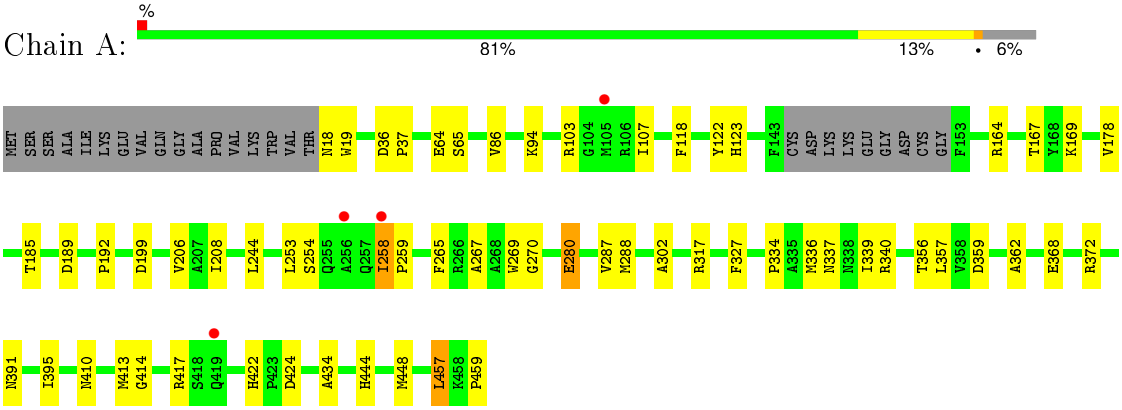
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	X	37	37	37	0	0

3 Residue-property plots (i)

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

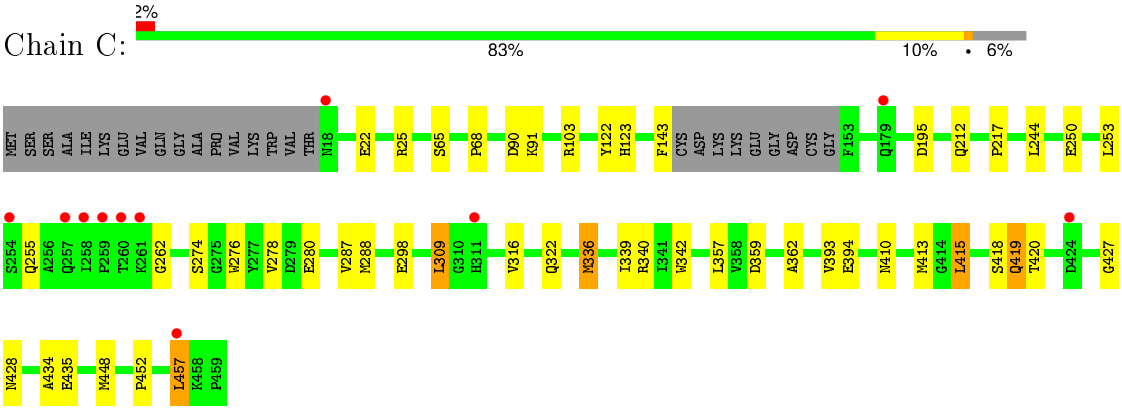
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain A:



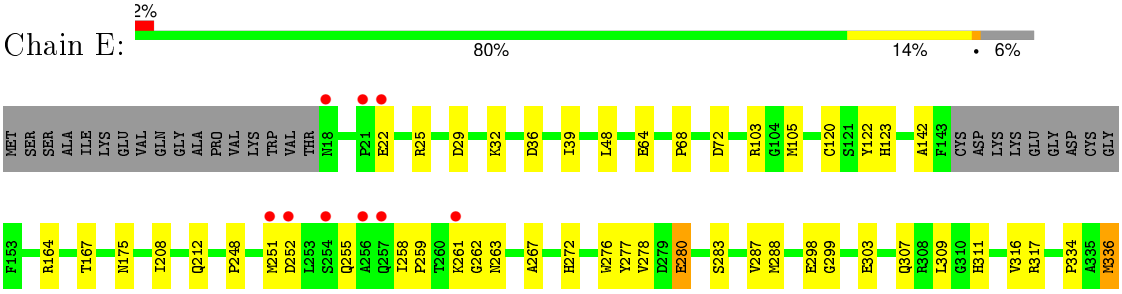
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain C:



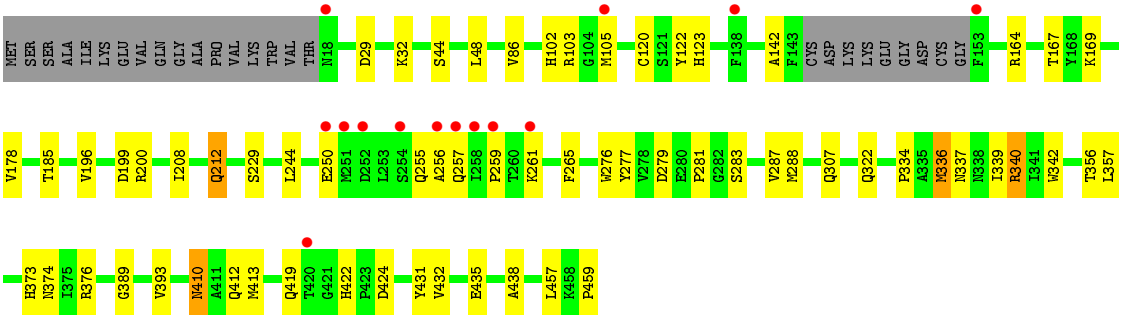
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain E:



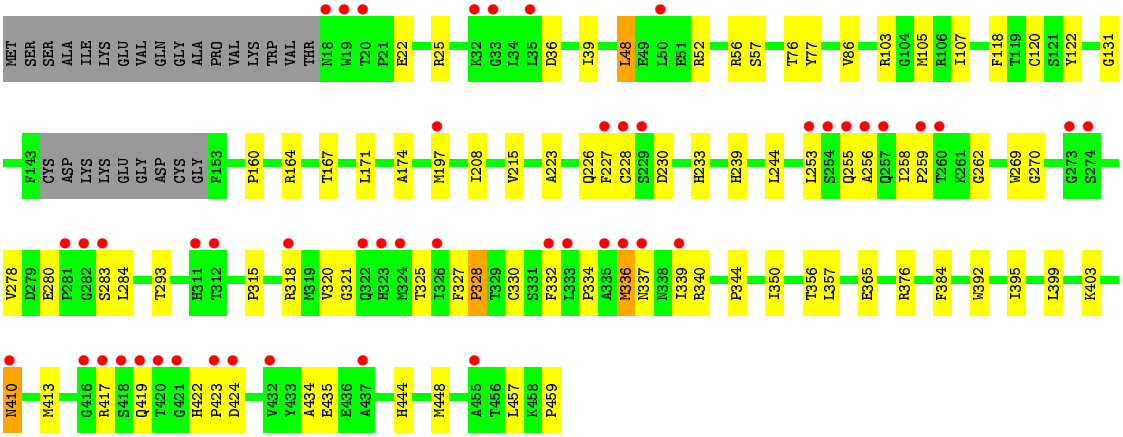
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain G:



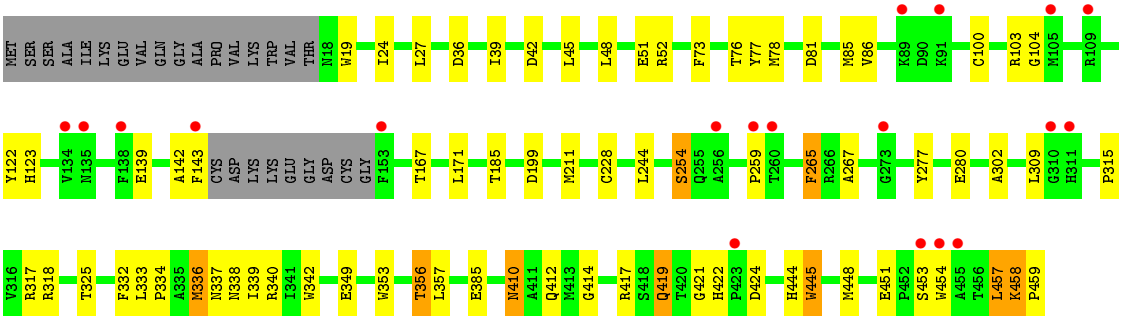
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain I:



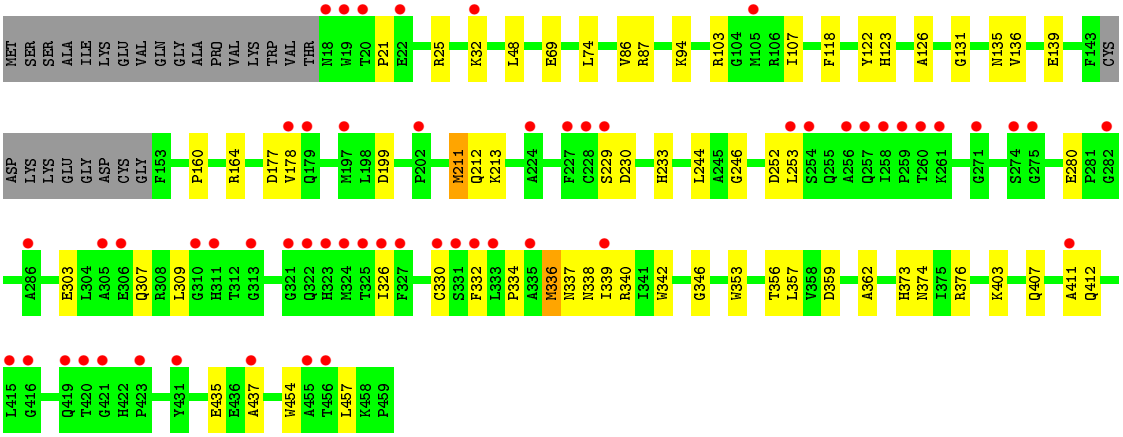
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain K:



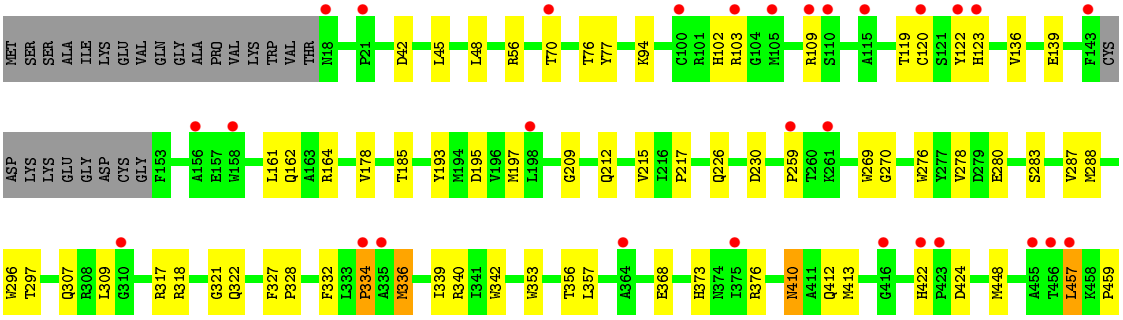
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain M:



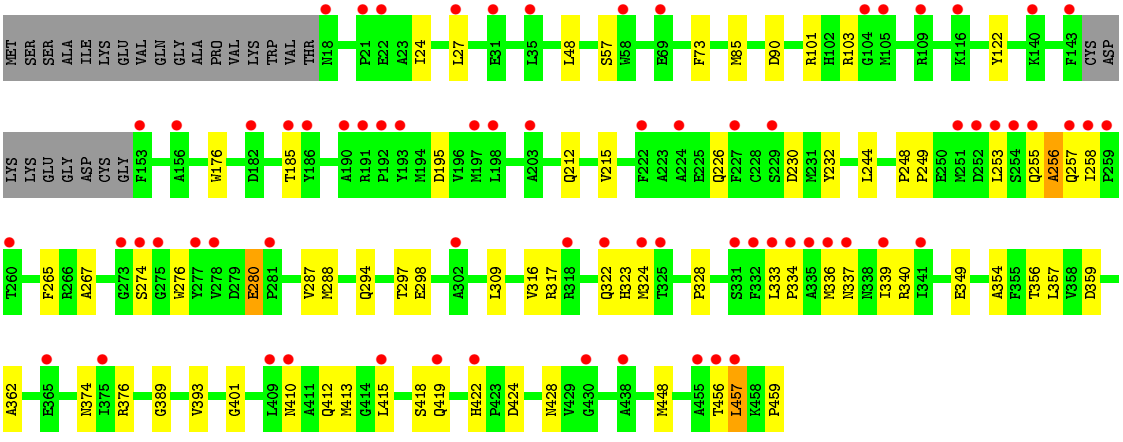
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain O:



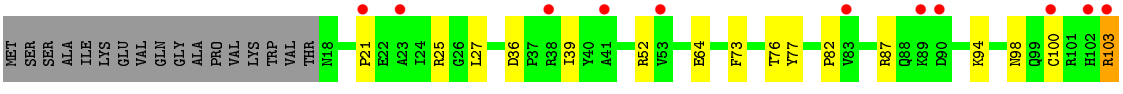
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

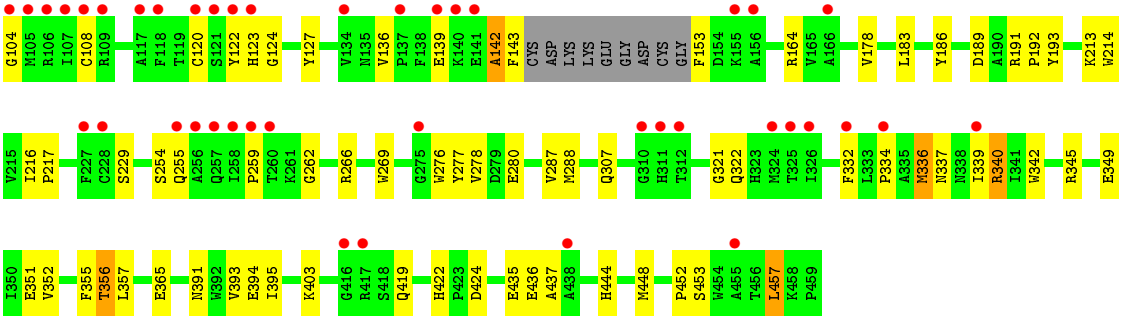
Chain Q:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

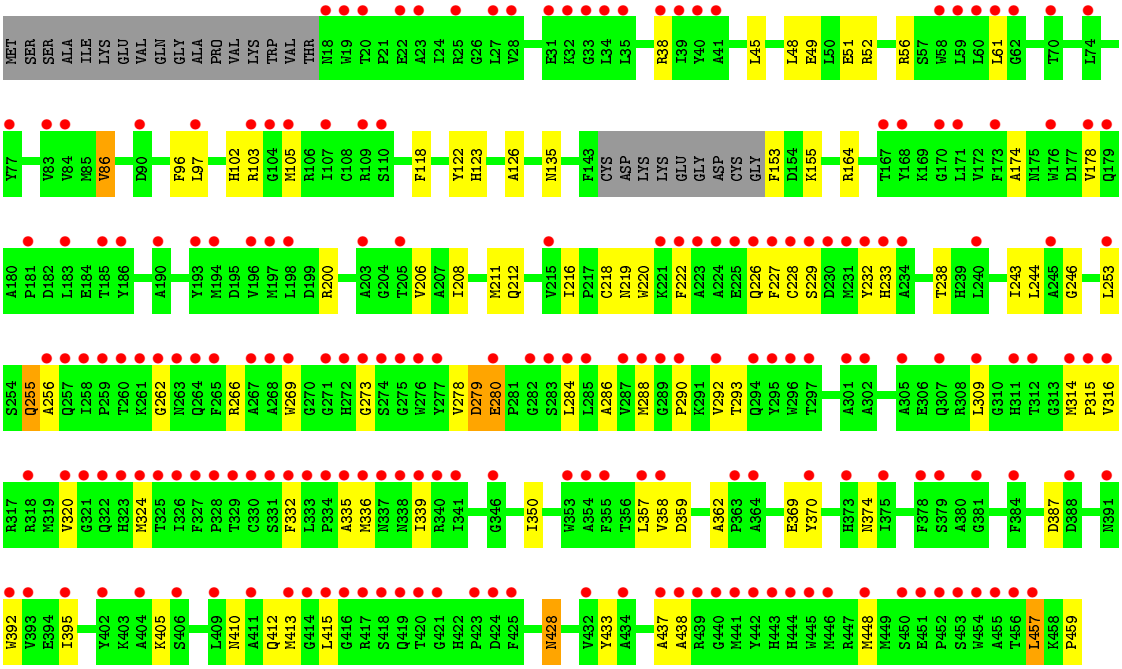
Chain S:





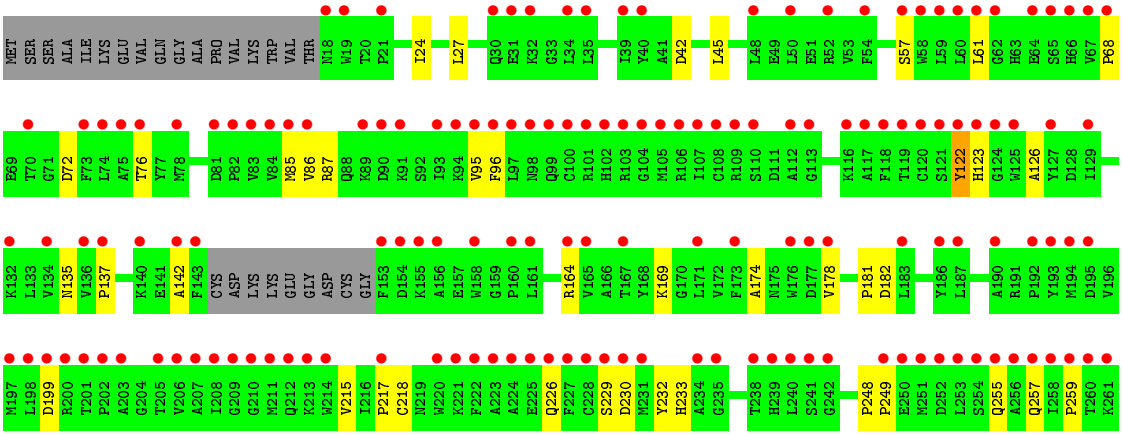
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

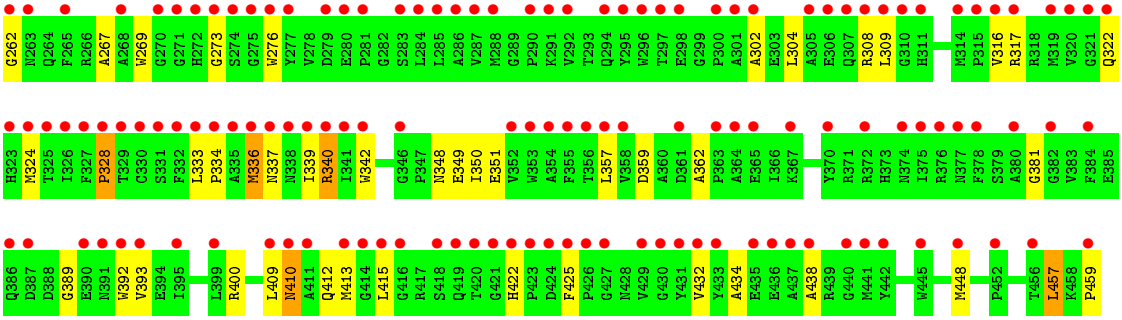
Chain U:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

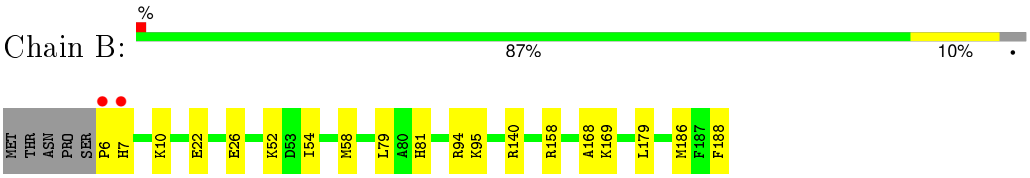
Chain W:





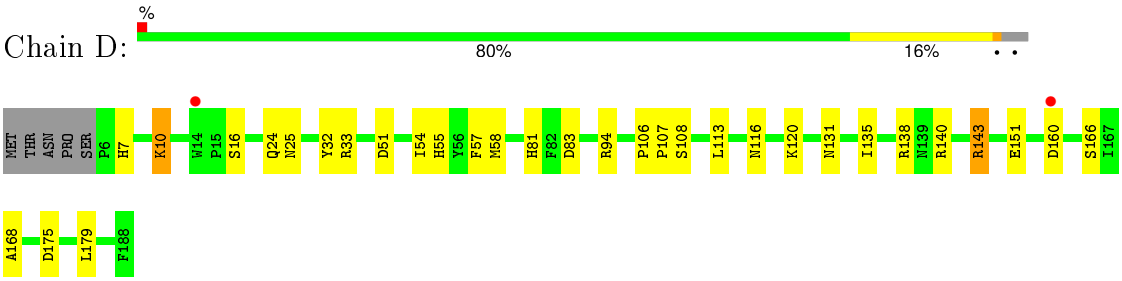
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain B:



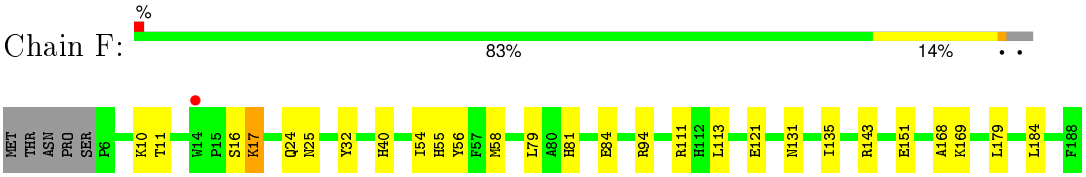
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain D:



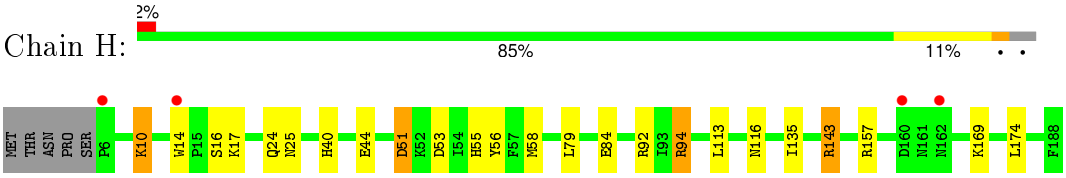
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain F:



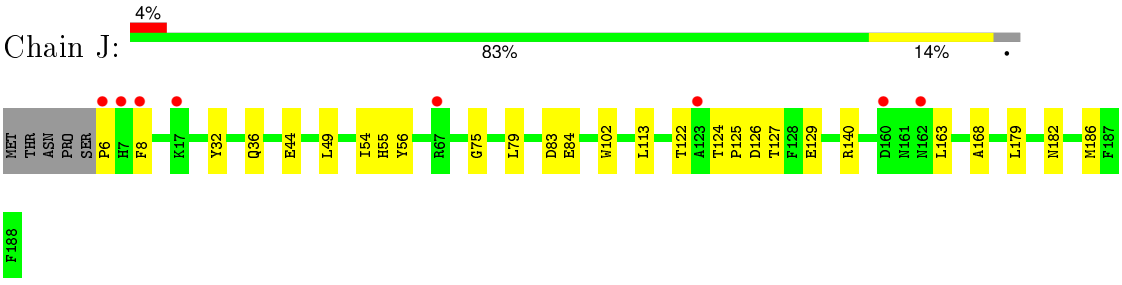
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain H:



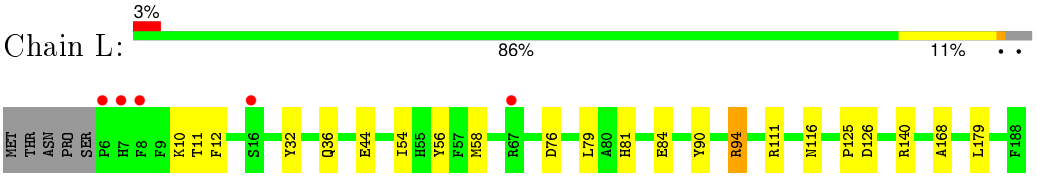
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain J:



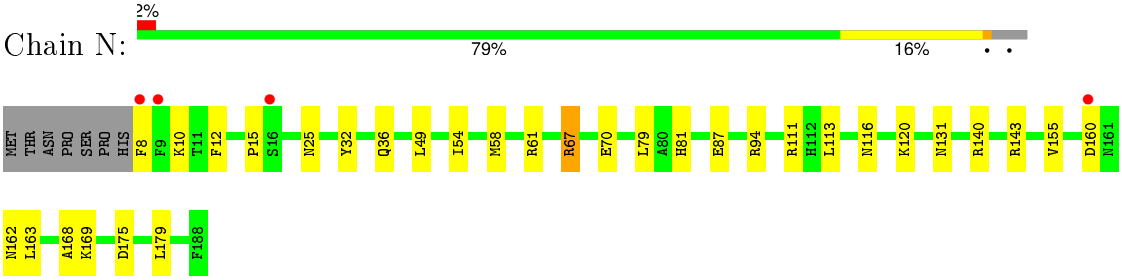
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain L:



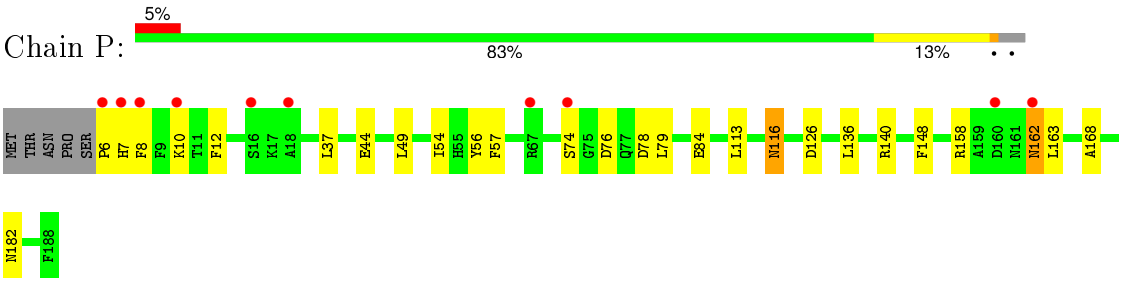
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain N:



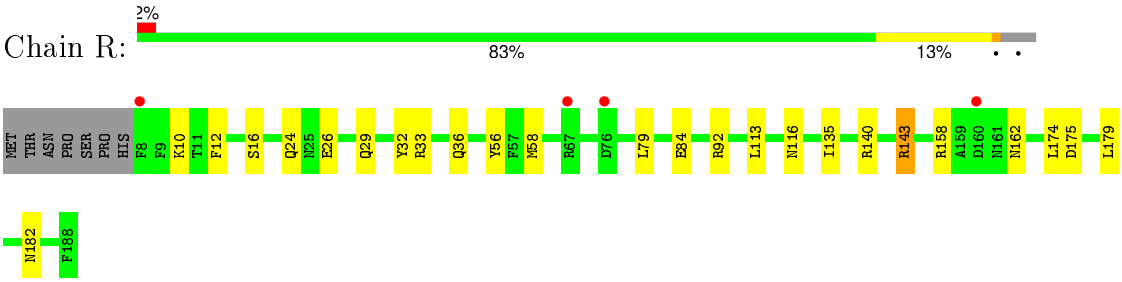
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain P:



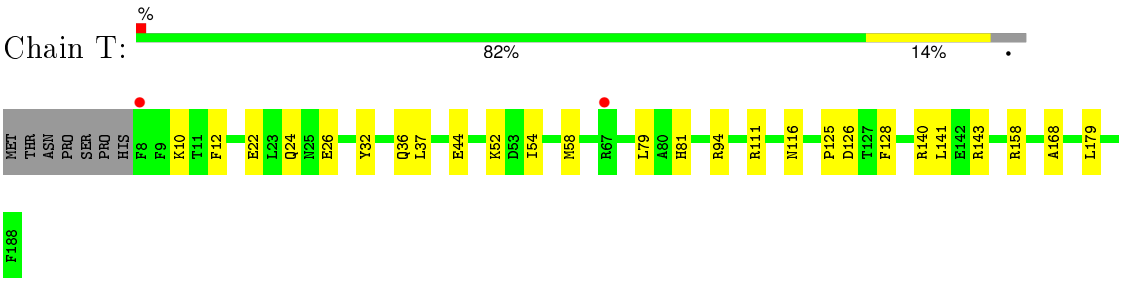
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain R:



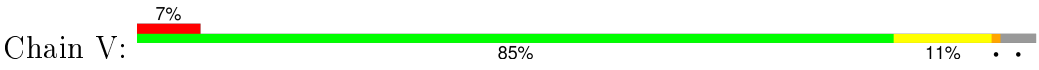
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

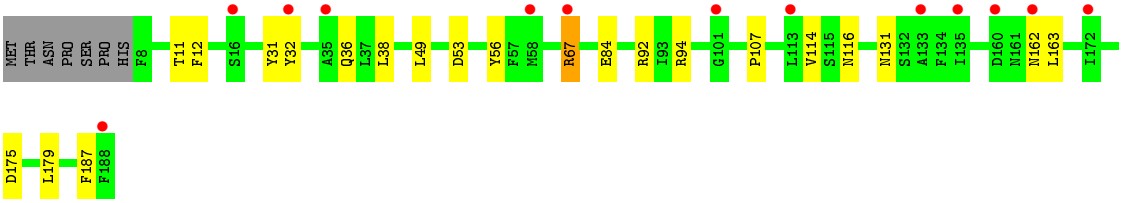
Chain T:



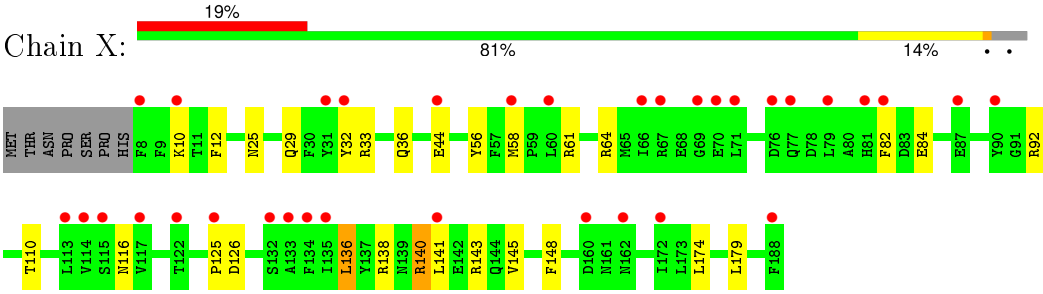
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain V:





- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



4 Data and refinement statistics (i)

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) 74.8 (28.40-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.266 0.233 , 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)	0.33 , 37.7	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[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 339687 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
1:I:422:HIS:CD2	1:I:424:ASP:H	2.04	0.74
5:A:2110:HOH:O	2:H:40:HIS:HD2	1.69	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:T:12:PHE:H	2:X:36:GLN:HE21	1.41	0.69
2:X:143:ARG:O	5:X:2029:HOH:O	2.10	0.69
1:W:123:HIS:N	3:W:900:FES:S2	2.64	0.69
3:S:900:FES:S1	5:S:2021:HOH:O	2.51	0.69
1:U:232:TYR:HA	1:U:433:TYR:CD1	2.27	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:G:422:HIS:CD2	1:G:424:ASP:H	2.14	0.66
1:A:422:HIS:HD2	1:A:424:ASP:H	1.44	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:K:142:ALA:HB1	1:Q:413:MET:CG	2.28	0.64
1:M:340:ARG:HD3	1:M:342:TRP:CH2	2.33	0.64
1:S:332:PHE:HB3	1:S:339:ILE:HG13	1.79	0.63
1:M:339:ILE:CD1	1:M:357:LEU:HG	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:GLU:OE1	1:G:102:HIS:NE2	2.26	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
2:R:26:GLU:OE1	2:R:158:ARG:NH2	2.31	0.63
1:Q:297:THR:O	1:Q:317:ARG:HD2	1.99	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:W:126:ALA:HB3	1:W:135:ASN:HB3	1.81	0.62
2:T:44:GLU:HG3	5:T:2011:HOH:O	1.99	0.62
1:Q:276:TRP:HB3	1:Q:322:GLN:HG3	1.80	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:U:123:HIS:HB2	3:U:900:FES:S2	2.39	0.62
1:I:259:PRO:HG2	1:I:283:SER:HB3	1.82	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
1:K:451:GLU:HB2	1:K:457:LEU:HD12	1.82	0.61
2:H:169:LYS:CE	5:H:2110:HOH:O	2.49	0.61
2:F:24:GLN:HG2	2:H:25:ASN:HD21	1.65	0.61
1:E:309:LEU:HD22	1:E:316:VAL:HG11	1.81	0.61
2:H:53:ASP:OD2	2:H:157:ARG:NH2	2.31	0.61
1:C:448:MET:HA	1:C:457:LEU:HD11	1.81	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
2:T:58:MET:HE2	2:T:81:HIS:CB	2.30	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
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:O:103:ARG:N	3:O:900:FES:S1	2.75	0.60
1:A:422:HIS:CD2	1:A:424:ASP:H	2.20	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:Q:287:VAL:HG12	1:Q:288:MET:CE	2.33	0.59
1:C:420:THR:HA	1:C:427:GLY:O	2.03	0.59
1:E:422:HIS:CD2	1:E:424:ASP:H	2.21	0.59
1:C:420:THR:OG1	1:O:94:LYS:HD3	2.02	0.59
2:T:116:ASN:HA	2:X:32:TYR:CD1	2.38	0.59
1:U:219:ASN:HA	5:U:2096:HOH:O	2.02	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: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:S:103:ARG:HB2	5:S:2028:HOH:O	1.99	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: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
2:B:58:MET:HE2	2:B:81:HIS:CG	2.39	0.57
1:A:414:GLY:HA2	1:A:417:ARG:HD2	1.86	0.57
1:A:391:ASN:O	1:A:395:ILE:HG13	2.04	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:E:22:GLU:HG3	1:E:25:ARG:NH2	2.20	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
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
1:I:262:GLY:HA2	1:I:278:VAL:HG23	1.86	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:U:266:ARG:HB3	1:U:428:ASN:ND2	2.19	0.57
1:U:324:MET:HB3	1:U:332:PHE:CE1	2.40	0.57
1:Q:339:ILE:N	1:Q:339:ILE:HD12	2.20	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:W:273:GLY:O	1:W:324:MET:HG3	2.06	0.56
1:I:259:PRO:HG3	1:I:280:GLU:HG2	1.87	0.56
2:N:8:PHE:HE2	2:N:70:GLU:CB	2.13	0.56
1:E:287:VAL:HG12	1:E:288:MET:HE2	1.84	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
2:J:6:PRO:N	2:J:75:GLY:HA3	2.21	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
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
1:U:164:ARG:O	1:U:174:ALA:HA	2.07	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
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:T:12:PHE:H	2:X:36:GLN:NE2	2.02	0.55
2:V:49:LEU:HD21	2:V:163:LEU:HD13	1.88	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:U:56:ARG:NH2	1:U:448:MET:O	2.41	0.54
1:U:412:GLN:O	1:U:415:LEU:HB2	2.08	0.54
2:X:125:PRO:O	2:X:126:ASP:HB2	2.07	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
2:F:58:MET:CE	2:F:184:LEU:HD13	2.38	0.53
1:S:229:SER:HB2	1:S:437:ALA:HB3	1.90	0.53
2:L:90:TYR:HE1	5:L:2023:HOH:O	1.89	0.53
1:S:345:ARG:HG3	1:S:351:GLU:HG3	1.91	0.53
2:N:36:GLN:HE21	2:R:12:PHE:H	1.55	0.53
1:O:339:ILE:CD1	1:O:357:LEU:HG	2.35	0.53
1:O:123:HIS:CB	5:O:2035:HOH:O	2.57	0.53
2:N:87:GLU:HB2	5:N:2041:HOH:O	2.09	0.53
2:L:116:ASN:HA	2:R:32:TYR:CD1	2.44	0.53
1:I:269:TRP:CZ2	1:I:444:HIS:HE1	2.27	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
1:U:238:THR:OG1	1:W:122:TYR:O	2.27	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: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
1:U:413:MET:CG	1:W:142:ALA:HB1	2.37	0.52
1:U:309:LEU:HD13	1:U:316:VAL:HG11	1.91	0.52
1:W:217:PRO:HG2	1:W:393:VAL:HG22	1.91	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:Q:356:THR:HG21	1:Q:374:ASN:HB3	1.92	0.52
1:K:36:ASP:O	1:K:39:ILE:HG12	2.10	0.52
1:A:244:LEU:HD13	1:A:253:LEU:HG	1.91	0.52
1:Q:294:GLN:NE2	1:Q:298:GLU:HG3	2.23	0.52
1:E:334:PRO:O	1:E:337:ASN:OD1	2.27	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
1:S:334:PRO:O	1:S:337:ASN:OD1	2.28	0.52
1:O:70:THR:HA	5:O:2026:HOH:O	2.10	0.52
1:U:227:PHE:HD2	5:U:2094:HOH:O	1.92	0.52
1:O:296:TRP:CH2	1:O:334:PRO:O	2.63	0.52
2:F:55:HIS:HB2	5:F:2115:HOH:O	2.09	0.52
2:P:54:ILE:HA	2:P:168:ALA:O	2.10	0.52
1:I:365:GLU:CD	1:I:365:GLU:H	2.12	0.52
1:Q:418:SER:HB3	1:Q:428:ASN:OD1	2.10	0.52
1:Q:287:VAL:HG12	1:Q:288:MET:HE3	1.92	0.52
1:G:279:ASP:O	1:G:281:PRO:HD3	2.10	0.52
1:S:422:HIS:HD2	1:S:424:ASP:H	1.58	0.51
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:U:232:TYR:CE1	1:W:123:HIS:HB3	2.45	0.51
2:P:56:TYR:HB3	2:P:84:GLU:HB2	1.92	0.51
1:I:36:ASP:O	1:I:39:ILE:HG12	2.10	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:O:123:HIS:HB2	5:O:2035:HOH:O	2.10	0.51
1:A:164:ARG:HD2	1:A:178:VAL:HA	1.92	0.51
1:W:215:VAL:HG22	1:W:351:GLU:HG2	1.92	0.51
1:O:102:HIS:HB3	3:O:900:FES:S1	2.50	0.51
5:S:2110:HOH:O	1:U:97:LEU:HD22	2.11	0.51
1:O:56:ARG:NH2	1:O:448:MET:O	2.44	0.51
1:S:21:PRO:O	1:S:25:ARG:HG3	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
1:W:339:ILE:HD13	1:W:357:LEU:HG	1.92	0.51
2:L:58:MET:HE2	2:L:81:HIS:CB	2.41	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:U:61:LEU:HD11	1:U:174:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:GLN:O	1:G:259:PRO:HD3	2.11	0.50
2:D:32:TYR:CG	2:H:116:ASN:HA	2.46	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:S:287:VAL:HG12	1:S:288:MET:CE	2.41	0.50
1:Q:215:VAL:O	2:R:182:ASN:HA	2.11	0.50
2:F:58:MET:HE1	2:F:184:LEU:CD1	2.41	0.50
1:E:299:GLY:O	1:E:303:GLU:HG3	2.10	0.50
1:W:337:ASN:HB3	1:W:357:LEU:O	2.11	0.50
1:K:339:ILE:HD13	1:K:357:LEU:HG	1.93	0.50
1:A:18:ASN:CG	1:A:19:TRP:H	2.15	0.50
1:O:340:ARG:HD3	1:O:342:TRP:CH2	2.46	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:I:107:ILE:HG22	1:I:118:PHE:HB3	1.94	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:K:444:HIS:O	1:K:445:TRP:C	2.50	0.50
1:M:164:ARG:HD2	1:M:178:VAL:HA	1.93	0.50
1:K:139:GLU:HA	1:K:143:PHE:HD1	1.77	0.50
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:N:111:ARG:HB2	2:R:175:ASP:OD2	2.12	0.49
1:I:226:GLN:HA	1:I:230:ASP:HB3	1.93	0.49
2:H:169:LYS:HE3	5:H:2110:HOH:O	2.12	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:W:410:ASN:HD21	1:W:412:GLN:HB2	1.77	0.49
1:K:265:PHE:CZ	1:K:267:ALA:HA	2.48	0.49
2:D:120:LYS:HE2	5:D:2083:HOH:O	2.11	0.49
1:C:195:ASP:HB3	1:C:309:LEU:HD21	1.93	0.49
1:G:44:SER:O	1:G:48:LEU:HD13	2.13	0.49
1:Q:339:ILE:HD13	1:Q:357:LEU:HG	1.95	0.49
1:O:197:MET:HB2	1:O:334:PRO:HB3	1.95	0.49
1:S:269:TRP:CZ2	1:S:444:HIS:HE1	2.31	0.49
1:C:339:ILE:HD13	1:C:357:LEU:HG	1.95	0.49
1:S:259:PRO:HB3	1:S:280:GLU:CG	2.37	0.49
2:D:135:ILE:HG13	2:F:113:LEU:HD22	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:29:GLN:O	2:X:33:ARG:HG3	2.13	0.49
1:S:82:PRO:HB2	1:S:98:ASN:HB3	1.94	0.49
1:I:131:GLY:O	1:I:160:PRO:HD2	2.12	0.49
1:I:403:LYS:HD2	1:O:161:LEU:HD21	1.95	0.49
1:I:376:ARG:HB2	5:I:2074:HOH:O	2.13	0.49
1:Q:339:ILE:CD1	1:Q:357:LEU:HG	2.43	0.49
1:K:340:ARG:HH12	1:K:385:GLU:CD	2.16	0.49
2:H:55:HIS:HB2	5:H:2041:HOH:O	2.12	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:G:169:LYS:HD3	1:G:199:ASP:HB2	1.95	0.49
1:K:410:ASN:ND2	1:K:412:GLN:H	2.09	0.49
1:W:412:GLN:O	1:W:415:LEU:HB2	2.13	0.48
1:W:218:CYS:SG	1:W:392:TRP:HB3	2.53	0.48
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:A:259:PRO:HB3	1:A:280:GLU:HG3	1.94	0.48
1:K:27:LEU:HD13	1:K:39:ILE:HG22	1.95	0.48
1:O:209:GLY:HA3	2:P:78:ASP:OD1	2.12	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:O:193:TYR:CE2	1:O:276:TRP:CH2	3.01	0.48
1:A:65:SER:CB	1:A:206:VAL:HG23	2.43	0.48
2:P:162:ASN:ND2	2:P:162:ASN:H	2.10	0.48
1:M:332:PHE:HB3	1:M:339:ILE:HG23	1.96	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:W:340:ARG:HD3	1:W:342:TRP:CH2	2.48	0.48
1:A:287:VAL:HG12	1:A:288:MET:HE2	1.94	0.48
1:A:265:PHE:CZ	1:A:267:ALA:HA	2.49	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
1:S:123:HIS:HA	5:W:2055:HOH:O	2.14	0.48
2:H:10:LYS:HD2	1:S:254:SER:CB	2.41	0.48
1:W:267:ALA:N	5:W:2059:HOH:O	2.46	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: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)
2:V:32:TYR:CD1	2:X:116:ASN:HA	2.48	0.48
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
1:G:287:VAL:CG1	1:G:288:MET:HE2	2.30	0.48
2:D:58:MET:HE2	2:D:81:HIS:HB2	1.95	0.48
1:O:226:GLN:HA	1:O:230:ASP:HB3	1.96	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:M:32:LYS:O	1:M:412:GLN:HG2	2.14	0.48
1:O:120:CYS:SG	5:O:2036:HOH:O	2.61	0.47
1:K:143:PHE:HA	5:K:2035:HOH:O	2.12	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
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
1:E:303:GLU:HG2	1:E:317:ARG:NH1	2.30	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:S:435:GLU:OE1	1:U:102:HIS:NE2	2.48	0.47
1:Q:73:PHE:HA	1:Q:85:MET:O	2.14	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: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
1:W:339:ILE:N	1:W:339:ILE:HD12	2.30	0.47
1:E:25:ARG:HD3	5:E:2002:HOH:O	2.13	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
2:L:54:ILE:HA	2:L:168:ALA:O	2.15	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
1:I:239:HIS:HE1	1:I:384:PHE:O	1.98	0.47
1:U:218:CYS:CB	1:U:392:TRP:HB3	2.45	0.47
1:U:208:ILE:HA	5:U:2069:HOH:O	2.13	0.47
1:U:164:ARG:HD2	1:U:178:VAL:HA	1.97	0.47
1:M:177:ASP:OD2	1:M:454:TRP:NE1	2.47	0.47
1:I:57:SER:HB3	1:I:328:PRO:HD3	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

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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:I:228:CYS:HB2	1:I:325:THR:HB	1.96	0.47
1:A:185:THR:HG22	1:A:459:PRO:HG2	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:E:339:ILE:N	1:E:339:ILE:HD12	2.29	0.47
1:A:189:ASP:O	1:A:192:PRO:HD2	2.15	0.47
1:S:217:PRO:HG2	1:S:393:VAL:HG22	1.97	0.47
1:G:410:ASN:ND2	1:G:412:GLN:H	2.13	0.47
1:W:181:PRO:HA	5:W:2044:HOH:O	2.15	0.47
1:S:332:PHE:CB	1:S:339:ILE:HG13	2.45	0.46
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
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
1:O:322:GLN:HB3	1:O:334:PRO:HD2	1.97	0.46
1:E:448:MET:HA	1:E:457:LEU:HD11	1.97	0.46
2:N:113:LEU:HD21	2:R:113:LEU:HD23	1.98	0.46
1:O:340:ARG:HA	1:O:353:TRP:O	2.15	0.46
1:M:346:GLY:O	5:M:2066:HOH:O	2.20	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:O:373:HIS:HD2	1:O:376:ARG:HH21	1.62	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:E:123:HIS:HB2	3:E:900:FES:S2	2.55	0.46
1:S:214:TRP:HE1	1:S:216:ILE:HD11	1.81	0.46
1:M:123:HIS:HB2	3:M:900:FES:S2	2.55	0.46
1:Q:359:ASP:HB2	1:Q:362:ALA:HB2	1.98	0.46
1:W:233:HIS:HA	5:W:2055:HOH:O	2.16	0.46
1:G:413:MET:HB2	1:G:435:GLU:OE2	2.15	0.46
2:L:116:ASN:HA	2:R:32:TYR:CG	2.51	0.46
1:I:255:GLN:O	1:I:256:ALA:C	2.53	0.46
1:Q:48:LEU:HD12	5:Q:2013:HOH:O	2.15	0.46
1:Q:257:GLN:HG3	1:Q:258:ILE:N	2.30	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
1:E:263:ASN:HB2	1:E:276:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:199:ASP:HB3	1:M:309:LEU:HD21	1.98	0.46
1:G:373:HIS:CD2	1:G:376:ARG:HE	2.34	0.46
2:B:22:GLU:O	2:B:26:GLU:HG3	2.16	0.46
1:S:391:ASN:O	1:S:395:ILE:HG13	2.16	0.46
1:E:64:GLU:OE1	1:E:167:THR:HG21	2.15	0.46
2:T:37:LEU:HD23	2:V:11:THR:HG21	1.98	0.46
2:L:56:TYR:HB3	2:L:84:GLU:HB2	1.98	0.46
1:E:356:THR:HG21	1:E:374:ASN:CB	2.46	0.46
1:W:413:MET:HG2	1:W:434:ALA:HA	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
2:X:110:THR:HG22	2:X:138:ARG:HG2	1.97	0.45
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
1:I:269:TRP:CD2	1:I:459:PRO:HG3	2.51	0.45
1:O:410:ASN:ND2	1:O:412:GLN:H	2.13	0.45
1:K:349:GLU:OE2	2:R:143:ARG:NH2	2.42	0.45
2:T:32:TYR:CD1	2:V:116:ASN:HA	2.52	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: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:M:326:ILE:HB	1:M:330:CYS:HB3	1.97	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
1:U:262:GLY:HA2	1:U:278:VAL:HG23	1.98	0.45
2:N:58:MET:HE2	2:N:81:HIS:HB2	1.99	0.45
2:N:15:PRO:HD3	2:N:120:LYS:HG3	1.98	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:33:ARG:HD3	5:D:2015:HOH:O	2.16	0.45
1:M:69:GLU:O	1:M:87:ARG:HB3	2.17	0.45
1:K:419:GLN:HE21	1:K:421:GLY:H	1.65	0.45
5:H:2056:HOH:O	2:T:52:LYS:CD	2.56	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)
2:D:175:ASP:OD2	2:F:111:ARG:HB2	2.16	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:S:262:GLY:HA2	1:S:278:VAL:HG23	1.98	0.45
1:Q:57:SER:HB3	1:Q:328:PRO:HD3	1.97	0.45
1:S:259:PRO:HB2	1:S:277:TYR:CE2	2.52	0.44
1:C:413:MET:HG2	1:C:434:ALA:HA	1.99	0.44
1:Q:422:HIS:CD2	1:Q:424:ASP:H	2.35	0.44
2:D:116:ASN:HA	2:F:32:TYR:CD1	2.52	0.44
1:C:244:LEU:HD13	1:C:253:LEU:HG	1.99	0.44
1:G:340:ARG:HD3	1:G:342:TRP:CH2	2.52	0.44
1:C:262:GLY:HA2	1:C:278:VAL:HG23	1.99	0.44
2:F:58:MET:CE	2:F:184:LEU:CD1	2.96	0.44
1:Q:356:THR:HG23	2:R:79:LEU:HD11	1.99	0.44
1:M:373:HIS:HD2	1:M:376:ARG:HE	1.65	0.44
1:C:22:GLU:HG3	1:C:25:ARG:HH22	1.82	0.44
5:H:2055:HOH:O	2:T:52:LYS:HD2	2.17	0.44
1:S:183:LEU:O	1:S:186:TYR:HB3	2.17	0.44
1:C:419:GLN:HE22	1:O:162:GLN:HG3	1.83	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: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
3:S:900:FES:S1	5:S:2028:HOH:O	2.62	0.44
1:S:287:VAL:HG12	1:S:288:MET:HE3	1.98	0.44
1:S:143:PHE:HB3	1:S:153:PHE:HB3	1.99	0.44
1:O:278:VAL:HA	1:O:318:ARG:O	2.17	0.44
1:I:48:LEU:HD12	1:I:52:ARG:HG3	1.99	0.44
1:M:21:PRO:O	1:M:25:ARG:HG3	2.17	0.44
1:K:73:PHE:HA	1:K:85:MET:O	2.17	0.44
2:T:125:PRO:O	2:T:126:ASP:HB2	2.18	0.44
1:U:218:CYS:HB3	1:U:392:TRP:HB3	2.00	0.44
1:O:119:THR:HA	5:O:2037:HOH:O	2.17	0.44
2:H:17:LYS:H	2:V:67:ARG:NH1	2.16	0.44
1:I:270:GLY:O	1:I:327:PHE:HB3	2.17	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
2:F:17:LYS:NZ	2:F:121:GLU:H	2.16	0.44
1:S:193:TYR:CE2	1:S:276:TRP:CH2	3.06	0.44
2:J:122:THR:HG22	2:J:129:GLU:HG3	1.99	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:I:233:HIS:HB3	1:O:123:HIS:CD2	2.52	0.43
2:D:116:ASN:HA	2:F:32:TYR:CG	2.53	0.43
2:N:131:ASN:ND2	5:N:2055:HOH:O	2.51	0.43
1:W:42:ASP:HB3	1:W:45:LEU:HB2	1.99	0.43
1:K:42:ASP:HB3	1:K:45:LEU:HB2	2.00	0.43
2:P:136:LEU:HB3	2:P:148:PHE:HB2	2.00	0.43
1:C:217:PRO:HD2	1:C:393:VAL:HG22	2.00	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
2:V:67:ARG:HE	2:V:67:ARG:HA	1.84	0.43
1:I:413:MET:HG2	1:I:434:ALA:HA	2.00	0.43
2:T:128:PHE:HZ	2:T:158:ARG:NH1	2.15	0.43
1:S:100:CYS:SG	1:S:127:TYR:OH	2.77	0.43
1:C:336:MET:HG2	1:C:336:MET:H	1.55	0.43
1:K:19:TRP:HB3	1:K:24:ILE:HD11	1.98	0.43
1:U:266:ARG:HB2	1:U:437:ALA:HA	2.00	0.43
2:F:17:LYS:HD3	2:F:17:LYS:N	2.34	0.43
2:X:58:MET:HE3	2:X:174:LEU:HD22	1.99	0.43
2:D:54:ILE:HA	2:D:168:ALA:O	2.19	0.43
1:U:229:SER:HB3	1:U:438:ALA:HB2	1.99	0.43
1:A:64:GLU:OE1	1:A:167:THR:HG21	2.17	0.43
2:J:55:HIS:NE2	2:J:83:ASP:OD2	2.43	0.43
1:G:185:THR:HG22	1:G:459:PRO:HG2	1.99	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:K:167:THR:HA	1:K:171:LEU:O	2.18	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:S:103:ARG:HA	1:W:409:LEU:HD13	2.01	0.43
1:E:259:PRO:HB2	1:E:277:TYR:CD2	2.53	0.43
1:A:167:THR:CG2	5:A:2013:HOH:O	2.66	0.43
1:W:68:PRO:HD2	1:W:72:ASP:OD2	2.19	0.43
1:S:73:PHE:CE1	1:S:108:CYS:SG	3.12	0.43
2:J:102:TRP:O	1:O:109:ARG:NH2	2.51	0.43
1:A:302:ALA:HB1	1:A:317:ARG:HD3	2.00	0.43
1:O:332:PHE:HD1	1:O:334:PRO:HG3	1.83	0.43
1:I:392:TRP:HA	1:I:395:ILE:HD12	2.00	0.43
1:K:211:MET:CE	1:K:353:TRP:CE3	3.02	0.43
1:U:86:VAL:HG11	1:U:96:PHE:HE2	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
2:V:38:LEU:HD22	2:V:187:PHE:HB2	2.00	0.43
2:T:111:ARG:HB2	2:V:175:ASP:OD2	2.19	0.43
1:K:336:MET:HG2	1:K:336:MET:H	1.54	0.43
2:L:32:TYR:CG	2:N:116:ASN:HA	2.54	0.43
1:E:259:PRO:HB2	1:E:277:TYR:CE2	2.54	0.43
1:W:68:PRO:HA	1:W:87:ARG:HH21	1.84	0.43
1:E:298:GLU:HG3	5:E:2136:HOH:O	2.19	0.43
1:Q:212:GLN:HE21	1:Q:354:ALA:HB3	1.82	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
1:W:164:ARG:O	1:W:174:ALA:HA	2.19	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:K:123:HIS:HB3	1:Q:232:TYR:CE1	2.54	0.42
1:G:373:HIS:HD2	1:G:376:ARG:HE	1.67	0.42
2:T:26:GLU:OE1	2:T:158:ARG:NH2	2.52	0.42
1:S:336:MET:H	1:S:336:MET:HG2	1.64	0.42
1:W:257:GLN:O	1:W:259:PRO:HD3	2.19	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
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:E:390:GLU:OE2	1:E:390:GLU:HA	2.19	0.42
1:O:368:GLU:OE2	1:O:368:GLU:HA	2.19	0.42
1:K:142:ALA:CB	1:Q:413:MET:HG3	2.40	0.42
1:O:287:VAL:HG12	1:O:288:MET:HE2	2.01	0.42
2:F:55:HIS:HB3	2:F:169:LYS:HD3	2.01	0.42
2:L:58:MET:HE2	2:L:81:HIS:HB3	2.01	0.42
1:K:333:LEU:HB2	1:K:336:MET:HG3	2.00	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
1:G:356:THR:HG21	1:G:374:ASN:CB	2.49	0.42
1:S:104:GLY:N	5:S:2021:HOH:O	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:W:226:GLN:HA	1:W:230:ASP:HB3	2.00	0.42
1:M:212:GLN:HB2	1:M:212:GLN:HE21	1.61	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:P:49:LEU:HD21	2:P:163:LEU:HD13	2.00	0.42
2:J:54:ILE:HA	2:J:168:ALA:O	2.19	0.42
1:U:284:LEU:HD23	1:U:293:THR:HG23	2.02	0.42
1:O:288:MET:SD	1:O:336:MET:HB3	2.60	0.42
2:B:6:PRO:O	2:B:7:HIS:C	2.57	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:W:123:HIS:O	1:W:137:PRO:HG2	2.20	0.42
2:H:169:LYS:HG2	5:H:2110:HOH:O	2.20	0.42
2:H:51:ASP:OD2	2:H:157:ARG:NH1	2.53	0.42
1:W:334:PRO:HA	5:W:2067:HOH:O	2.20	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
1:U:288:MET:HE2	1:U:288:MET:HA	2.02	0.42
1:I:105:MET:HB3	1:I:120:CYS:SG	2.60	0.42
1:S:36:ASP:O	1:S:39:ILE:HG12	2.19	0.42
1:U:86:VAL:CG1	1:U:96:PHE:HE2	2.33	0.42
1:S:266:ARG:NH1	1:S:436:GLU:OE1	2.52	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
2:L:125:PRO:O	2:L:126:ASP:HB2	2.20	0.42
1:I:230:ASP:O	1:I:233:HIS:ND1	2.53	0.41
1:A:258:ILE:HA	1:A:259:PRO:HD3	1.70	0.41
1:U:200:ARG:CG	5:U:2065:HOH:O	2.64	0.41
1:G:277:TYR:HD1	1:G:283:SER:HG	1.67	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:251:MET:HG3	1:E:255:GLN:HE21	1.83	0.41
1:E:212:GLN:HE21	1:E:212:GLN:HB2	1.56	0.41
1:E:262:GLY:C	1:E:432:VAL:HB	2.41	0.41
1:I:226:GLN:HA	1:I:230:ASP:CB	2.51	0.41
2:V:56:TYR:HB3	2:V:84:GLU:HB2	2.02	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:E:68:PRO:HD2	1:E:72:ASP:OD2	2.20	0.41
1:O:270:GLY:O	1:O:327:PHE:HB3	2.20	0.41
1:W:57:SER:HB3	1:W:328:PRO:HD3	2.03	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:S:76:THR:OG1	1:S:77:TYR:N	2.54	0.41
1:W:359:ASP:HB2	1:W:362:ALA:HB2	2.03	0.41
2:F:17:LYS:HD3	2:F:17:LYS:H	1.85	0.41
1:W:389:GLY:O	1:W:393:VAL:HG23	2.20	0.41
1:M:244:LEU:HD11	2:N:94:ARG:HG2	2.02	0.41
1:G:431:TYR:CE1	1:G:432:VAL:HG12	2.55	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
2:L:11:THR:HG23	2:R:36:GLN:HB3	2.02	0.41
2:T:116:ASN:HA	2:X:32:TYR:CG	2.56	0.41
2:N:36:GLN:NE2	2:R:12:PHE:H	2.16	0.41
1:K:339:ILE:HD12	1:K:339:ILE:N	2.35	0.41
2:R:29:GLN:O	2:R:33:ARG:HG3	2.21	0.41
2:V:53:ASP:OD1	2:V:53:ASP:N	2.48	0.41
1:S:355:PHE:HE1	1:S:357:LEU:HD21	1.86	0.41
1:I:208:ILE:HD12	1:I:356:THR:OG1	2.21	0.41
2:H:55:HIS:HB3	2:H:169:LYS:HE2	2.02	0.41
1:K:52:ARG:HB3	1:K:448:MET:O	2.20	0.41
1:G:376:ARG:HA	2:H:92:ARG:NH2	2.36	0.41
1:S:136:VAL:O	1:S:139:GLU:HB2	2.21	0.41
1:W:248:PRO:HA	1:W:249:PRO:HD3	1.98	0.41
1:Q:248:PRO:HA	1:Q:249:PRO:HD3	1.95	0.41
1:I:422:HIS:CD2	1:I:423:PRO:HD2	2.55	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
2:N:113:LEU:CD2	2:R:113:LEU:HD23	2.50	0.41
1:M:356:THR:HG21	1:M:374:ASN:CB	2.51	0.41
2:J:36:GLN:HE21	2:P:12:PHE:H	1.68	0.41
1:U:314:MET:HA	1:U:315:PRO:HD3	1.96	0.41
1:A:269:TRP:CZ2	1:A:444:HIS:HE1	2.39	0.41
1:S:52:ARG:NH2	1:S:452:PRO:HB3	2.36	0.41
2:B:52:LYS:NZ	5:B:2041:HOH:O	2.53	0.41
1:S:365:GLU:CD	1:S:365:GLU:H	2.24	0.41
1:C:65:SER:O	1:C:68:PRO:HD3	2.21	0.41
1:Q:280:GLU:HB2	5:Q:2054:HOH:O	2.19	0.41
2:P:126:ASP:HB3	2:P:158:ARG:HB2	2.03	0.41
1:E:164:ARG:HB2	1:E:175:ASN:O	2.20	0.41
2:D:55:HIS:CE1	2:D:57:PHE:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:259:PRO:HB2	1:K:277:TYR:CE2	2.55	0.41
2:F:121:GLU:HB3	5:F:2090:HOH:O	2.20	0.41
1:K:81:ASP:OD1	1:Q:401:GLY:HA3	2.21	0.41
1:K:185:THR:HG22	1:K:459:PRO:HG2	2.02	0.41
2:N:155:VAL:HB	2:N:169:LYS:HB2	2.02	0.41
1:G:164:ARG:HD2	1:G:178:VAL:HA	2.03	0.41
1:A:36:ASP:HA	1:A:37:PRO:HD3	1.97	0.41
1:O:42:ASP:HB3	1:O:45:LEU:HD12	2.03	0.41
1:M:136:VAL:O	1:M:139:GLU:HB2	2.20	0.41
2:B:169:LYS:HG2	5:E:2167:HOH:O	2.21	0.40
1:U:220:TRP:HA	1:U:350:ILE:HG21	2.01	0.40
1:E:267:ALA:HB2	1:E:272:HIS:HB2	2.03	0.40
1:U:255:GLN:O	1:U:256:ALA:C	2.58	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:G:29:ASP:OD1	1:G:32:LYS:HD2	2.21	0.40
1:C:359:ASP:HB2	1:C:362:ALA:HB2	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: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:A:270:GLY:O	1:A:327:PHE:HB3	2.21	0.40
1:W:229:SER:HB3	1:W:438:ALA:HB2	2.02	0.40
1:U:208:ILE:HD11	1:U:358:VAL:HG13	2.03	0.40
1:M:373:HIS:CD2	1:M:376:ARG:HE	2.39	0.40
2:B:54:ILE:HA	2:B:168:ALA:O	2.21	0.40
2:T:158:ARG:NH1	5:T:2059:HOH:O	2.54	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
1:U:335:ALA:HB2	5:U:2091:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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%)	52	59
1	G	429/459 (94%)	407 (95%)	22 (5%)	0	100	100
1	I	429/459 (94%)	414 (96%)	14 (3%)	1 (0%)	52	59
1	K	429/459 (94%)	407 (95%)	21 (5%)	1 (0%)	52	59
1	M	429/459 (94%)	402 (94%)	26 (6%)	1 (0%)	52	59
1	O	429/459 (94%)	407 (95%)	20 (5%)	2 (0%)	34	35
1	Q	429/459 (94%)	405 (94%)	23 (5%)	1 (0%)	52	59
1	S	429/459 (94%)	412 (96%)	15 (4%)	2 (0%)	34	35
1	U	429/459 (94%)	401 (94%)	24 (6%)	4 (1%)	21	19
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%)	30	29
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%)	17	14
2	R	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
2	T	179/188 (95%)	172 (96%)	6 (3%)	1 (1%)	30	29
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%)	52	59

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 (i)

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%)	50	62
1	C	350/372 (94%)	338 (97%)	12 (3%)	44	54
1	E	350/372 (94%)	335 (96%)	15 (4%)	35	43
1	G	350/372 (94%)	336 (96%)	14 (4%)	38	47
1	I	350/372 (94%)	339 (97%)	11 (3%)	47	59
1	K	350/372 (94%)	336 (96%)	14 (4%)	38	47
1	M	350/372 (94%)	340 (97%)	10 (3%)	50	62
1	O	350/372 (94%)	340 (97%)	10 (3%)	50	62
1	Q	350/372 (94%)	340 (97%)	10 (3%)	50	62
1	S	350/372 (94%)	340 (97%)	10 (3%)	50	62
1	U	350/372 (94%)	336 (96%)	14 (4%)	38	47
1	W	350/372 (94%)	342 (98%)	8 (2%)	58	71
2	B	162/167 (97%)	157 (97%)	5 (3%)	47	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	162/167 (97%)	154 (95%)	8 (5%)	31 36
2	F	162/167 (97%)	155 (96%)	7 (4%)	35 43
2	H	162/167 (97%)	155 (96%)	7 (4%)	35 43
2	J	162/167 (97%)	159 (98%)	3 (2%)	65 77
2	L	162/167 (97%)	157 (97%)	5 (3%)	47 59
2	N	160/167 (96%)	154 (96%)	6 (4%)	40 49
2	P	162/167 (97%)	156 (96%)	6 (4%)	41 50
2	R	160/167 (96%)	155 (97%)	5 (3%)	47 59
2	T	160/167 (96%)	155 (97%)	5 (3%)	47 59
2	V	160/167 (96%)	156 (98%)	4 (2%)	55 67
2	X	160/167 (96%)	153 (96%)	7 (4%)	35 42
All	All	6134/6468 (95%)	5928 (97%)	206 (3%)	44 54

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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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	0/1/1/1
3	FES	C	900	1	-	0/0/4/4	0/1/1/1
3	FES	E	900	1	-	0/0/4/4	0/1/1/1
3	FES	G	900	1	-	0/0/4/4	0/1/1/1
3	FES	I	900	1	-	0/0/4/4	0/1/1/1
3	FES	K	900	1,5	-	0/0/4/4	0/1/1/1
3	FES	M	900	1	-	0/0/4/4	0/1/1/1
3	FES	O	900	1,5	-	0/0/4/4	0/1/1/1
3	FES	Q	900	1	-	0/0/4/4	0/1/1/1
3	FES	S	900	1,5	-	0/0/4/4	0/1/1/1
3	FES	U	900	1	-	0/0/4/4	0/1/1/1
3	FES	W	900	1,5	-	0/0/4/4	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	A	900	FES	1	0
3	C	900	FES	1	0
3	E	900	FES	1	0
3	G	900	FES	1	0
3	K	900	FES	2	0
3	M	900	FES	1	0
3	O	900	FES	3	0
3	S	900	FES	4	0
3	U	900	FES	1	0
3	W	900	FES	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.39	4 (0%) 85 85	-7, 10, 35, 51	18 (4%)
1	C	433/459 (94%)	0.06	11 (2%) 61 60	3, 29, 56, 66	18 (4%)
1	E	433/459 (94%)	-0.39	9 (2%) 67 65	-11, 7, 33, 47	18 (4%)
1	G	433/459 (94%)	-0.10	14 (3%) 51 50	-3, 17, 42, 60	18 (4%)
1	I	433/459 (94%)	0.58	48 (11%) 7 7	7, 50, 89, 101	18 (4%)
1	K	433/459 (94%)	0.10	19 (4%) 38 37	12, 29, 54, 99	18 (4%)
1	M	433/459 (94%)	0.69	56 (12%) 5 4	17, 47, 83, 92	18 (4%)
1	O	433/459 (94%)	0.54	29 (6%) 21 20	20, 49, 71, 100	18 (4%)
1	Q	433/459 (94%)	1.07	71 (16%) 2 2	37, 64, 92, 108	18 (4%)
1	S	433/459 (94%)	0.70	53 (12%) 5 5	15, 48, 80, 113	18 (4%)
1	U	433/459 (94%)	2.20	198 (45%) 0 0	43, 88, 126, 135	18 (4%)
1	W	433/459 (94%)	2.93	284 (65%) 0 0	71, 111, 142, 155	18 (4%)
2	B	183/188 (97%)	-0.55	2 (1%) 82 82	-12, -2, 16, 28	4 (2%)
2	D	183/188 (97%)	-0.55	2 (1%) 82 82	-12, 2, 28, 40	4 (2%)
2	F	183/188 (97%)	-0.54	1 (0%) 91 91	-16, -5, 19, 32	4 (2%)
2	H	183/188 (97%)	-0.46	4 (2%) 65 64	-15, -4, 33, 48	4 (2%)
2	J	183/188 (97%)	0.04	8 (4%) 38 37	1, 22, 47, 58	4 (2%)
2	L	183/188 (97%)	-0.39	5 (2%) 58 57	3, 12, 33, 52	4 (2%)
2	N	181/188 (96%)	-0.10	4 (2%) 65 64	8, 25, 40, 46	4 (2%)
2	P	183/188 (97%)	-0.11	10 (5%) 29 28	-11, 12, 45, 67	4 (2%)
2	R	181/188 (96%)	-0.35	4 (2%) 65 64	7, 22, 41, 53	4 (2%)
2	T	181/188 (96%)	-0.27	2 (1%) 82 82	5, 20, 49, 75	4 (2%)
2	V	181/188 (96%)	0.57	13 (7%) 18 18	25, 50, 81, 99	4 (2%)
2	X	181/188 (96%)	1.12	35 (19%) 2 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%)	0.43	886 (12%) 6 5	-16, 33, 105, 155	264 (3%)

All (886) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	421	GLY	8.2
1	G	256	ALA	8.1
1	W	429	VAL	7.9
1	U	259	PRO	7.8
1	U	321	GLY	7.8
1	W	333	LEU	7.7
1	W	332	PHE	7.7
1	U	273	GLY	7.5
1	W	227	PHE	7.3
1	W	105	MET	7.3
1	W	207	ALA	7.2
1	W	193	TYR	7.0
1	W	113	GLY	7.0
1	U	301	ALA	6.9
1	W	153	PHE	6.9
1	U	260	THR	6.9
1	U	332	PHE	6.9
1	Q	456	THR	6.8
1	W	419	GLN	6.8
1	U	416	GLY	6.8
1	W	339	ILE	6.7
1	U	330	CYS	6.7
1	U	324	MET	6.6
1	U	105	MET	6.5
1	U	437	ALA	6.4
1	W	334	PRO	6.4
1	U	228	CYS	6.4
1	W	317	ARG	6.4
1	U	322	GLN	6.4
1	U	227	PHE	6.4
1	W	228	CYS	6.3
2	X	8	PHE	6.3
1	W	442	TYR	6.3
1	U	378	PHE	6.2
1	W	355	PHE	6.2
1	U	326	ILE	6.2
1	W	296	TRP	6.1

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Mol	Chain	Res	Type	RSRZ
1	W	341	ILE	6.1
1	E	256	ALA	6.1
1	U	253	LEU	6.1
1	W	100	CYS	6.1
1	U	323	HIS	6.0
1	W	253	LEU	6.0
1	W	322	GLN	6.0
1	W	337	ASN	6.0
2	N	8	PHE	5.9
1	U	289	GLY	5.9
1	U	224	ALA	5.9
1	W	431	TYR	5.9
1	W	109	ARG	5.8
1	W	273	GLY	5.8
1	W	331	SER	5.7
1	U	35	LEU	5.7
1	W	384	PHE	5.7
1	U	415	LEU	5.7
2	J	6	PRO	5.7
1	W	335	ALA	5.7
1	W	183	LEU	5.6
1	U	438	ALA	5.6
2	J	8	PHE	5.6
1	W	103	ARG	5.6
1	U	339	ILE	5.6
1	W	194	MET	5.6
1	U	274	SER	5.6
1	W	338	ASN	5.6
1	W	154	ASP	5.6
1	W	143	PHE	5.5
1	M	257	GLN	5.5
1	W	425	PHE	5.5
1	W	420	THR	5.5
1	W	261	LYS	5.5
1	W	107	ILE	5.5
1	W	285	LEU	5.5
1	W	357	LEU	5.5
1	W	74	LEU	5.4
1	W	324	MET	5.4
1	S	122	TYR	5.4
1	W	122	TYR	5.4
1	U	409	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	U	364	ALA	5.3
1	U	320	VAL	5.3
1	W	86	VAL	5.3
1	Q	455	ALA	5.3
2	X	77	GLN	5.3
1	W	354	ALA	5.2
1	W	58	TRP	5.2
1	U	325	THR	5.2
1	W	356	THR	5.2
1	O	105	MET	5.2
1	W	258	ILE	5.2
1	W	430	GLY	5.2
1	U	334	PRO	5.2
1	M	261	LYS	5.1
1	W	156	ALA	5.1
1	W	197	MET	5.1
1	W	257	GLN	5.1
1	W	414	GLY	5.1
2	J	160	ASP	5.1
1	W	203	ALA	5.1
2	L	6	PRO	5.1
1	U	275	GLY	5.1
1	U	456	THR	5.1
1	U	333	LEU	5.0
1	W	198	LEU	5.0
1	M	18	ASN	5.0
1	U	406	SER	5.0
1	W	93	ILE	5.0
1	U	40	TYR	5.0
1	U	331	SER	5.0
1	S	105	MET	5.0
1	W	325	THR	5.0
1	W	320	VAL	5.0
1	U	257	GLN	4.9
1	W	104	GLY	4.9
1	W	330	CYS	4.9
1	W	409	LEU	4.9
1	S	109	ARG	4.9
1	U	178	VAL	4.9
1	U	337	ASN	4.9
1	W	200	ARG	4.9
1	W	106	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	M	256	ALA	4.8
1	U	314	MET	4.8
1	W	160	PRO	4.8
1	U	258	ILE	4.8
1	W	270	GLY	4.8
1	W	226	GLN	4.8
1	W	316	VAL	4.8
1	S	107	ILE	4.8
1	W	268	ALA	4.7
1	W	336	MET	4.7
1	Q	258	ILE	4.7
2	X	71	LEU	4.7
1	U	32	LYS	4.7
1	W	176	TRP	4.7
2	J	162	ASN	4.7
1	W	59	LEU	4.7
1	W	118	PHE	4.7
1	W	224	ALA	4.7
1	W	311	HIS	4.7
1	W	84	VAL	4.7
1	W	76	THR	4.6
1	U	231	MET	4.6
2	X	58	MET	4.6
1	W	410	ASN	4.6
1	W	125	TRP	4.6
1	Q	190	ALA	4.6
1	K	153	PHE	4.6
2	P	16	SER	4.6
1	Q	257	GLN	4.6
1	G	257	GLN	4.6
2	H	14	TRP	4.5
1	W	375	ILE	4.5
1	W	124	GLY	4.5
1	W	459	PRO	4.5
1	Q	22	GLU	4.5
1	M	258	ILE	4.5
1	W	309	LEU	4.5
1	M	254	SER	4.5
1	U	341	ILE	4.4
1	M	313	GLY	4.4
1	W	206	VAL	4.4
1	U	277	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	U	197	MET	4.4
1	W	95	VAL	4.4
1	W	99	GLN	4.4
1	W	275	GLY	4.4
1	W	374	ASN	4.4
1	O	109	ARG	4.4
1	S	89	LYS	4.4
1	W	353	TRP	4.4
1	U	229	SER	4.3
1	W	378	PHE	4.3
1	W	294	GLN	4.3
1	W	274	SER	4.3
1	W	108	CYS	4.3
1	W	48	LEU	4.3
1	I	18	ASN	4.3
1	I	260	THR	4.3
1	W	60	LEU	4.3
1	W	97	LEU	4.3
1	W	212	GLN	4.3
1	K	455	ALA	4.3
1	U	296	TRP	4.3
1	W	256	ALA	4.2
1	W	438	ALA	4.2
1	W	142	ALA	4.2
1	W	186	TYR	4.2
1	W	340	ARG	4.2
1	W	123	HIS	4.2
1	W	250	GLU	4.2
1	U	18	ASN	4.2
1	U	256	ALA	4.1
1	U	28	VAL	4.1
2	R	8	PHE	4.1
1	U	335	ALA	4.1
1	U	327	PHE	4.1
1	M	421	GLY	4.1
1	W	161	LEU	4.1
1	I	256	ALA	4.1
1	M	310	GLY	4.1
1	W	423	PRO	4.1
1	Q	260	THR	4.1
1	U	271	GLY	4.1
1	W	286	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	U	315	PRO	4.1
1	U	329	THR	4.0
1	W	456	THR	4.0
1	Q	105	MET	4.0
1	U	20	THR	4.0
1	W	238	THR	4.0
1	C	18	ASN	4.0
1	W	326	ILE	4.0
1	O	70	THR	4.0
1	U	425	PHE	4.0
1	W	177	ASP	4.0
1	W	158	TRP	4.0
1	K	109	ARG	4.0
2	P	7	HIS	4.0
1	M	19	TRP	4.0
1	W	321	GLY	4.0
1	W	370	TYR	4.0
1	W	287	VAL	4.0
2	X	76	ASP	4.0
1	U	452	PRO	4.0
1	W	255	GLN	4.0
1	S	103	ARG	3.9
1	U	263	ASN	3.9
1	W	98	ASN	3.9
1	M	423	PRO	3.9
1	W	319	MET	3.9
1	Q	253	LEU	3.9
1	W	61	LEU	3.9
1	U	58	TRP	3.9
2	D	14	TRP	3.9
1	W	323	HIS	3.9
1	M	253	LEU	3.9
1	M	260	THR	3.9
1	M	282	GLY	3.9
1	U	393	VAL	3.9
1	W	91	LYS	3.9
1	W	209	GLY	3.9
1	U	276	TRP	3.9
1	U	264	GLN	3.8
1	W	83	VAL	3.8
1	O	143	PHE	3.8
1	Q	109	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	S	416	GLY	3.8
1	W	440	GLY	3.8
1	W	66	HIS	3.8
1	U	19	TRP	3.8
1	U	392	TRP	3.8
1	W	452	PRO	3.8
1	I	20	THR	3.8
1	W	301	ALA	3.8
1	U	419	GLN	3.8
1	Q	335	ALA	3.8
1	U	311	HIS	3.8
1	W	230	ASP	3.8
1	Q	143	PHE	3.8
1	U	39	ILE	3.8
1	E	257	GLN	3.8
1	W	89	LYS	3.7
1	W	120	CYS	3.7
1	W	18	ASN	3.7
1	W	31	GLU	3.7
1	W	241	SER	3.7
1	U	287	VAL	3.7
1	U	442	TYR	3.7
1	W	327	PHE	3.7
1	S	104	GLY	3.7
1	U	269	TRP	3.7
1	C	258	ILE	3.7
1	W	132	LYS	3.7
1	K	138	PHE	3.7
1	U	457	LEU	3.7
1	W	314	MET	3.7
1	U	384	PHE	3.7
1	M	324	MET	3.7
1	U	423	PRO	3.7
1	S	140	LYS	3.7
1	U	355	PHE	3.7
1	W	75	ALA	3.7
1	U	288	MET	3.6
1	W	129	ILE	3.6
1	U	234	ALA	3.6
1	M	332	PHE	3.6
1	W	217	PRO	3.6
1	W	358	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	U	230	ASP	3.6
1	U	223	ALA	3.6
1	U	455	ALA	3.6
1	W	85	MET	3.6
1	U	316	VAL	3.6
1	I	333	LEU	3.6
1	Q	35	LEU	3.6
1	U	22	GLU	3.6
1	U	215	VAL	3.6
1	C	259	PRO	3.6
1	S	137	PRO	3.6
1	W	67	VAL	3.6
2	H	6	PRO	3.6
2	X	10	LYS	3.5
2	J	7	HIS	3.5
1	W	231	MET	3.5
2	X	113	LEU	3.5
2	X	67	ARG	3.5
1	W	110	SER	3.5
1	M	311	HIS	3.5
1	U	357	LEU	3.5
1	E	254	SER	3.5
1	U	363	PRO	3.5
1	S	311	HIS	3.5
1	W	116	LYS	3.5
2	L	67	ARG	3.5
1	W	73	PHE	3.5
2	V	16	SER	3.5
1	M	271	GLY	3.5
1	Q	203	ALA	3.5
1	W	411	ALA	3.5
1	U	417	ARG	3.4
1	W	416	GLY	3.4
1	G	259	PRO	3.4
1	U	297	THR	3.4
1	W	102	HIS	3.4
2	X	160	ASP	3.4
1	W	94	LYS	3.4
1	U	420	THR	3.4
1	Q	251	MET	3.4
2	X	79	LEU	3.4
1	S	332	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
2	T	8	PHE	3.4
1	G	258	ILE	3.4
1	U	292	VAL	3.4
1	W	202	PRO	3.4
2	P	6	PRO	3.4
1	W	288	MET	3.4
1	W	329	THR	3.4
1	O	156	ALA	3.4
1	U	391	ASN	3.4
1	W	40	TYR	3.4
1	W	377	ASN	3.4
1	Q	339	ILE	3.4
1	U	104	GLY	3.4
1	U	443	HIS	3.4
1	W	136	VAL	3.4
1	W	82	PRO	3.4
1	W	448	MET	3.3
1	U	23	ALA	3.3
1	I	253	LEU	3.3
1	S	23	ALA	3.3
1	U	27	LEU	3.3
1	Q	254	SER	3.3
1	S	455	ALA	3.3
1	G	261	LYS	3.3
1	I	257	GLN	3.3
1	U	312	THR	3.3
1	U	84	VAL	3.3
1	U	441	MET	3.3
1	W	213	LYS	3.3
1	U	265	PHE	3.3
1	S	121	SER	3.3
1	S	155	LYS	3.3
2	V	113	LEU	3.3
2	V	188	PHE	3.3
1	O	261	LYS	3.3
1	M	105	MET	3.3
1	U	233	HIS	3.3
2	X	117	VAL	3.3
1	K	256	ALA	3.3
1	O	18	ASN	3.2
1	W	376	ARG	3.2
1	G	254	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	U	272	HIS	3.2
1	K	134	VAL	3.2
1	W	372	ARG	3.2
1	M	306	GLU	3.2
1	W	310	GLY	3.2
1	I	332	PHE	3.2
1	Q	410	ASN	3.2
1	U	340	ARG	3.2
1	W	415	LEU	3.2
1	O	416	GLY	3.2
1	U	25	ARG	3.2
1	W	34	LEU	3.2
1	Q	281	PRO	3.2
1	S	156	ALA	3.2
1	U	59	LEU	3.2
1	W	211	MET	3.2
1	I	410	ASN	3.2
1	W	422	HIS	3.2
1	U	60	LEU	3.1
1	U	336	MET	3.1
1	U	338	ASN	3.1
1	W	251	MET	3.1
1	U	232	TYR	3.1
1	M	227	PHE	3.1
2	L	8	PHE	3.1
1	E	261	LYS	3.1
1	W	437	ALA	3.1
1	C	257	GLN	3.1
1	U	358	VAL	3.1
1	I	19	TRP	3.1
1	W	445	TRP	3.1
2	X	102	TRP	3.1
1	G	153	PHE	3.1
1	Q	430	GLY	3.1
1	W	96	PHE	3.1
1	O	364	ALA	3.1
1	W	305	ALA	3.1
1	W	432	VAL	3.1
2	H	160	ASP	3.1
1	Q	375	ILE	3.1
1	W	208	ILE	3.1
1	W	386	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	X	133	ALA	3.1
1	U	62	GLY	3.1
1	I	423	PRO	3.1
1	W	281	PRO	3.1
1	W	291	LYS	3.1
1	U	375	ILE	3.1
1	W	171	LEU	3.1
1	U	109	ARG	3.1
2	V	160	ASP	3.1
1	Q	422	HIS	3.1
1	W	39	ILE	3.0
1	W	392	TRP	3.1
1	U	74	LEU	3.0
1	U	448	MET	3.0
1	W	155	LYS	3.0
1	W	165	VAL	3.0
1	W	192	PRO	3.0
1	S	256	ALA	3.0
1	I	336	MET	3.0
1	U	434	ALA	3.0
1	W	302	ALA	3.0
1	U	194	MET	3.0
1	W	19	TRP	3.0
1	W	276	TRP	3.0
1	M	323	HIS	3.0
1	O	335	ALA	3.0
1	U	107	ILE	3.0
1	W	280	GLU	3.0
1	Q	252	ASP	3.0
1	W	178	VAL	3.0
1	U	307	GLN	3.0
1	I	312	THR	3.0
1	K	105	MET	3.0
1	U	240	LEU	3.0
1	U	284	LEU	3.0
1	W	70	THR	3.0
1	W	205	THR	3.0
1	Q	334	PRO	2.9
1	K	310	GLY	2.9
1	U	305	ALA	2.9
1	K	453	SER	2.9
1	S	108	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	318	ARG	2.9
1	K	311	HIS	2.9
1	M	339	ILE	2.9
1	M	456	THR	2.9
1	M	333	LEU	2.9
1	W	382	GLY	2.9
1	U	318	ARG	2.9
1	U	176	TRP	2.9
1	U	411	ALA	2.9
1	W	134	VAL	2.9
1	U	373	HIS	2.9
1	I	227	PHE	2.9
1	K	423	PRO	2.9
1	W	54	PHE	2.9
2	T	67	ARG	2.9
1	O	115	ALA	2.9
1	W	225	GLU	2.9
1	M	419	GLN	2.9
1	U	226	GLN	2.9
1	Q	259	PRO	2.9
1	U	328	PRO	2.9
1	W	413	MET	2.9
1	W	390	GLU	2.9
1	Q	337	ASN	2.9
1	W	254	SER	2.9
2	X	115	SER	2.9
1	O	103	ARG	2.9
1	U	454	TRP	2.9
1	W	210	GLY	2.9
2	X	66	ILE	2.9
2	X	188	PHE	2.9
1	C	179	GLN	2.9
1	W	307	GLN	2.9
1	M	331	SER	2.9
1	W	57	SER	2.9
1	I	259	PRO	2.8
1	M	327	PHE	2.8
1	S	324	MET	2.8
1	U	83	VAL	2.8
1	W	140	LYS	2.8
1	W	395	ILE	2.8
1	W	78	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	110	SER	2.8
1	M	202	PRO	2.8
1	U	290	PRO	2.8
1	U	90	ASP	2.8
1	W	64	GLU	2.8
1	I	339	ILE	2.8
1	K	273	GLY	2.8
1	U	440	GLY	2.8
2	X	162	ASN	2.8
1	Q	333	LEU	2.8
1	S	102	HIS	2.8
1	U	309	LEU	2.8
1	U	221	LYS	2.8
2	X	114	VAL	2.8
1	Q	324	MET	2.8
1	Q	332	PHE	2.8
1	U	424	ASP	2.8
1	W	35	LEU	2.8
1	W	399	LEU	2.8
1	G	18	ASN	2.8
1	W	342	TRP	2.8
2	F	14	TRP	2.8
1	W	352	VAL	2.7
1	W	199	ASP	2.7
1	W	252	ASP	2.7
1	W	308	ARG	2.7
1	U	395	ILE	2.7
1	Q	224	ALA	2.7
1	Q	302	ALA	2.7
1	W	298	GLU	2.7
1	W	260	THR	2.7
1	S	90	ASP	2.7
2	N	160	ASP	2.7
1	K	135	ASN	2.7
1	M	321	GLY	2.7
1	Q	198	LEU	2.7
1	W	127	TYR	2.7
1	W	81	ASP	2.7
1	W	229	SER	2.7
1	W	220	TRP	2.7
1	S	339	ILE	2.7
1	U	97	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	U	183	LEU	2.7
1	W	32	LYS	2.7
1	I	455	ALA	2.7
1	U	203	ALA	2.7
1	W	112	ALA	2.7
1	U	110	SER	2.7
1	U	193	TYR	2.7
2	P	74	SER	2.7
1	M	22	GLU	2.7
1	A	258	ILE	2.7
1	O	123	HIS	2.7
1	S	325	THR	2.7
1	O	310	GLY	2.7
1	Q	255	GLN	2.7
1	G	252	ASP	2.7
1	U	432	VAL	2.7
1	W	259	PRO	2.7
1	W	279	ASP	2.7
1	U	267	ALA	2.7
1	W	222	PHE	2.7
1	W	391	ASN	2.7
1	W	418	SER	2.7
2	X	82	PHE	2.7
1	O	158	TRP	2.7
1	W	363	PRO	2.7
1	U	453	SER	2.6
2	P	162	ASN	2.6
1	W	30	GLN	2.6
1	M	325	THR	2.6
1	O	120	CYS	2.6
1	W	68	PRO	2.6
1	W	249	PRO	2.6
2	B	6	PRO	2.6
1	S	38	ARG	2.6
1	U	171	LEU	2.6
1	U	379	SER	2.6
1	W	240	LEU	2.6
1	W	167	THR	2.6
2	V	32	TYR	2.6
1	W	101	ARG	2.6
1	W	436	GLU	2.6
2	X	44	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	197	MET	2.6
1	M	20	THR	2.6
1	Q	182	ASP	2.6
1	W	265	PHE	2.6
1	U	179	GLN	2.6
1	M	259	PRO	2.6
1	W	328	PRO	2.6
1	C	254	SER	2.6
1	I	254	SER	2.6
1	U	418	SER	2.6
1	U	450	SER	2.6
1	W	121	SER	2.6
1	W	367	LYS	2.6
1	M	415	LEU	2.6
1	M	437	ALA	2.6
1	W	393	VAL	2.6
1	W	441	MET	2.6
1	W	435	GLU	2.6
1	O	122	TYR	2.6
1	W	21	PRO	2.6
1	A	105	MET	2.6
1	O	198	LEU	2.6
1	S	83	VAL	2.6
1	W	284	LEU	2.6
1	U	38	ARG	2.6
1	U	185	THR	2.6
2	H	162	ASN	2.6
1	U	388	ASP	2.6
1	W	262	GLY	2.6
2	B	7	HIS	2.6
1	M	224	ALA	2.6
1	S	258	ILE	2.6
1	U	181	PRO	2.5
1	W	361	ASP	2.5
1	Q	58	TRP	2.5
1	U	445	TRP	2.5
1	W	235	GLY	2.5
1	W	271	GLY	2.5
2	X	69	GLY	2.5
1	K	89	LYS	2.5
1	U	402	TYR	2.5
1	W	117	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	22	GLU	2.5
1	G	251	MET	2.5
1	Q	197	MET	2.5
1	U	196	VAL	2.5
1	Q	341	ILE	2.5
1	M	228	CYS	2.5
1	C	261	LYS	2.5
1	U	294	GLN	2.5
1	U	225	GLU	2.5
1	S	117	ALA	2.5
1	I	324	MET	2.5
1	I	229	SER	2.5
1	U	222	PHE	2.5
1	W	223	ALA	2.5
1	W	364	ALA	2.5
1	I	273	GLY	2.5
1	W	283	SER	2.5
1	W	346	GLY	2.5
1	Q	365	GLU	2.5
1	W	272	HIS	2.5
1	Q	193	TYR	2.5
1	U	167	THR	2.5
1	W	50	LEU	2.5
1	W	62	GLY	2.5
1	U	31	GLU	2.5
1	M	455	ALA	2.5
1	S	100	CYS	2.5
1	U	70	THR	2.5
1	W	119	THR	2.5
1	U	370	TYR	2.5
2	N	16	SER	2.5
1	I	311	HIS	2.5
1	W	221	LYS	2.5
1	W	387	ASP	2.5
1	U	404	ALA	2.4
2	J	123	ALA	2.4
1	S	228	CYS	2.4
2	L	7	HIS	2.4
1	W	433	TYR	2.4
1	W	421	GLY	2.4
1	I	283	SER	2.4
2	V	35	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	419	GLN	2.4
1	O	334	PRO	2.4
1	W	315	PRO	2.4
1	Q	415	LEU	2.4
1	M	431	TYR	2.4
1	O	100	CYS	2.4
1	U	353	TRP	2.4
1	Q	156	ALA	2.4
1	U	302	ALA	2.4
2	V	133	ALA	2.4
1	U	280	GLU	2.4
1	W	164	ARG	2.4
1	G	138	PHE	2.4
1	I	274	SER	2.4
2	P	8	PHE	2.4
1	U	444	HIS	2.4
1	A	256	ALA	2.4
1	Q	325	THR	2.4
1	U	190	ALA	2.4
1	W	297	THR	2.4
1	Q	21	PRO	2.4
1	S	334	PRO	2.4
1	U	61	LEU	2.4
1	U	439	ARG	2.4
1	W	52	ARG	2.4
2	X	90	TYR	2.4
1	S	275	GLY	2.4
1	U	261	LYS	2.4
1	Q	331	SER	2.4
1	M	286	ALA	2.4
1	M	179	GLN	2.4
1	O	457	LEU	2.4
1	S	257	GLN	2.4
2	J	67	ARG	2.4
1	I	416	GLY	2.4
2	R	160	ASP	2.4
1	U	186	TYR	2.4
1	Q	229	SER	2.4
2	L	16	SER	2.4
2	X	172	ILE	2.4
1	U	173	PHE	2.4
1	O	21	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	259	PRO	2.4
1	O	456	THR	2.4
1	U	354	ALA	2.4
1	I	421	GLY	2.3
1	M	416	GLY	2.3
1	I	326	ILE	2.3
1	U	33	GLY	2.3
1	W	242	GLY	2.3
1	I	35	LEU	2.3
1	W	239	HIS	2.3
1	U	168	TYR	2.3
2	X	31	TYR	2.3
1	M	335	ALA	2.3
1	S	312	THR	2.3
2	X	125	PRO	2.3
1	W	263	ASN	2.3
2	X	134	PHE	2.3
1	S	120	CYS	2.3
1	C	311	HIS	2.3
1	E	251	MET	2.3
1	Q	457	LEU	2.3
1	M	178	VAL	2.3
1	W	300	PRO	2.3
2	X	32	TYR	2.3
1	M	305	ALA	2.3
1	K	143	PHE	2.3
1	S	118	PHE	2.3
2	N	9	PHE	2.3
1	K	454	TRP	2.3
1	I	432	VAL	2.3
1	O	423	PRO	2.3
1	W	290	PRO	2.3
1	O	455	ALA	2.3
1	Q	185	THR	2.3
1	U	77	TYR	2.3
2	R	67	ARG	2.3
1	M	322	GLN	2.3
1	M	229	SER	2.3
1	G	105	MET	2.3
1	K	91	LYS	2.3
1	W	214	TRP	2.3
2	V	162	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	192	PRO	2.3
1	S	21	PRO	2.3
2	X	87	GLU	2.3
1	I	33	GLY	2.3
1	Q	104	GLY	2.3
1	U	170	GLY	2.3
1	U	268	ALA	2.3
1	W	190	ALA	2.3
1	W	427	GLY	2.3
1	S	227	PHE	2.3
1	I	323	HIS	2.3
1	I	424	ASP	2.3
2	P	160	ASP	2.3
1	I	337	ASN	2.3
1	M	197	MET	2.3
2	P	67	ARG	2.3
1	I	419	GLN	2.2
1	S	255	GLN	2.2
1	M	32	LYS	2.2
1	W	65	SER	2.2
1	W	295	TYR	2.2
1	W	424	ASP	2.2
1	U	103	ARG	2.2
1	I	255	GLN	2.2
1	I	322	GLN	2.2
1	U	198	LEU	2.2
1	S	310	GLY	2.2
1	M	411	ALA	2.2
1	W	277	TYR	2.2
1	Q	227	PHE	2.2
1	C	260	THR	2.2
1	U	283	SER	2.2
1	W	234	ALA	2.2
1	S	326	ILE	2.2
1	I	32	LYS	2.2
1	Q	336	MET	2.2
1	U	446	MET	2.2
1	I	418	SER	2.2
1	E	18	ASN	2.2
1	O	422	HIS	2.2
2	V	172	ILE	2.2
1	Q	222	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	275	GLY	2.2
1	U	282	GLY	2.2
1	W	187	LEU	2.2
1	Q	140	LYS	2.2
1	G	420	THR	2.2
1	K	260	THR	2.2
1	S	260	THR	2.2
1	Q	275	GLY	2.2
1	U	381	GLY	2.2
1	W	195	ASP	2.2
2	V	101	GLY	2.2
1	U	34	LEU	2.2
1	I	228	CYS	2.2
2	X	132	SER	2.2
1	W	380	ALA	2.2
2	J	17	LYS	2.1
1	S	134	VAL	2.1
1	U	262	GLY	2.1
1	M	420	THR	2.1
1	C	424	ASP	2.1
2	P	10	LYS	2.1
2	P	18	ALA	2.1
1	Q	31	GLU	2.1
1	Q	273	GLY	2.1
1	W	306	GLU	2.1
1	W	292	VAL	2.1
1	Q	274	SER	2.1
1	I	50	LEU	2.1
1	S	417	ARG	2.1
2	D	160	ASP	2.1
1	Q	438	ALA	2.1
1	U	245	ALA	2.1
1	U	414	GLY	2.1
1	K	259	PRO	2.1
1	W	137	PRO	2.1
1	W	426	PRO	2.1
1	Q	153	PHE	2.1
1	U	451	GLU	2.1
1	W	365	GLU	2.1
2	X	70	GLU	2.1
1	I	420	THR	2.1
1	Q	409	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	282	GLY	2.1
1	S	166	ALA	2.1
1	U	41	ALA	2.1
1	Q	18	ASN	2.1
1	Q	69	GLU	2.1
1	Q	419	GLN	2.1
1	W	173	PHE	2.1
1	Q	27	LEU	2.1
1	U	205	THR	2.1
2	V	58	MET	2.1
1	I	437	ALA	2.1
1	U	346	GLY	2.1
1	S	139	GLU	2.1
2	V	67	ARG	2.1
1	Q	322	GLN	2.1
2	V	135	ILE	2.1
1	S	53	VAL	2.1
1	Q	186	TYR	2.1
1	U	295	TYR	2.1
2	X	81	HIS	2.1
1	M	326	ILE	2.1
2	X	135	ILE	2.1
1	S	141	GLU	2.0
1	I	417	ARG	2.0
1	Q	318	ARG	2.0
1	W	201	THR	2.0
2	X	122	THR	2.0
1	I	335	ALA	2.0
1	E	252	ASP	2.0
1	Q	277	TYR	2.0
1	S	41	ALA	2.0
1	W	90	ASP	2.0
2	R	76	ASP	2.0
1	M	274	SER	2.0
1	O	375	ILE	2.0
1	Q	191	ARG	2.0
1	S	106	ARG	2.0
1	Q	278	VAL	2.0
1	C	457	LEU	2.0
1	Q	116	LYS	2.0
1	S	438	ALA	2.0
1	U	413	MET	2.0

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Mol	Chain	Res	Type	RSRZ
2	X	141	LEU	2.0
1	M	330	CYS	2.0
1	E	21	PRO	2.0
1	S	259	PRO	2.0
1	G	250	GLU	2.0
1	U	285	LEU	2.0
2	X	60	LEU	2.0
1	S	123	HIS	2.0
1	I	281	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	FE2	G	901	1/1	0.99	0.14	2.05	14,14,14,14	0
4	FE2	O	901	1/1	0.98	0.16	0.59	32,32,32,32	0
4	FE2	E	901	1/1	0.99	0.12	0.44	20,20,20,20	0
3	FES	E	900	4/4	0.98	0.10	0.07	13,13,14,15	0
3	FES	I	900	4/4	0.97	0.10	-0.33	14,15,15,17	0
3	FES	C	900	4/4	0.99	0.10	-0.45	17,18,19,19	0
4	FE2	I	901	1/1	0.96	0.14	-0.55	48,48,48,48	0
3	FES	G	900	4/4	0.97	0.10	-0.60	25,26,26,27	0
3	FES	A	900	4/4	0.98	0.09	-0.73	19,20,22,22	0
3	FES	M	900	4/4	0.98	0.09	-0.85	21,21,21,21	0
4	FE2	U	901	1/1	0.82	0.27	-1.01	67,67,67,67	0
3	FES	U	900	4/4	0.96	0.07	-1.50	21,23,23,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FES	Q	900	4/4	0.98	0.08	-2.06	31,32,37,37	0
3	FES	S	900	4/4	0.93	0.09	-2.14	48,48,50,50	0
3	FES	K	900	4/4	0.97	0.05	-2.81	32,33,34,35	0
4	FE2	W	901	1/1	0.96	0.08	-2.84	57,57,57,57	0
3	FES	O	900	4/4	0.94	0.06	-2.96	41,42,43,43	0
4	FE2	M	901	1/1	0.98	0.08	-3.06	37,37,37,37	0
3	FES	W	900	4/4	0.91	0.10	-3.67	65,67,68,69	0
4	FE2	Q	901	1/1	0.93	0.08	-4.09	45,45,45,45	0
4	FE2	S	901	1/1	0.96	0.11	-	26,26,26,26	0
4	FE2	C	901	1/1	0.99	0.14	-	29,29,29,29	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

6.5 Other polymers (i)

There are no such residues in this entry.