



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 AM GMT

PDB ID : 2XR8  
Title : CRYSTAL STRUCTURE OF BIPHENYL DIOXYGENASE FROM  
BURKHOLDERIA XENOVORANS LB400  
Authors : Kumar, P.; Bolin, J.T.  
Deposited on : 2010-09-12  
Resolution : 2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

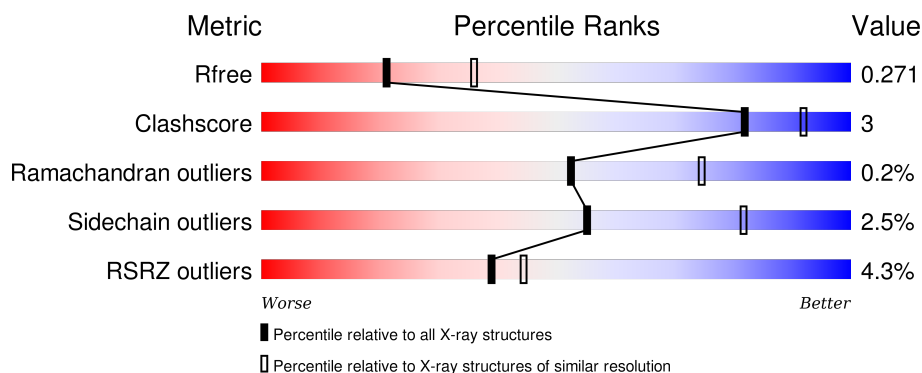
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	459	<div> <div>2%</div> <div>83% 10% 6%</div> </div>
1	C	459	<div> <div>4%</div> <div>87% 7% 6%</div> </div>
1	E	459	<div> <div>4%</div> <div>85% 8% 6%</div> </div>
1	G	459	<div> <div>7%</div> <div>85% 9% 6%</div> </div>
1	I	459	<div> <div>9%</div> <div>87% 7% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
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 59924 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
			3436	2187	603	623	23			
1	C	433	Total	C	N	O	S	0	0	0
			3436	2187	603	623	23			
1	E	433	Total	C	N	O	S	0	0	0
			3436	2187	603	623	23			
1	G	433	Total	C	N	O	S	0	0	0
			3436	2187	603	623	23			
1	I	433	Total	C	N	O	S	0	0	0
			3436	2187	603	623	23			
1	K	433	Total	C	N	O	S	0	0	0
			3436	2187	603	623	23			
1	M	433	Total	C	N	O	S	0	0	0
			3432	2185	602	622	23			
1	O	433	Total	C	N	O	S	0	0	0
			3432	2185	602	622	23			
1	Q	433	Total	C	N	O	S	0	0	0
			3432	2185	602	622	23			
1	S	433	Total	C	N	O	S	0	0	0
			3436	2187	603	623	23			
1	U	433	Total	C	N	O	S	0	0	0
			3436	2187	603	623	23			
1	W	433	Total	C	N	O	S	0	0	0
			3436	2187	603	623	23			

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

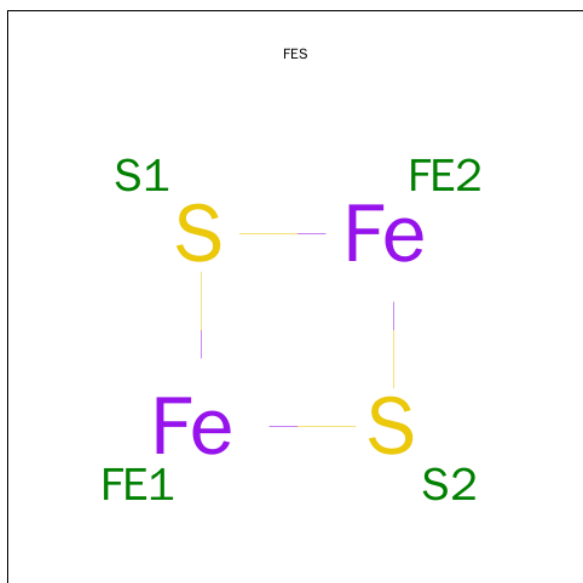
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	D	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	H	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	J	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	L	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	N	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	P	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	R	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	T	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	V	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			
2	X	180	Total	C	N	O	S	0	0	0
			1496	948	265	279	4			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	44	Total 44	O 44	0	0
5	B	26	Total 26	O 26	0	0
5	C	28	Total 28	O 28	0	0
5	D	24	Total 24	O 24	0	0
5	E	35	Total 35	O 35	0	0
5	F	19	Total 19	O 19	0	0
5	G	23	Total 23	O 23	0	0
5	H	14	Total 14	O 14	0	0
5	I	23	Total 23	O 23	0	0
5	J	14	Total 14	O 14	0	0
5	K	49	Total 49	O 49	0	0
5	L	16	Total 16	O 16	0	0
5	M	49	Total 49	O 49	0	0
5	N	31	Total 31	O 31	0	0
5	O	58	Total 58	O 58	0	0

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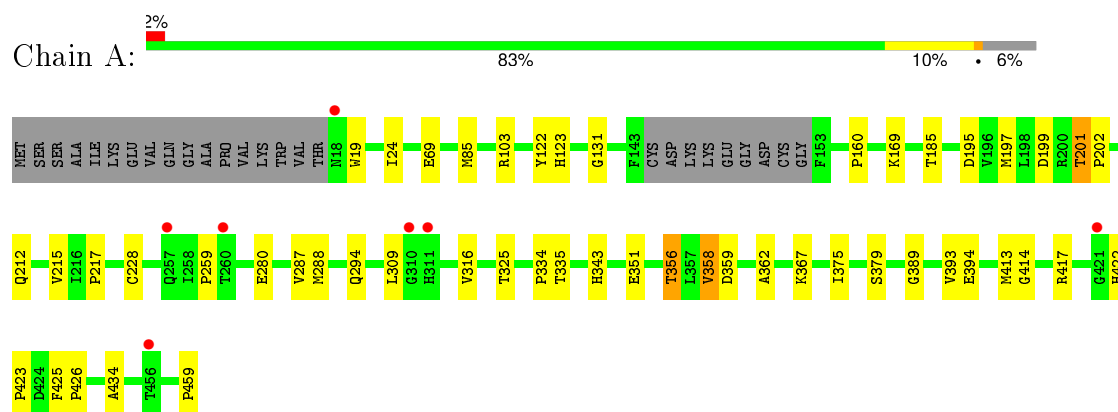
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	35	Total 35	O 35	0	0
5	Q	42	Total 42	O 42	0	0
5	R	24	Total 24	O 24	0	0
5	S	34	Total 34	O 34	0	0
5	T	23	Total 23	O 23	0	0
5	U	22	Total 22	O 22	0	0
5	V	15	Total 15	O 15	0	0
5	W	22	Total 22	O 22	0	0
5	X	22	Total 22	O 22	0	0



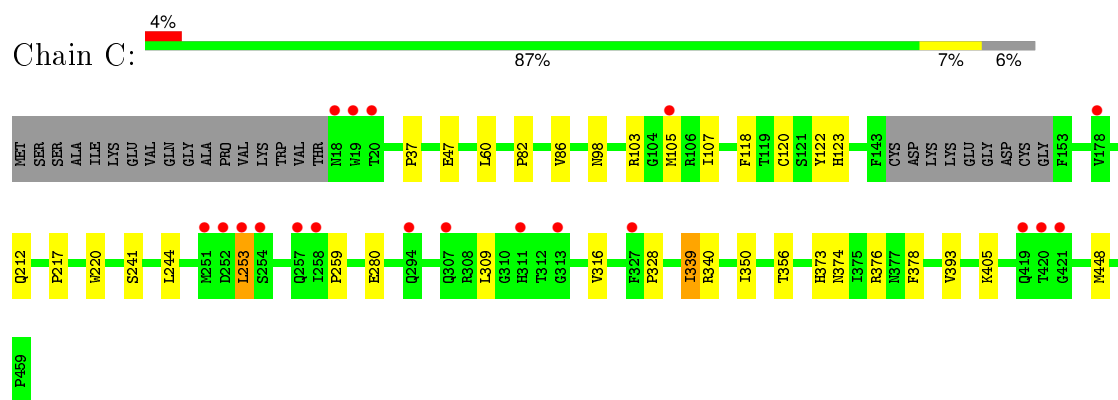
### 3 Residue-property plots

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.

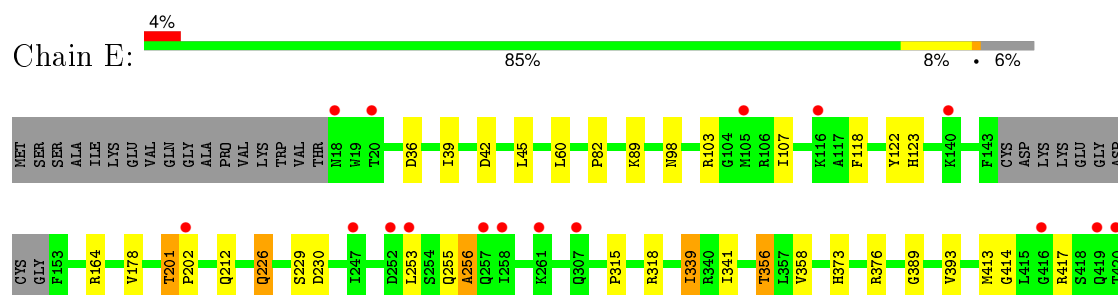
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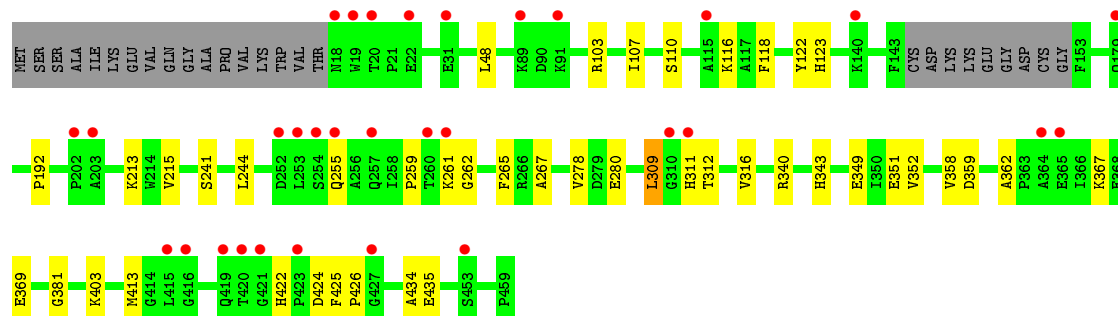
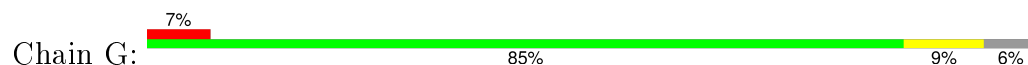


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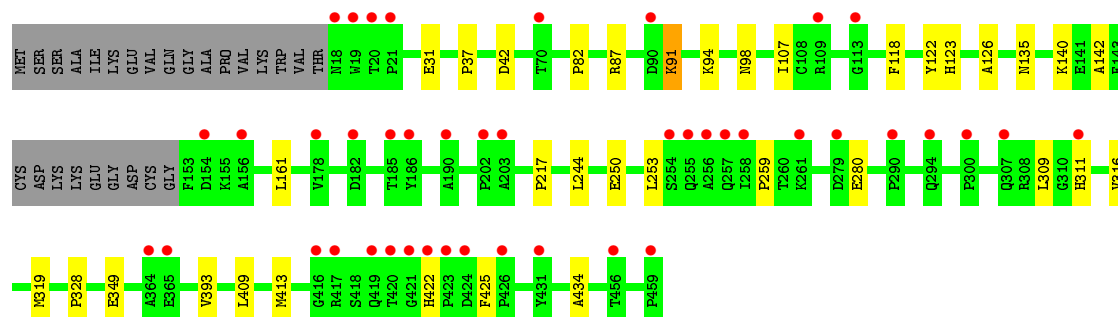
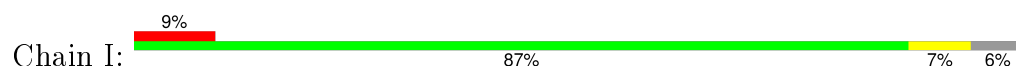




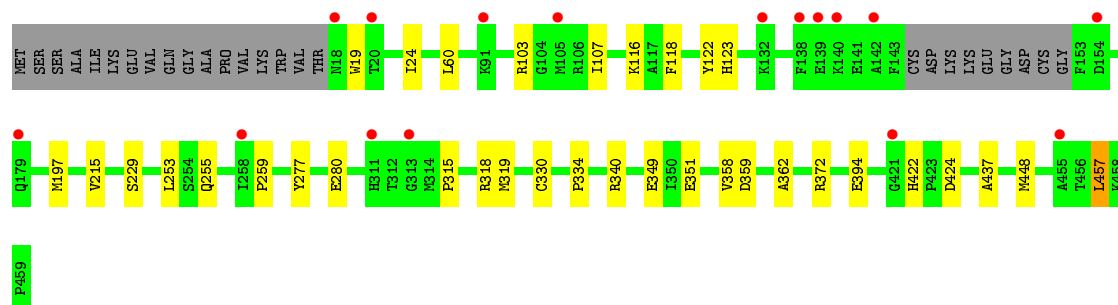
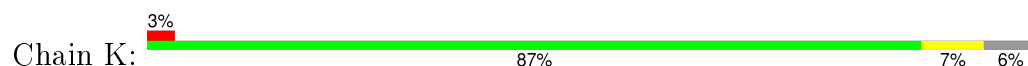
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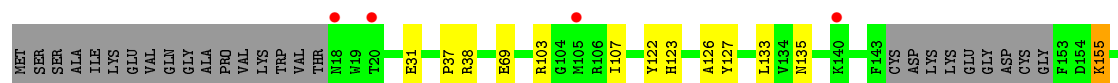
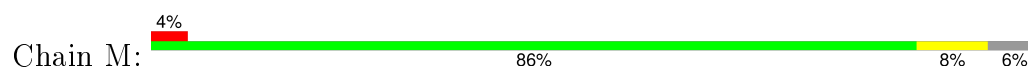
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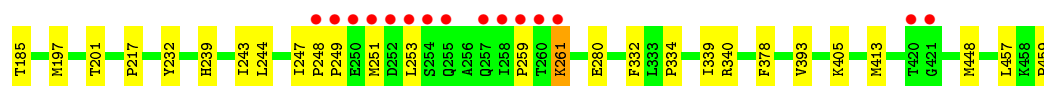


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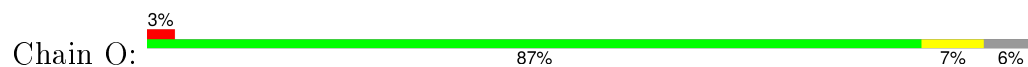


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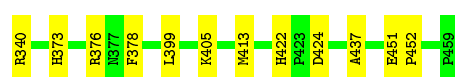
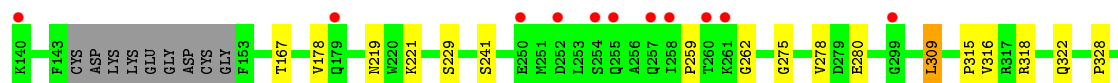
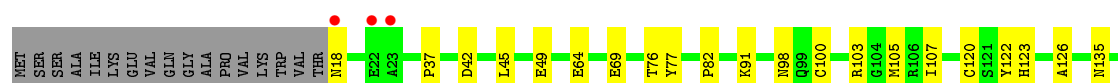
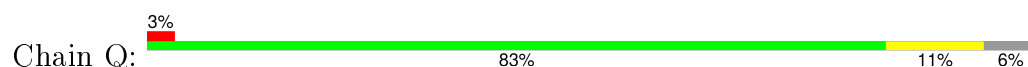




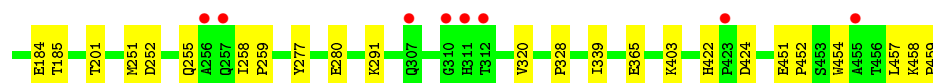
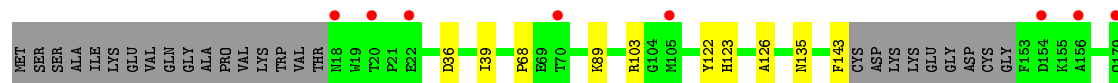
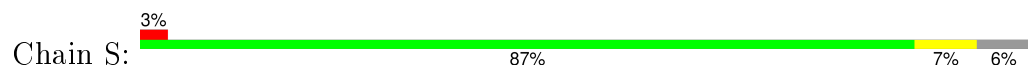
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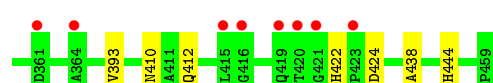
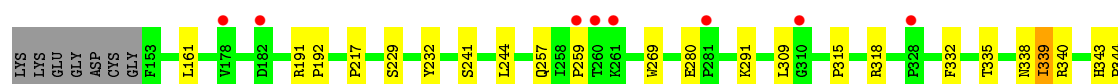
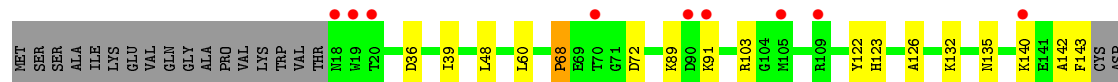
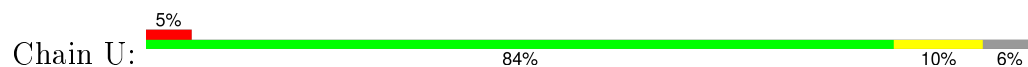
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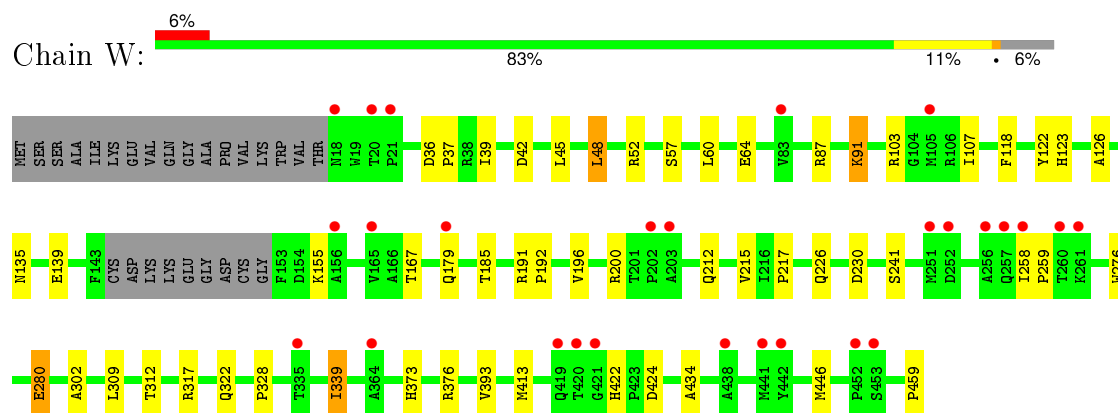
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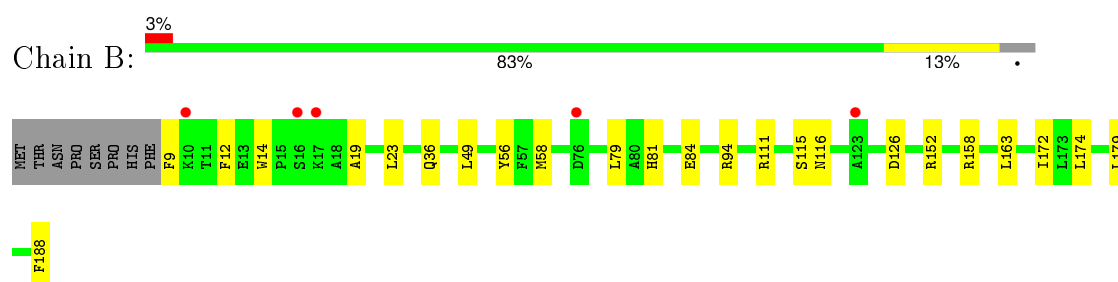
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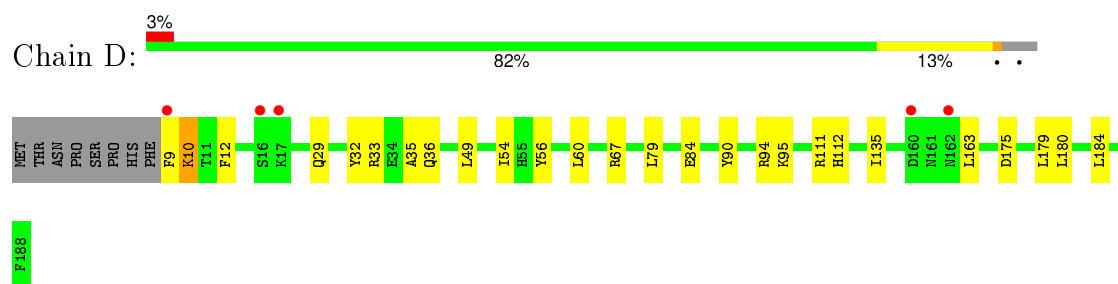
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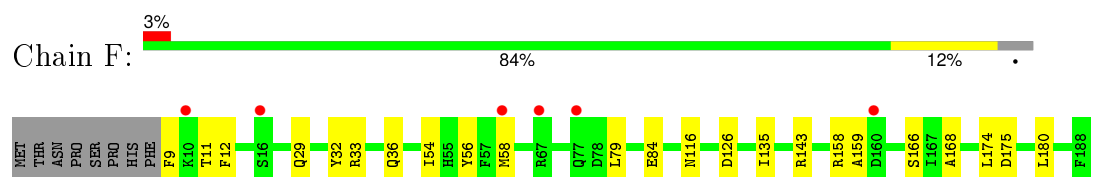
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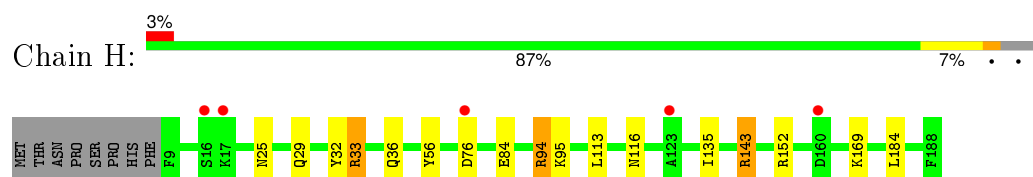
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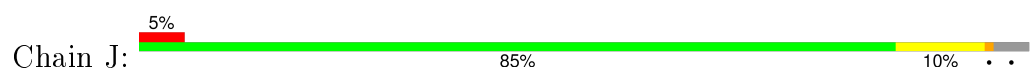
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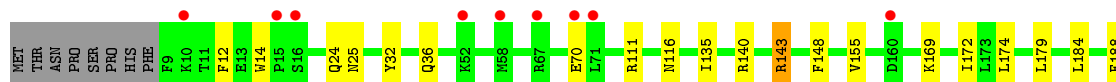


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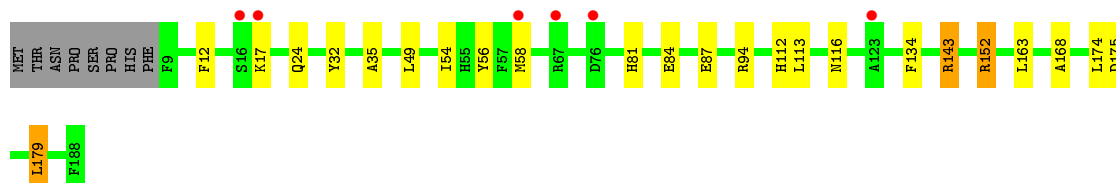
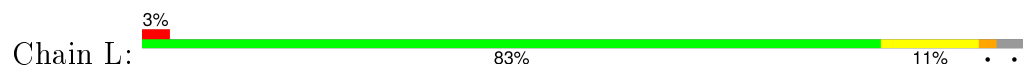


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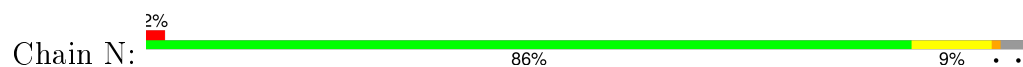




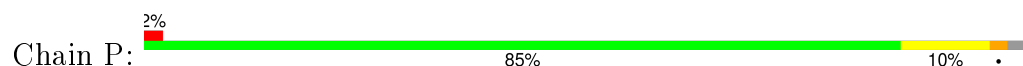
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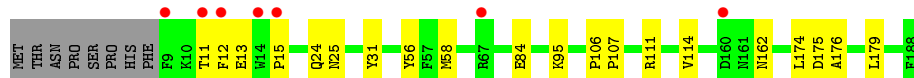
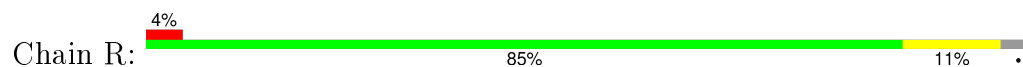
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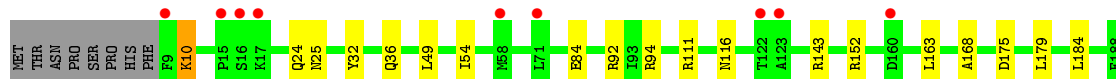
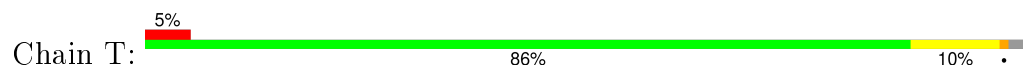
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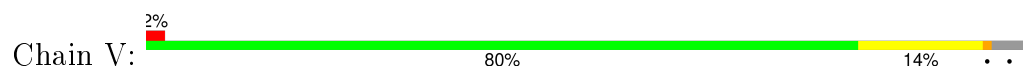
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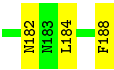
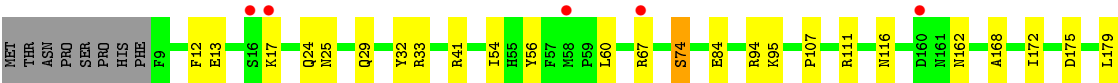
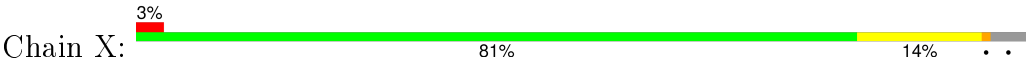


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA





● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.59Å 132.35Å 132.98Å 102.60° 102.68° 104.61°	Depositor
Resolution (Å)	129.10 – 2.49 26.25 – 2.49	Depositor EDS
% Data completeness (in resolution range)	89.3 (129.10-2.49) 63.1 (26.25-2.49)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.216 , 0.267 0.229 , 0.271	Depositor DCC
$R_{free}$ test set	514 reflections (0.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.2	EDS
Estimated twinning fraction	0.025 for l,h,k 0.025 for k,l,h 0.016 for -k,-h,-l 0.016 for -h,-l,-k 0.006 for -l,-k,-h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 185934 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	59924	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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	0.34	0/3539	0.47	0/4804
1	C	0.34	0/3539	0.48	0/4804
1	E	0.35	0/3539	0.48	0/4804
1	G	0.33	0/3539	0.47	0/4804
1	I	0.34	0/3539	0.47	0/4804
1	K	0.33	0/3539	0.48	0/4804
1	M	0.34	0/3535	0.49	0/4799
1	O	0.35	0/3535	0.49	0/4799
1	Q	0.35	0/3535	0.49	0/4799
1	S	0.35	0/3539	0.47	0/4804
1	U	0.35	0/3539	0.48	0/4804
1	W	0.35	0/3539	0.47	0/4804
2	B	0.37	0/1530	0.51	0/2068
2	D	0.35	0/1530	0.51	0/2068
2	F	0.35	0/1530	0.50	0/2068
2	H	0.34	0/1530	0.49	0/2068
2	J	0.35	0/1530	0.49	0/2068
2	L	0.35	0/1530	0.50	0/2068
2	N	0.36	0/1530	0.51	0/2068
2	P	0.36	0/1530	0.54	0/2068
2	R	0.35	0/1530	0.51	0/2068
2	T	0.35	0/1530	0.51	0/2068
2	V	0.36	0/1530	0.51	0/2068
2	X	0.36	0/1530	0.50	0/2068
All	All	0.35	0/60816	0.49	0/82449

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3436	0	3289	30	0
1	C	3436	0	3289	18	0
1	E	3436	0	3289	24	0
1	G	3436	0	3289	23	0
1	I	3436	0	3289	16	0
1	K	3436	0	3289	20	0
1	M	3432	0	3283	22	0
1	O	3432	0	3283	21	0
1	Q	3432	0	3283	26	0
1	S	3436	0	3289	16	0
1	U	3436	0	3289	22	0
1	W	3436	0	3289	29	0
2	B	1496	0	1447	18	0
2	D	1496	0	1447	18	0
2	F	1496	0	1447	17	0
2	H	1496	0	1447	13	0
2	J	1496	0	1447	14	0
2	L	1496	0	1447	17	0
2	N	1496	0	1447	10	0
2	P	1496	0	1447	12	0
2	R	1496	0	1447	12	0
2	T	1496	0	1447	13	0
2	V	1496	0	1447	18	0
2	X	1496	0	1447	19	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	1	0
3	K	4	0	0	1	0
3	M	4	0	0	1	0
3	O	4	0	0	1	0
3	Q	4	0	0	1	0
3	S	4	0	0	1	0
3	U	4	0	0	1	0
3	W	4	0	0	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	44	0	0	1	0
5	B	26	0	0	1	0
5	C	28	0	0	0	0
5	D	24	0	0	0	0
5	E	35	0	0	0	0
5	F	19	0	0	1	0
5	G	23	0	0	1	0
5	H	14	0	0	0	0
5	I	23	0	0	0	0
5	J	14	0	0	0	0
5	K	49	0	0	2	0
5	L	16	0	0	0	0
5	M	49	0	0	0	0
5	N	31	0	0	0	0
5	O	58	0	0	0	0
5	P	35	0	0	0	0
5	Q	42	0	0	0	0
5	R	24	0	0	0	0
5	S	34	0	0	1	0
5	T	23	0	0	0	0
5	U	22	0	0	0	0
5	V	15	0	0	0	0
5	W	22	0	0	1	0
5	X	22	0	0	0	0
All	All	59924	0	56814	374	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 3.

All (374) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:259:PRO:HB3	1:O:280:GLU:HG2	1.53	0.89
1:E:255:GLN:O	1:E:256:ALA:O	1.93	0.87
1:A:259:PRO:HB3	1:A:280:GLU:HG2	1.55	0.86
2:R:58:MET:HE1	2:R:174:LEU:HD22	1.58	0.85
1:I:123:HIS:HB2	3:I:900:FES:S2	2.17	0.84
1:C:259:PRO:HB3	1:C:280:GLU:HG2	1.58	0.83
1:K:259:PRO:HB3	1:K:280:GLU:HG2	1.60	0.82
1:U:259:PRO:HB3	1:U:280:GLU:HG2	1.65	0.79
1:W:123:HIS:HB2	3:W:900:FES:S2	2.23	0.78
2:P:11:THR:O	2:P:13:GLU:N	2.17	0.78
1:E:255:GLN:O	1:E:256:ALA:C	2.24	0.76
1:E:123:HIS:HB2	3:E:900:FES:S2	2.27	0.75
1:W:259:PRO:HB3	1:W:280:GLU:HG2	1.66	0.75
2:R:58:MET:CE	2:R:174:LEU:HD22	2.19	0.73
1:G:123:HIS:HB2	3:G:900:FES:S2	2.29	0.73
2:L:58:MET:HE1	2:L:174:LEU:HD22	1.70	0.73
1:O:100:CYS:HB2	1:O:107:ILE:HD11	1.71	0.70
1:M:259:PRO:HB3	1:M:280:GLU:HG2	1.73	0.70
1:C:373:HIS:HD2	1:C:376:ARG:HE	1.39	0.69
2:N:24:GLN:HG2	2:R:25:ASN:HD21	1.59	0.68
1:K:123:HIS:HB2	3:K:900:FES:S2	2.34	0.67
1:O:123:HIS:HB2	3:O:900:FES:S2	2.35	0.67
1:G:422:HIS:HD2	1:G:424:ASP:H	1.43	0.66
1:I:259:PRO:HB3	1:I:280:GLU:HG2	1.78	0.65
2:B:36:GLN:HE21	2:D:12:PHE:H	1.42	0.65
2:N:56:TYR:HB3	2:N:84:GLU:HB2	1.79	0.64
2:B:81:HIS:CE1	2:B:179:LEU:HD21	2.31	0.64
1:M:133:LEU:HG	1:M:155:LYS:HG2	1.79	0.64
1:A:294:GLN:HG2	5:A:2028:HOH:O	1.96	0.64
1:C:123:HIS:HB2	3:C:900:FES:S2	2.38	0.64
1:S:123:HIS:HB2	3:S:900:FES:S2	2.38	0.64
1:G:403:LYS:HE3	1:I:161:LEU:HD21	1.78	0.63
1:O:422:HIS:HD2	1:O:424:ASP:H	1.46	0.63
2:T:25:ASN:HD21	2:V:24:GLN:HG2	1.64	0.63
1:Q:422:HIS:HD2	1:Q:424:ASP:H	1.47	0.62
1:M:185:THR:HG22	1:M:459:PRO:HG2	1.82	0.61
1:M:123:HIS:HB2	3:M:900:FES:S2	2.39	0.61
1:Q:309:LEU:HD13	1:Q:316:VAL:HG21	1.82	0.61
1:Q:259:PRO:HB3	1:Q:280:GLU:HG2	1.83	0.61
1:A:413:MET:HG2	1:A:434:ALA:HA	1.83	0.60
1:E:413:MET:HG2	1:E:434:ALA:HA	1.84	0.60
2:T:49:LEU:HD21	2:T:163:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:HG22	1:A:202:PRO:HD2	1.84	0.60
1:E:201:THR:HG22	1:E:202:PRO:HD2	1.83	0.60
1:S:251:MET:O	2:T:94:ARG:NH2	2.34	0.59
1:M:126:ALA:HB3	1:M:135:ASN:HB3	1.85	0.59
1:S:126:ALA:HB3	1:S:135:ASN:HB3	1.84	0.59
2:D:9:PHE:O	2:D:10:LYS:HG2	2.03	0.59
2:B:9:PHE:HA	5:B:2002:HOH:O	2.01	0.59
1:U:123:HIS:HB2	3:U:900:FES:S2	2.42	0.59
1:M:244:LEU:HD13	1:M:253:LEU:HG	1.85	0.59
1:O:49:GLU:OE1	1:O:221:LYS:HE3	2.02	0.59
2:L:54:ILE:HA	2:L:168:ALA:O	2.03	0.59
1:K:448:MET:HA	1:K:457:LEU:HD11	1.83	0.59
2:N:26:GLU:OE1	2:N:158:ARG:NH2	2.36	0.58
1:W:373:HIS:HD2	1:W:376:ARG:HH21	1.52	0.58
1:U:60:LEU:HD22	1:U:339:ILE:HD11	1.86	0.58
2:D:36:GLN:NE2	2:F:12:PHE:H	2.01	0.58
1:U:91:LYS:HE2	1:U:91:LYS:HA	1.85	0.57
1:K:315:PRO:HB2	1:K:318:ARG:HG3	1.87	0.57
2:L:87:GLU:HG3	2:P:76:ASP:OD1	2.04	0.57
1:K:422:HIS:HD2	1:K:424:ASP:H	1.53	0.57
1:W:60:LEU:CD2	1:W:339:ILE:HD11	2.34	0.57
1:Q:123:HIS:HB2	3:Q:900:FES:S2	2.45	0.57
2:T:36:GLN:HE21	2:V:12:PHE:H	1.50	0.56
1:Q:229:SER:HB2	1:Q:437:ALA:HB3	1.87	0.56
1:Q:100:CYS:HB2	1:Q:107:ILE:HD11	1.88	0.56
2:J:172:ILE:HD13	2:J:188:PHE:HB2	1.87	0.55
2:B:36:GLN:NE2	2:D:12:PHE:H	2.04	0.55
2:B:14:TRP:CE2	2:F:33:ARG:HD3	2.41	0.55
1:A:123:HIS:HB2	3:A:900:FES:S2	2.47	0.55
1:K:422:HIS:CD2	1:K:424:ASP:H	2.24	0.55
2:N:111:ARG:HB2	2:P:175:ASP:OD2	2.08	0.54
1:G:413:MET:HG3	1:I:142:ALA:HB1	1.89	0.54
2:V:26:GLU:OE1	2:V:158:ARG:NH2	2.41	0.54
1:U:232:TYR:CE1	1:W:123:HIS:HB3	2.42	0.54
1:W:42:ASP:HB3	1:W:45:LEU:HB2	1.89	0.54
1:A:228:CYS:HB2	1:A:325:THR:HB	1.90	0.54
1:W:107:ILE:HG22	1:W:118:PHE:HB3	1.90	0.54
1:G:422:HIS:CD2	1:G:424:ASP:H	2.23	0.54
2:B:172:ILE:HD13	2:B:188:PHE:HB2	1.90	0.54
2:P:25:ASN:HD21	2:R:24:GLN:HG2	1.72	0.54
1:C:82:PRO:HB2	1:C:98:ASN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:126:ALA:HB3	1:Q:135:ASN:HB3	1.90	0.53
1:M:244:LEU:HG	2:N:94:ARG:HG2	1.90	0.53
1:Q:82:PRO:HB2	1:Q:98:ASN:HB3	1.89	0.53
2:F:54:ILE:HA	2:F:168:ALA:O	2.08	0.53
2:X:41:ARG:HE	2:X:107:PRO:HB2	1.73	0.53
2:D:56:TYR:HB3	2:D:84:GLU:HB2	1.90	0.53
1:Q:241:SER:HB2	2:R:95:LYS:HG3	1.90	0.53
2:D:36:GLN:HE21	2:F:12:PHE:H	1.55	0.53
1:M:239:HIS:O	1:M:243:ILE:HG12	2.08	0.53
2:T:111:ARG:HB2	2:V:175:ASP:OD2	2.09	0.53
1:C:241:SER:HB2	2:D:95:LYS:HG2	1.91	0.53
2:J:32:TYR:CD1	2:L:116:ASN:HA	2.43	0.53
1:O:107:ILE:HG22	1:O:118:PHE:HB3	1.91	0.53
2:L:58:MET:CE	2:L:174:LEU:HD22	2.38	0.52
2:J:111:ARG:HB2	2:L:175:ASP:OD2	2.09	0.52
1:K:253:LEU:HB3	2:P:10:LYS:HB2	1.91	0.52
1:W:413:MET:HB3	1:W:434:ALA:HA	1.91	0.52
2:H:25:ASN:HD21	2:J:24:GLN:HG2	1.73	0.52
1:I:87:ARG:HD2	1:I:91:LYS:HD3	1.90	0.52
1:E:60:LEU:HD23	1:E:341:ILE:HG12	1.91	0.52
1:W:422:HIS:HD2	1:W:424:ASP:H	1.56	0.52
2:L:81:HIS:CE1	2:L:179:LEU:HD21	2.43	0.52
1:M:340:ARG:HH21	1:M:378:PHE:HB3	1.73	0.52
1:E:356:THR:HG23	2:F:79:LEU:HD11	1.92	0.52
1:U:315:PRO:HB2	1:U:318:ARG:HG3	1.91	0.51
2:D:90:TYR:CE2	2:D:94:ARG:HD2	2.45	0.51
1:E:454:TRP:HA	1:E:457:LEU:HB2	1.90	0.51
1:W:48:LEU:HD23	1:W:52:ARG:HG3	1.91	0.51
2:T:175:ASP:OD2	2:X:111:ARG:HB2	2.10	0.51
1:I:316:VAL:HA	1:I:319:MET:HG2	1.92	0.51
1:A:309:LEU:HD13	1:A:316:VAL:HG11	1.93	0.51
1:W:191:ARG:N	1:W:192:PRO:HD2	2.25	0.51
1:E:42:ASP:HB3	1:E:45:LEU:HB2	1.93	0.51
2:B:126:ASP:HB3	2:B:158:ARG:HB2	1.90	0.51
1:S:403:LYS:HE3	1:U:161:LEU:HD21	1.92	0.51
1:M:37:PRO:HG2	1:M:405:LYS:HA	1.93	0.51
2:B:116:ASN:HA	2:F:32:TYR:CD1	2.45	0.51
1:Q:373:HIS:HD2	1:Q:376:ARG:HE	1.58	0.51
1:I:244:LEU:HD13	1:I:253:LEU:HG	1.93	0.51
2:H:33:ARG:HG2	2:J:14:TRP:CE2	2.46	0.51
1:E:164:ARG:HD2	1:E:178:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:ILE:HG22	1:G:118:PHE:HB3	1.92	0.50
1:W:126:ALA:HB3	1:W:135:ASN:HB3	1.92	0.50
1:C:107:ILE:HG22	1:C:118:PHE:HB3	1.92	0.50
1:U:191:ARG:N	1:U:192:PRO:HD2	2.27	0.50
1:Q:49:GLU:OE1	1:Q:221:LYS:HE3	2.12	0.50
1:S:36:ASP:O	1:S:39:ILE:HG12	2.11	0.50
1:U:244:LEU:HG	2:V:94:ARG:HG2	1.92	0.50
1:I:422:HIS:HD2	1:I:425:PHE:H	1.59	0.50
1:C:60:LEU:CD2	1:C:339:ILE:HD11	2.42	0.50
2:V:9:PHE:O	2:V:10:LYS:HB3	2.11	0.50
1:U:217:PRO:HD2	1:U:393:VAL:HG22	1.93	0.50
1:A:389:GLY:O	1:A:393:VAL:HG23	2.12	0.49
1:O:100:CYS:CB	1:O:107:ILE:HD11	2.42	0.49
1:O:340:ARG:HH21	1:O:378:PHE:HB3	1.77	0.49
1:S:185:THR:HG22	1:S:459:PRO:HG2	1.93	0.49
1:G:413:MET:HG2	1:G:434:ALA:HA	1.94	0.49
1:G:309:LEU:HD13	1:G:316:VAL:HG11	1.94	0.49
1:M:38:ARG:HG2	1:M:405:LYS:HD2	1.94	0.49
1:I:217:PRO:HD2	1:I:393:VAL:HG22	1.94	0.49
1:U:229:SER:OG	1:U:438:ALA:HB2	2.13	0.49
1:C:244:LEU:HD12	1:C:253:LEU:HD12	1.94	0.49
1:E:229:SER:HB2	1:E:437:ALA:HB3	1.95	0.49
2:X:54:ILE:HA	2:X:168:ALA:O	2.12	0.49
2:J:143:ARG:NH2	1:K:349:GLU:OE2	2.46	0.49
2:P:111:ARG:HB2	2:R:175:ASP:OD2	2.13	0.49
2:V:54:ILE:HA	2:V:168:ALA:O	2.12	0.48
1:I:309:LEU:HD13	1:I:316:VAL:HG11	1.95	0.48
1:G:259:PRO:HB3	1:G:280:GLU:HG2	1.94	0.48
2:N:13:GLU:O	2:N:14:TRP:HB2	2.13	0.48
1:E:414:GLY:HA2	1:E:417:ARG:HD2	1.93	0.48
1:W:185:THR:HG22	1:W:459:PRO:HG2	1.95	0.48
2:X:56:TYR:HB3	2:X:84:GLU:HB2	1.95	0.48
2:F:56:TYR:HB3	2:F:84:GLU:HB2	1.96	0.48
1:S:143:PHE:HA	5:W:2020:HOH:O	2.13	0.48
1:W:217:PRO:HG2	1:W:393:VAL:HG22	1.95	0.48
1:Q:64:GLU:OE2	1:Q:167:THR:HG21	2.13	0.48
1:C:309:LEU:HD13	1:C:316:VAL:HG11	1.95	0.48
1:E:82:PRO:HB2	1:E:98:ASN:HB3	1.96	0.48
1:M:448:MET:HE2	1:M:457:LEU:HD22	1.95	0.47
1:M:413:MET:HG2	1:O:142:ALA:HB1	1.95	0.47
1:Q:399:LEU:O	1:Q:405:LYS:HE3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:422:HIS:CD2	1:O:424:ASP:H	2.28	0.47
1:E:60:LEU:CD2	1:E:339:ILE:HD11	2.44	0.47
1:A:359:ASP:HB2	1:A:362:ALA:HB2	1.96	0.47
1:A:131:GLY:O	1:A:160:PRO:HD2	2.13	0.47
2:L:35:ALA:HB1	2:L:112:HIS:HB2	1.96	0.47
1:S:184:GLU:HG2	5:S:2010:HOH:O	2.14	0.47
2:B:111:ARG:HB2	2:D:175:ASP:OD2	2.14	0.47
1:G:213:LYS:HA	1:G:352:VAL:O	2.15	0.47
1:A:217:PRO:HD2	1:A:393:VAL:HG22	1.97	0.47
2:N:32:TYR:CD1	2:P:116:ASN:HA	2.49	0.47
1:G:343:HIS:HB2	1:G:351:GLU:HB2	1.96	0.47
1:A:185:THR:HG22	1:A:459:PRO:HG2	1.96	0.47
2:T:179:LEU:HD21	2:T:184:LEU:HD11	1.96	0.47
1:O:219:ASN:OD1	1:O:221:LYS:NZ	2.48	0.47
2:J:25:ASN:HD21	2:L:24:GLN:HG2	1.80	0.47
1:C:356:THR:HG21	1:C:374:ASN:HB3	1.97	0.47
1:Q:219:ASN:OD1	1:Q:221:LYS:NZ	2.47	0.47
1:W:212:GLN:HG2	2:X:60:LEU:HD21	1.96	0.47
2:B:58:MET:CE	2:B:174:LEU:HD22	2.45	0.47
1:O:100:CYS:HB2	1:O:107:ILE:CD1	2.44	0.46
2:H:32:TYR:CD1	2:J:116:ASN:HA	2.49	0.46
1:Q:42:ASP:HB3	1:Q:45:LEU:HB2	1.96	0.46
1:K:229:SER:HB2	1:K:437:ALA:HB3	1.98	0.46
1:Q:100:CYS:CB	1:Q:107:ILE:HD11	2.45	0.46
1:I:126:ALA:HB3	1:I:135:ASN:HB3	1.98	0.46
2:B:12:PHE:H	2:F:36:GLN:HE21	1.62	0.46
1:O:244:LEU:HD13	1:O:253:LEU:HG	1.97	0.46
1:O:448:MET:HE2	1:O:457:LEU:HD22	1.96	0.46
2:T:32:TYR:CD1	2:V:116:ASN:HA	2.50	0.46
1:U:338:ASN:OD1	1:U:340:ARG:HD3	2.16	0.46
1:W:60:LEU:HD22	1:W:339:ILE:HD11	1.97	0.46
1:E:373:HIS:HD2	1:E:376:ARG:HH21	1.63	0.46
1:A:287:VAL:HG12	1:A:288:MET:CE	2.46	0.46
1:E:226:GLN:HA	1:E:230:ASP:HB3	1.96	0.46
1:G:425:PHE:HA	1:G:426:PRO:HD3	1.79	0.46
1:M:332:PHE:HB3	1:M:339:ILE:HD13	1.96	0.46
2:N:32:TYR:CG	2:P:116:ASN:HA	2.51	0.46
1:C:356:THR:HG23	2:D:79:LEU:HD11	1.98	0.46
2:N:175:ASP:OD2	2:R:111:ARG:HB2	2.16	0.46
2:V:36:GLN:NE2	2:X:12:PHE:H	2.14	0.45
1:Q:262:GLY:HA2	1:Q:278:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:51:ASP:OD2	2:P:157:ARG:NH1	2.50	0.45
1:A:358:VAL:HG11	1:A:367:LYS:HA	1.99	0.45
1:S:259:PRO:HB3	1:S:280:GLU:HG2	1.99	0.45
2:P:134:PHE:CD2	2:P:152:ARG:HD3	2.51	0.45
2:D:49:LEU:HD21	2:D:163:LEU:HD13	1.98	0.45
1:W:87:ARG:HD2	1:W:91:LYS:HE3	1.99	0.45
2:R:11:THR:C	2:R:13:GLU:H	2.20	0.45
1:E:107:ILE:HG22	1:E:118:PHE:HB3	1.98	0.45
1:Q:315:PRO:HB2	1:Q:318:ARG:HD3	1.97	0.45
2:V:56:TYR:HB3	2:V:84:GLU:HB2	1.99	0.45
1:G:241:SER:HB2	2:H:95:LYS:HG3	1.99	0.44
2:F:159:ALA:HB2	2:F:166:SER:HB2	1.99	0.44
1:S:252:ASP:H	1:S:255:GLN:HE21	1.64	0.44
2:D:29:GLN:O	2:D:33:ARG:HG3	2.16	0.44
1:G:358:VAL:HG11	1:G:367:LYS:HA	1.98	0.44
1:Q:275:GLY:O	1:Q:322:GLN:HA	2.17	0.44
1:S:454:TRP:HA	1:S:457:LEU:HB2	1.98	0.44
2:D:32:TYR:CD1	2:F:116:ASN:HA	2.51	0.44
1:E:389:GLY:O	1:E:393:VAL:HG23	2.18	0.44
2:P:9:PHE:O	2:P:11:THR:N	2.51	0.44
2:X:172:ILE:HD13	2:X:188:PHE:HB2	1.99	0.44
2:V:93:ILE:HA	2:V:96:VAL:HG12	2.00	0.44
2:D:179:LEU:HD21	2:D:184:LEU:HD11	2.00	0.44
1:U:142:ALA:O	1:U:143:PHE:HB2	2.17	0.44
1:I:413:MET:HG2	1:I:434:ALA:HA	1.99	0.44
1:K:359:ASP:HB2	1:K:362:ALA:HB2	1.99	0.44
2:T:84:GLU:CD	2:T:92:ARG:HE	2.21	0.44
1:C:217:PRO:HG2	1:C:393:VAL:HG22	2.00	0.44
1:O:265:PHE:CZ	1:O:267:ALA:HA	2.53	0.44
2:V:36:GLN:HE21	2:X:12:PHE:H	1.65	0.43
1:C:37:PRO:HG2	1:C:405:LYS:HA	1.99	0.43
1:O:413:MET:HE3	1:O:435:GLU:HG3	2.00	0.43
1:G:381:GLY:HA3	2:H:184:LEU:HB2	2.00	0.43
1:K:60:LEU:HD22	1:K:330:CYS:SG	2.58	0.43
2:L:134:PHE:CD2	2:L:152:ARG:HD3	2.52	0.43
1:K:448:MET:HG2	1:K:457:LEU:HD21	1.99	0.43
2:B:58:MET:HE1	2:B:174:LEU:HD22	1.99	0.43
2:T:24:GLN:HG2	2:X:25:ASN:HD21	1.82	0.43
1:A:375:ILE:O	1:A:379:SER:HB3	2.18	0.43
2:R:56:TYR:HB3	2:R:84:GLU:HB2	1.99	0.43
1:I:37:PRO:HG3	1:I:409:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:HIS:HD2	1:A:425:PHE:H	1.66	0.43
1:K:215:VAL:HG22	1:K:351:GLU:HG2	1.99	0.43
1:U:68:PRO:HD2	1:U:72:ASP:OD2	2.18	0.43
1:Q:340:ARG:HH21	1:Q:378:PHE:HB3	1.84	0.43
1:O:425:PHE:HA	1:O:426:PRO:HD3	1.90	0.43
2:H:56:TYR:HB3	2:H:84:GLU:HB2	2.00	0.43
1:I:107:ILE:HG22	1:I:118:PHE:HB3	2.00	0.43
1:K:259:PRO:HB2	1:K:277:TYR:CE2	2.54	0.43
1:K:372:ARG:HD2	5:K:2037:HOH:O	2.18	0.43
1:U:410:ASN:ND2	1:U:412:GLN:H	2.16	0.43
1:K:107:ILE:HG22	1:K:118:PHE:HB3	2.01	0.43
2:X:162:ASN:H	2:X:162:ASN:HD22	1.66	0.43
1:S:277:TYR:HB2	1:S:320:VAL:HG23	2.01	0.43
1:A:169:LYS:HE2	1:A:199:ASP:CG	2.39	0.43
1:G:359:ASP:HB2	1:G:362:ALA:HB2	2.00	0.43
2:H:143:ARG:NH2	1:I:349:GLU:OE2	2.51	0.43
1:G:349:GLU:OE2	2:L:143:ARG:NH2	2.51	0.43
1:Q:451:GLU:HA	1:Q:452:PRO:HD3	1.85	0.43
1:M:232:TYR:CE1	1:O:123:HIS:HB3	2.54	0.43
2:V:111:ARG:HB2	2:X:175:ASP:OD2	2.18	0.43
2:J:179:LEU:HD21	2:J:184:LEU:HD11	2.01	0.43
1:C:340:ARG:NH2	1:C:378:PHE:HB3	2.34	0.43
2:T:54:ILE:HA	2:T:168:ALA:O	2.19	0.43
1:K:394:GLU:HG2	5:K:2043:HOH:O	2.17	0.42
2:J:155:VAL:HB	2:J:169:LYS:HB2	2.01	0.42
2:L:56:TYR:HB3	2:L:84:GLU:HB2	2.00	0.42
2:N:106:PRO:HA	2:N:107:PRO:HD3	1.90	0.42
1:S:422:HIS:HD2	1:S:424:ASP:H	1.66	0.42
1:G:244:LEU:HG	2:H:94:ARG:HG2	2.01	0.42
2:X:29:GLN:O	2:X:33:ARG:HG3	2.20	0.42
1:U:241:SER:HB2	2:V:95:LYS:HG3	1.99	0.42
1:W:241:SER:HB2	2:X:95:LYS:HG3	2.01	0.42
1:W:57:SER:HB3	1:W:328:PRO:HD3	1.99	0.42
1:Q:422:HIS:CD2	1:Q:424:ASP:H	2.32	0.42
1:A:425:PHE:HA	1:A:426:PRO:HD3	1.77	0.42
1:C:105:MET:HB3	1:C:120:CYS:SG	2.60	0.42
1:S:451:GLU:HA	1:S:452:PRO:HD3	1.84	0.42
1:M:197:MET:HB2	1:M:334:PRO:HB3	2.00	0.42
1:G:192:PRO:HB3	1:G:312:THR:HG21	2.00	0.42
1:U:269:TRP:CZ2	1:U:444:HIS:HE1	2.38	0.42
1:A:212:GLN:HE21	1:A:212:GLN:HB2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:332:PHE:CE2	1:U:339:ILE:HD13	2.54	0.42
2:R:106:PRO:HA	2:R:107:PRO:HD3	1.89	0.42
1:E:422:HIS:HD2	1:E:424:ASP:H	1.68	0.42
1:E:212:GLN:HE21	1:E:212:GLN:HB2	1.67	0.42
1:K:19:TRP:HB3	1:K:24:ILE:HD11	2.01	0.42
2:V:25:ASN:HD21	2:X:24:GLN:HG2	1.84	0.42
1:C:212:GLN:HG2	2:D:60:LEU:HD21	2.01	0.42
1:W:215:VAL:O	2:X:182:ASN:HA	2.19	0.42
2:F:9:PHE:HA	5:F:2001:HOH:O	2.19	0.42
1:W:64:GLU:OE2	1:W:167:THR:HG21	2.20	0.42
2:D:35:ALA:HB1	2:D:112:HIS:HB2	2.01	0.42
2:P:139:ASN:OD1	2:R:176:ALA:HA	2.19	0.42
2:R:31:TYR:HB3	2:R:114:VAL:HG11	2.01	0.42
1:O:191:ARG:N	1:O:192:PRO:HD2	2.34	0.42
1:C:356:THR:HG21	1:C:374:ASN:CB	2.50	0.42
1:A:343:HIS:HB2	1:A:351:GLU:HB2	2.01	0.42
2:L:49:LEU:HD21	2:L:163:LEU:HD13	2.00	0.42
1:A:197:MET:HB2	1:A:334:PRO:HB3	2.01	0.42
1:W:276:TRP:HB3	1:W:322:GLN:HG3	2.01	0.42
1:K:277:TYR:O	1:K:319:MET:HA	2.19	0.42
1:A:195:ASP:HB3	1:A:309:LEU:HD21	2.02	0.42
2:X:60:LEU:H	2:X:74:SER:HB3	1.85	0.42
2:T:116:ASN:HA	2:X:32:TYR:CG	2.55	0.42
2:H:36:GLN:NE2	2:J:12:PHE:H	2.18	0.42
2:H:113:LEU:HD22	2:J:135:ILE:HG13	2.02	0.42
1:U:126:ALA:HB3	1:U:135:ASN:HB3	2.02	0.42
1:A:356:THR:HG21	2:B:79:LEU:HD21	2.02	0.42
1:U:422:HIS:HD2	1:U:424:ASP:H	1.68	0.42
1:G:265:PHE:CZ	1:G:267:ALA:HA	2.55	0.41
1:O:226:GLN:HA	1:O:230:ASP:HB3	2.02	0.41
1:W:258:ILE:HA	1:W:259:PRO:HD3	1.90	0.41
2:B:49:LEU:HD11	2:B:163:LEU:HD22	2.02	0.41
1:G:262:GLY:HA2	1:G:278:VAL:HG23	2.02	0.41
1:U:343:HIS:HA	1:U:344:PRO:HD2	1.92	0.41
1:E:315:PRO:HB2	1:E:318:ARG:HD3	2.02	0.41
1:W:36:ASP:HA	1:W:37:PRO:HD3	1.93	0.41
1:W:139:GLU:OE1	1:W:155:LYS:HE3	2.21	0.41
2:J:36:GLN:HE21	2:L:12:PHE:H	1.68	0.41
1:O:454:TRP:HA	1:O:457:LEU:HB2	2.03	0.41
1:A:287:VAL:HG12	1:A:288:MET:HE3	2.02	0.41
1:M:107:ILE:HD12	1:M:127:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:TYR:HB3	2:B:84:GLU:HB2	2.03	0.41
1:W:36:ASP:O	1:W:39:ILE:HG12	2.20	0.41
2:F:58:MET:CE	2:F:174:LEU:HD22	2.51	0.41
1:I:82:PRO:HB2	1:I:98:ASN:HB3	2.02	0.41
2:F:126:ASP:HB3	2:F:158:ARG:HB2	2.02	0.41
1:E:60:LEU:HD22	1:E:339:ILE:HD11	2.01	0.41
2:D:111:ARG:HB2	2:F:175:ASP:OD2	2.20	0.41
1:Q:76:THR:OG1	1:Q:77:TYR:N	2.52	0.41
2:V:49:LEU:HD21	2:V:163:LEU:HD13	2.01	0.41
1:M:217:PRO:HG2	1:M:393:VAL:HG22	2.03	0.41
1:U:36:ASP:O	1:U:39:ILE:HG12	2.21	0.41
1:S:259:PRO:HB2	1:S:277:TYR:CE2	2.56	0.41
1:Q:105:MET:HB3	1:Q:120:CYS:SG	2.60	0.41
1:W:196:VAL:O	1:W:200:ARG:HD3	2.21	0.41
1:W:302:ALA:HB1	1:W:317:ARG:HG2	2.01	0.41
2:X:179:LEU:HD21	2:X:184:LEU:HD11	2.03	0.41
2:F:29:GLN:O	2:F:33:ARG:HG3	2.20	0.41
2:H:29:GLN:O	2:H:33:ARG:HD3	2.20	0.41
1:M:448:MET:CE	1:M:457:LEU:HD22	2.49	0.41
1:K:197:MET:HB2	1:K:334:PRO:HB3	2.03	0.41
1:G:311:HIS:HB2	5:G:2017:HOH:O	2.20	0.41
1:C:220:TRP:HA	1:C:350:ILE:HG21	2.02	0.41
1:M:261:LYS:HD3	1:M:261:LYS:HA	1.90	0.41
2:T:32:TYR:CG	2:V:116:ASN:HA	2.56	0.41
2:V:32:TYR:CD1	2:X:116:ASN:HA	2.56	0.41
2:D:36:GLN:HB3	2:F:11:THR:HG23	2.03	0.40
1:Q:37:PRO:HG2	1:Q:405:LYS:HA	2.03	0.40
1:A:422:HIS:HA	1:A:423:PRO:HD3	1.95	0.40
2:B:19:ALA:HB1	2:B:23:LEU:HD23	2.03	0.40
1:Q:413:MET:HB2	1:Q:413:MET:HE2	1.78	0.40
2:H:116:ASN:HA	2:L:32:TYR:CD1	2.56	0.40
1:A:414:GLY:HA2	1:A:417:ARG:HD2	2.03	0.40
1:A:356:THR:CG2	2:B:79:LEU:HD21	2.52	0.40
1:A:19:TRP:HB3	1:A:24:ILE:HD11	2.03	0.40
1:M:248:PRO:HA	1:M:249:PRO:HD3	1.87	0.40
1:E:448:MET:HE2	1:E:457:LEU:HD22	2.03	0.40
1:S:258:ILE:HA	1:S:259:PRO:HD3	1.96	0.40
1:G:215:VAL:HG21	2:L:143:ARG:NH1	2.37	0.40
2:H:135:ILE:HD12	2:L:113:LEU:HD22	2.04	0.40
1:A:356:THR:HG22	2:B:79:LEU:HD11	2.02	0.40
1:A:215:VAL:HG21	2:F:143:ARG:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:226:GLN:HA	1:W:230:ASP:HB3	2.03	0.40
2:J:148:PHE:HB3	2:J:174:LEU:HD11	2.04	0.40
1:M:247:ILE:HD12	1:M:251:MET:HG3	2.04	0.40
1:E:36:ASP:O	1:E:39:ILE:HG12	2.22	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%)	415 (97%)	14 (3%)	0	100	100
1	C	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	52	75
1	E	429/459 (94%)	410 (96%)	18 (4%)	1 (0%)	52	75
1	G	429/459 (94%)	418 (97%)	11 (3%)	0	100	100
1	I	429/459 (94%)	410 (96%)	18 (4%)	1 (0%)	52	75
1	K	429/459 (94%)	414 (96%)	15 (4%)	0	100	100
1	M	429/459 (94%)	418 (97%)	11 (3%)	0	100	100
1	O	429/459 (94%)	412 (96%)	17 (4%)	0	100	100
1	Q	429/459 (94%)	420 (98%)	8 (2%)	1 (0%)	52	75
1	S	429/459 (94%)	415 (97%)	12 (3%)	2 (0%)	34	55
1	U	429/459 (94%)	411 (96%)	17 (4%)	1 (0%)	52	75
1	W	429/459 (94%)	408 (95%)	21 (5%)	0	100	100
2	B	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
2	D	178/188 (95%)	172 (97%)	6 (3%)	0	100	100
2	F	178/188 (95%)	172 (97%)	6 (3%)	0	100	100
2	H	178/188 (95%)	170 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
2	L	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
2	N	178/188 (95%)	173 (97%)	4 (2%)	1 (1%)	30	50
2	P	178/188 (95%)	167 (94%)	8 (4%)	3 (2%)	11	19
2	R	178/188 (95%)	167 (94%)	9 (5%)	2 (1%)	17	31
2	T	178/188 (95%)	172 (97%)	5 (3%)	1 (1%)	30	50
2	V	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
2	X	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
All	All	7284/7764 (94%)	7013 (96%)	257 (4%)	14 (0%)	52	75

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	256	ALA
2	P	12	PHE
2	P	10	LYS
2	R	12	PHE
2	R	15	PRO
2	T	10	LYS
2	N	14	TRP
2	P	14	TRP
1	S	68	PRO
1	U	68	PRO
1	C	328	PRO
1	I	328	PRO
1	S	328	PRO
1	Q	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	352/373 (94%)	343 (97%)	9 (3%)	54	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	352/373 (94%)	345 (98%)	7 (2%)	63	86
1	E	352/373 (94%)	343 (97%)	9 (3%)	54	81
1	G	352/373 (94%)	341 (97%)	11 (3%)	47	75
1	I	352/373 (94%)	344 (98%)	8 (2%)	58	83
1	K	352/373 (94%)	345 (98%)	7 (2%)	63	86
1	M	351/373 (94%)	344 (98%)	7 (2%)	63	86
1	O	351/373 (94%)	345 (98%)	6 (2%)	68	89
1	Q	351/373 (94%)	344 (98%)	7 (2%)	63	86
1	S	352/373 (94%)	344 (98%)	8 (2%)	58	83
1	U	352/373 (94%)	341 (97%)	11 (3%)	47	75
1	W	352/373 (94%)	342 (97%)	10 (3%)	51	78
2	B	159/167 (95%)	156 (98%)	3 (2%)	65	87
2	D	159/167 (95%)	154 (97%)	5 (3%)	47	75
2	F	159/167 (95%)	157 (99%)	2 (1%)	76	92
2	H	159/167 (95%)	153 (96%)	6 (4%)	40	67
2	J	159/167 (95%)	156 (98%)	3 (2%)	65	87
2	L	159/167 (95%)	154 (97%)	5 (3%)	47	75
2	N	159/167 (95%)	153 (96%)	6 (4%)	40	67
2	P	159/167 (95%)	152 (96%)	7 (4%)	35	60
2	R	159/167 (95%)	157 (99%)	2 (1%)	76	92
2	T	159/167 (95%)	156 (98%)	3 (2%)	65	87
2	V	159/167 (95%)	150 (94%)	9 (6%)	25	46
2	X	159/167 (95%)	154 (97%)	5 (3%)	47	75
All	All	6129/6480 (95%)	5973 (98%)	156 (2%)	55	82

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLU
1	A	85	MET
1	A	103	ARG
1	A	122	TYR
1	A	201	THR
1	A	335	THR

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Mol	Chain	Res	Type
1	A	356	THR
1	A	358	VAL
1	A	394	GLU
2	B	94	ARG
2	B	115	SER
2	B	152	ARG
1	C	47	GLU
1	C	86	VAL
1	C	103	ARG
1	C	122	TYR
1	C	253	LEU
1	C	339	ILE
1	C	448	MET
2	D	10	LYS
2	D	54	ILE
2	D	67	ARG
2	D	135	ILE
2	D	180	LEU
1	E	89	LYS
1	E	103	ARG
1	E	122	TYR
1	E	201	THR
1	E	226	GLN
1	E	253	LEU
1	E	339	ILE
1	E	356	THR
1	E	358	VAL
2	F	135	ILE
2	F	180	LEU
1	G	48	LEU
1	G	103	ARG
1	G	110	SER
1	G	116	LYS
1	G	122	TYR
1	G	255	GLN
1	G	261	LYS
1	G	309	LEU
1	G	340	ARG
1	G	369	GLU
1	G	435	GLU
2	H	33	ARG
2	H	76	ASP

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Mol	Chain	Res	Type
2	H	94	ARG
2	H	143	ARG
2	H	152	ARG
2	H	169	LYS
1	I	31	GLU
1	I	42	ASP
1	I	91	LYS
1	I	94	LYS
1	I	122	TYR
1	I	140	LYS
1	I	250	GLU
1	I	311	HIS
2	J	70	GLU
2	J	140	ARG
2	J	143	ARG
1	K	103	ARG
1	K	116	LYS
1	K	122	TYR
1	K	255	GLN
1	K	340	ARG
1	K	358	VAL
1	K	457	LEU
2	L	17	LYS
2	L	94	ARG
2	L	143	ARG
2	L	152	ARG
2	L	179	LEU
1	M	31	GLU
1	M	69	GLU
1	M	103	ARG
1	M	122	TYR
1	M	155	LYS
1	M	201	THR
1	M	261	LYS
2	N	51	ASP
2	N	94	ARG
2	N	140	ARG
2	N	143	ARG
2	N	174	LEU
2	N	179	LEU
1	O	69	GLU
1	O	86	VAL

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Mol	Chain	Res	Type
1	O	103	ARG
1	O	122	TYR
1	O	258	ILE
1	O	280	GLU
2	P	14	TRP
2	P	17	LYS
2	P	95	LYS
2	P	98	SER
2	P	143	ARG
2	P	152	ARG
2	P	179	LEU
1	Q	18	ASN
1	Q	69	GLU
1	Q	91	LYS
1	Q	103	ARG
1	Q	122	TYR
1	Q	178	VAL
1	Q	309	LEU
2	R	162	ASN
2	R	179	LEU
1	S	89	LYS
1	S	103	ARG
1	S	122	TYR
1	S	201	THR
1	S	291	LYS
1	S	339	ILE
1	S	365	GLU
1	S	458	LYS
2	T	10	LYS
2	T	143	ARG
2	T	152	ARG
1	U	48	LEU
1	U	89	LYS
1	U	103	ARG
1	U	122	TYR
1	U	132	LYS
1	U	140	LYS
1	U	257	GLN
1	U	291	LYS
1	U	309	LEU
1	U	335	THR
1	U	339	ILE

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Mol	Chain	Res	Type
2	V	9	PHE
2	V	17	LYS
2	V	52	LYS
2	V	64	ARG
2	V	94	ARG
2	V	121	GLU
2	V	143	ARG
2	V	160	ASP
2	V	179	LEU
1	W	48	LEU
1	W	91	LYS
1	W	103	ARG
1	W	122	TYR
1	W	179	GLN
1	W	280	GLU
1	W	309	LEU
1	W	312	THR
1	W	339	ILE
1	W	446	MET
2	X	13	GLU
2	X	17	LYS
2	X	67	ARG
2	X	74	SER
2	X	94	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	263	ASN
1	A	343	HIS
1	A	410	ASN
1	A	422	HIS
1	A	444	HIS
2	B	25	ASN
2	B	36	GLN
2	B	131	ASN
1	C	212	GLN
1	C	373	HIS
1	C	391	ASN
1	C	410	ASN
1	C	419	GLN

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Mol	Chain	Res	Type
1	C	422	HIS
1	C	444	HIS
2	D	25	ASN
2	D	36	GLN
1	E	212	GLN
1	E	391	ASN
1	E	410	ASN
1	E	422	HIS
1	E	444	HIS
2	F	36	GLN
2	F	77	GLN
2	F	131	ASN
1	G	343	HIS
1	G	391	ASN
1	G	410	ASN
1	G	422	HIS
1	G	444	HIS
2	H	25	ASN
2	H	36	GLN
1	I	410	ASN
1	I	422	HIS
1	I	444	HIS
2	J	25	ASN
2	J	36	GLN
2	J	131	ASN
1	K	255	GLN
1	K	391	ASN
1	K	410	ASN
1	K	419	GLN
1	K	422	HIS
1	K	444	HIS
2	L	25	ASN
2	L	36	GLN
2	L	131	ASN
1	M	212	GLN
1	M	255	GLN
1	M	263	ASN
1	M	311	HIS
1	M	391	ASN
1	M	410	ASN
1	M	422	HIS
2	N	25	ASN

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Mol	Chain	Res	Type
2	N	77	GLN
2	N	162	ASN
1	O	18	ASN
1	O	212	GLN
1	O	311	HIS
1	O	391	ASN
1	O	410	ASN
1	O	422	HIS
1	O	444	HIS
2	P	25	ASN
2	P	162	ASN
1	Q	255	GLN
1	Q	311	HIS
1	Q	373	HIS
1	Q	410	ASN
1	Q	422	HIS
2	R	25	ASN
2	R	36	GLN
2	R	162	ASN
1	S	255	GLN
1	S	263	ASN
1	S	391	ASN
1	S	410	ASN
1	S	422	HIS
2	T	25	ASN
2	T	36	GLN
2	T	131	ASN
1	U	88	GLN
1	U	343	HIS
1	U	391	ASN
1	U	410	ASN
1	U	422	HIS
1	U	444	HIS
2	V	25	ASN
2	V	36	GLN
2	V	162	ASN
1	W	391	ASN
1	W	410	ASN
1	W	422	HIS
1	W	444	HIS
2	X	25	ASN
2	X	36	GLN

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Mol	Chain	Res	Type
2	X	131	ASN
2	X	162	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	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	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	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	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	-	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	-	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	-	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	-	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.

12 monomers are involved in 12 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	I	900	FES	1	0
3	K	900	FES	1	0
3	M	900	FES	1	0
3	O	900	FES	1	0
3	Q	900	FES	1	0
3	S	900	FES	1	0
3	U	900	FES	1	0
3	W	900	FES	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	433/459 (94%)	0.02	7 (1%) 74 78	14, 26, 32, 44	18 (4%)
1	C	433/459 (94%)	0.17	19 (4%) 38 43	18, 27, 37, 43	18 (4%)
1	E	433/459 (94%)	0.06	17 (3%) 43 48	22, 26, 34, 39	18 (4%)
1	G	433/459 (94%)	0.21	31 (7%) 18 20	20, 29, 39, 43	18 (4%)
1	I	433/459 (94%)	0.38	43 (9%) 9 10	22, 31, 39, 44	18 (4%)
1	K	433/459 (94%)	0.10	16 (3%) 45 50	17, 26, 34, 41	18 (4%)
1	M	433/459 (94%)	0.08	19 (4%) 38 43	19, 25, 35, 45	18 (4%)
1	O	433/459 (94%)	0.02	15 (3%) 48 53	18, 25, 34, 44	18 (4%)
1	Q	433/459 (94%)	0.05	14 (3%) 51 56	19, 26, 35, 44	18 (4%)
1	S	433/459 (94%)	0.27	16 (3%) 45 50	26, 37, 49, 53	18 (4%)
1	U	433/459 (94%)	0.34	25 (5%) 26 30	26, 36, 47, 51	18 (4%)
1	W	433/459 (94%)	0.45	27 (6%) 24 27	29, 39, 50, 54	18 (4%)
2	B	180/188 (95%)	-0.04	5 (2%) 56 61	21, 25, 33, 43	4 (2%)
2	D	180/188 (95%)	-0.02	5 (2%) 56 61	18, 25, 32, 39	4 (2%)
2	F	180/188 (95%)	-0.07	6 (3%) 50 55	21, 25, 35, 40	4 (2%)
2	H	180/188 (95%)	-0.04	5 (2%) 56 61	20, 27, 33, 39	4 (2%)
2	J	180/188 (95%)	-0.07	9 (5%) 32 37	20, 26, 36, 46	4 (2%)
2	L	180/188 (95%)	-0.05	6 (3%) 50 55	20, 26, 33, 38	4 (2%)
2	N	180/188 (95%)	-0.14	3 (1%) 73 76	17, 24, 35, 44	4 (2%)
2	P	180/188 (95%)	-0.05	4 (2%) 65 69	19, 25, 36, 44	4 (2%)
2	R	180/188 (95%)	-0.06	7 (3%) 43 48	19, 24, 45, 65	4 (2%)
2	T	180/188 (95%)	0.05	9 (5%) 32 37	24, 30, 43, 49	4 (2%)
2	V	180/188 (95%)	0.01	4 (2%) 65 69	24, 28, 35, 39	4 (2%)
2	X	180/188 (95%)	-0.02	5 (2%) 56 61	24, 31, 38, 40	4 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	7356/7764 (94%)	0.11	317 (4%)	39	44	14, 28, 42, 65	264 (3%)

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	15	PRO	6.0
1	A	18	ASN	5.3
1	M	254	SER	5.3
1	W	18	ASN	5.2
1	Q	258	ILE	5.1
2	R	12	PHE	5.1
1	C	18	ASN	4.9
2	X	160	ASP	4.8
1	G	18	ASN	4.8
1	S	257	GLN	4.8
2	F	16	SER	4.7
1	W	421	GLY	4.7
1	U	421	GLY	4.6
1	M	257	GLN	4.6
1	M	261	LYS	4.5
1	I	156	ALA	4.5
1	C	421	GLY	4.4
1	K	18	ASN	4.4
1	Q	18	ASN	4.4
1	G	203	ALA	4.4
1	G	416	GLY	4.4
2	R	14	TRP	4.3
1	M	250	GLU	4.3
2	T	123	ALA	4.3
1	G	423	PRO	4.3
1	C	20	THR	4.3
1	O	18	ASN	4.2
2	J	16	SER	4.2
1	O	257	GLN	4.1
1	O	258	ILE	4.1
1	G	202	PRO	4.1
1	C	258	ILE	4.1
1	W	257	GLN	4.1
1	W	258	ILE	4.0
1	A	421	GLY	4.0
2	B	123	ALA	4.0
2	H	160	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
2	V	16	SER	3.9
2	R	9	PHE	3.9
1	G	364	ALA	3.8
1	S	311	HIS	3.8
2	L	123	ALA	3.8
1	C	257	GLN	3.8
1	O	255	GLN	3.8
1	W	260	THR	3.8
1	K	140	LYS	3.8
1	W	20	THR	3.6
1	S	18	ASN	3.6
1	E	140	LYS	3.6
2	V	160	ASP	3.6
2	L	16	SER	3.6
1	I	417	ARG	3.6
1	M	255	GLN	3.6
1	O	260	THR	3.5
1	W	179	GLN	3.5
1	U	140	LYS	3.5
1	G	311	HIS	3.5
1	U	91	LYS	3.5
2	F	160	ASP	3.4
1	I	423	PRO	3.4
1	G	419	GLN	3.4
1	M	253	LEU	3.4
1	G	420	THR	3.4
2	N	11	THR	3.4
2	P	11	THR	3.4
1	W	261	LYS	3.4
2	X	16	SER	3.4
1	W	202	PRO	3.3
2	P	58	MET	3.3
1	E	257	GLN	3.3
2	D	160	ASP	3.3
2	F	67	ARG	3.3
2	B	16	SER	3.3
2	T	16	SER	3.3
2	D	16	SER	3.2
1	M	18	ASN	3.2
1	U	261	LYS	3.2
2	T	17	LYS	3.2
1	K	455	ALA	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	Q	255	GLN	3.2
1	O	261	LYS	3.2
1	U	419	GLN	3.2
1	M	251	MET	3.2
1	C	254	SER	3.2
1	K	313	GLY	3.2
1	W	105	MET	3.2
1	U	18	ASN	3.2
2	D	17	LYS	3.1
2	N	160	ASP	3.1
1	E	18	ASN	3.1
1	I	257	GLN	3.1
1	U	364	ALA	3.1
1	K	105	MET	3.1
1	W	256	ALA	3.1
2	J	71	LEU	3.1
1	M	421	GLY	3.1
1	G	20	THR	3.1
1	I	154	ASP	3.1
1	S	156	ALA	3.1
1	U	310	GLY	3.1
1	E	105	MET	3.0
1	Q	254	SER	3.0
1	K	154	ASP	3.0
1	K	258	ILE	3.0
1	G	260	THR	3.0
2	H	16	SER	3.0
1	K	138	PHE	3.0
1	C	178	VAL	3.0
1	O	251	MET	3.0
1	A	310	GLY	3.0
1	C	253	LEU	3.0
1	U	415	LEU	3.0
1	S	22	GLU	3.0
1	I	254	SER	2.9
1	C	19	TRP	2.9
1	S	310	GLY	2.9
2	R	160	ASP	2.9
1	K	421	GLY	2.9
2	J	67	ARG	2.9
1	G	252	ASP	2.9
1	W	438	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	U	90	ASP	2.9
1	I	178	VAL	2.8
2	L	58	MET	2.8
1	O	22	GLU	2.8
1	Q	261	LYS	2.8
1	U	178	VAL	2.8
1	E	258	ILE	2.8
1	I	294	GLN	2.8
1	E	253	LEU	2.8
1	E	252	ASP	2.8
2	T	58	MET	2.8
1	E	420	THR	2.8
1	U	416	GLY	2.8
1	I	256	ALA	2.8
1	A	260	THR	2.8
1	C	419	GLN	2.8
2	B	17	LYS	2.7
1	C	420	THR	2.7
1	W	21	PRO	2.7
1	K	132	LYS	2.7
1	I	416	GLY	2.7
1	I	90	ASP	2.7
1	U	423	PRO	2.7
1	G	257	GLN	2.7
2	P	14	TRP	2.7
2	D	9	PHE	2.7
1	M	258	ILE	2.7
1	M	249	PRO	2.7
1	W	203	ALA	2.7
1	W	452	PRO	2.6
2	J	58	MET	2.6
2	B	10	LYS	2.6
1	W	419	GLN	2.6
1	I	20	THR	2.6
2	F	77	GLN	2.6
1	I	255	GLN	2.6
1	I	18	ASN	2.6
1	Q	23	ALA	2.6
1	U	19	TRP	2.6
1	S	20	THR	2.6
2	T	122	THR	2.6
1	W	156	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	67	ARG	2.6
1	U	281	PRO	2.6
1	C	252	ASP	2.5
1	M	259	PRO	2.5
1	S	179	GLN	2.5
1	U	105	MET	2.5
1	G	261	LYS	2.5
1	I	261	LYS	2.5
1	M	252	ASP	2.5
1	U	182	ASP	2.5
1	E	419	GLN	2.5
1	G	89	LYS	2.5
1	I	190	ALA	2.5
1	E	416	GLY	2.5
1	A	257	GLN	2.5
1	I	419	GLN	2.5
1	I	459	PRO	2.5
2	F	10	LYS	2.5
2	V	17	LYS	2.5
1	I	420	THR	2.5
2	J	70	GLU	2.5
1	S	423	PRO	2.5
1	I	290	PRO	2.5
1	G	255	GLN	2.5
1	G	421	GLY	2.5
2	H	123	ALA	2.5
1	O	250	GLU	2.5
1	G	19	TRP	2.5
2	H	17	LYS	2.5
2	T	71	LEU	2.5
2	X	17	LYS	2.4
1	I	300	PRO	2.4
1	O	252	ASP	2.4
1	Q	22	GLU	2.4
2	V	162	ASN	2.4
1	K	311	HIS	2.4
2	J	10	LYS	2.4
1	I	456	THR	2.4
1	U	259	PRO	2.4
1	K	20	THR	2.4
2	X	67	ARG	2.4
2	J	52	LYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	L	76	ASP	2.4
1	U	260	THR	2.4
1	W	364	ALA	2.4
1	U	420	THR	2.3
1	W	335	THR	2.3
1	I	202	PRO	2.3
1	Q	260	THR	2.3
2	D	162	ASN	2.3
1	G	310	GLY	2.3
1	C	294	GLN	2.3
1	I	279	ASP	2.3
1	Q	252	ASP	2.3
1	I	19	TRP	2.3
1	Q	140	LYS	2.3
1	W	442	TYR	2.3
1	G	365	GLU	2.3
1	I	70	THR	2.3
1	W	83	VAL	2.3
1	W	420	THR	2.3
1	S	307	GLN	2.3
1	C	105	MET	2.3
1	I	364	ALA	2.3
2	F	58	MET	2.3
1	Q	257	GLN	2.3
2	J	160	ASP	2.3
1	E	247	ILE	2.3
1	I	422	HIS	2.3
1	I	421	GLY	2.3
1	S	70	THR	2.3
2	H	76	ASP	2.3
2	T	160	ASP	2.3
1	C	311	HIS	2.2
1	U	361	ASP	2.2
1	M	260	THR	2.2
1	O	249	PRO	2.2
1	G	254	SER	2.2
2	R	67	ARG	2.2
1	E	261	LYS	2.2
1	G	140	LYS	2.2
1	G	115	ALA	2.2
1	O	254	SER	2.2
2	T	9	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	253	LEU	2.2
1	K	139	GLU	2.2
1	K	142	ALA	2.2
1	W	252	ASP	2.2
1	Q	299	GLY	2.2
2	N	14	TRP	2.2
1	A	456	THR	2.2
1	I	185	THR	2.2
1	O	259	PRO	2.2
1	C	251	MET	2.2
2	R	11	THR	2.2
1	M	248	PRO	2.2
1	S	154	ASP	2.2
1	I	203	ALA	2.2
2	X	58	MET	2.2
1	I	307	GLN	2.2
1	E	20	THR	2.2
1	M	20	THR	2.2
1	S	312	THR	2.2
1	U	70	THR	2.2
1	I	113	GLY	2.1
1	Q	250	GLU	2.1
1	U	328	PRO	2.1
1	I	311	HIS	2.1
1	K	91	LYS	2.1
1	O	256	ALA	2.1
1	S	455	ALA	2.1
1	W	251	MET	2.1
1	C	327	PHE	2.1
1	U	20	THR	2.1
1	G	179	GLN	2.1
1	K	179	GLN	2.1
1	O	179	GLN	2.1
1	S	256	ALA	2.1
1	E	307	GLN	2.1
1	G	91	LYS	2.1
2	P	17	LYS	2.1
1	I	109	ARG	2.1
1	W	165	VAL	2.1
1	I	182	ASP	2.1
1	I	186	TYR	2.1
1	I	431	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	311	HIS	2.1
1	E	202	PRO	2.1
1	G	427	GLY	2.1
1	M	420	THR	2.1
1	G	453	SER	2.1
1	E	116	LYS	2.1
1	M	140	LYS	2.1
1	G	31	GLU	2.1
1	W	453	SER	2.1
2	B	76	ASP	2.1
1	W	441	MET	2.1
1	U	109	ARG	2.1
1	I	258	ILE	2.1
1	G	22	GLU	2.1
1	I	365	GLU	2.1
1	I	21	PRO	2.1
2	J	15	PRO	2.1
2	T	15	PRO	2.1
1	I	424	ASP	2.1
1	C	307	GLN	2.0
1	G	415	LEU	2.0
1	M	105	MET	2.0
1	C	313	GLY	2.0
1	E	452	PRO	2.0
1	I	426	PRO	2.0
1	Q	179	GLN	2.0
2	L	17	LYS	2.0
1	S	105	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron



density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FES	I	900	4/4	0.91	0.12	-0.61	47,48,49,51	0
3	FES	E	900	4/4	0.93	0.11	-0.68	39,40,42,44	0
3	FES	K	900	4/4	0.97	0.11	-0.82	46,47,48,49	0
4	FE2	U	901	1/1	0.99	0.11	-0.99	33,33,33,33	0
3	FES	S	900	4/4	0.92	0.12	-1.00	48,49,49,51	0
3	FES	Q	900	4/4	0.96	0.10	-1.03	36,38,38,41	0
3	FES	M	900	4/4	0.97	0.10	-1.08	36,38,39,43	0
4	FE2	K	901	1/1	0.98	0.10	-1.21	31,31,31,31	0
3	FES	A	900	4/4	0.92	0.10	-1.23	37,39,39,43	0
3	FES	U	900	4/4	0.94	0.11	-1.23	37,38,39,41	0
3	FES	O	900	4/4	0.92	0.12	-1.28	29,30,32,35	0
3	FES	W	900	4/4	0.97	0.09	-1.49	34,35,36,38	0
3	FES	G	900	4/4	0.96	0.08	-1.50	35,36,37,40	0
3	FES	C	900	4/4	0.97	0.09	-1.94	29,29,30,34	0
4	FE2	E	901	1/1	0.98	0.13	-	33,33,33,33	0
4	FE2	M	901	1/1	0.98	0.12	-	29,29,29,29	0
4	FE2	C	901	1/1	0.99	0.07	-	33,33,33,33	0
4	FE2	W	901	1/1	0.98	0.10	-	38,38,38,38	0
4	FE2	S	901	1/1	0.97	0.12	-	42,42,42,42	0
4	FE2	I	901	1/1	0.99	0.10	-	39,39,39,39	0
4	FE2	Q	901	1/1	0.95	0.15	-	30,30,30,30	0
4	FE2	A	901	1/1	0.98	0.11	-	31,31,31,31	0
4	FE2	O	901	1/1	0.99	0.13	-	29,29,29,29	0
4	FE2	G	901	1/1	0.99	0.12	-	39,39,39,39	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.