



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 08:06 pm BST

PDB ID : 2XRX  
Title : CRYSTAL STRUCTURE OF BIPHENYL DIOXYGENASE IN COMPLEX  
WITH BIPHENYL FROM BURKHOLDERIA XENOVORANS LB400  
Authors : Kumar, P.; Bolin, J.T.  
Deposited on : 2010-09-23  
Resolution : 2.42 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

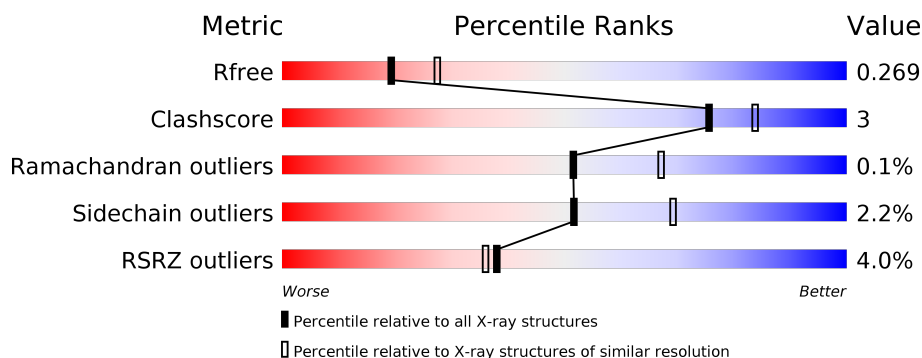
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	459	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>
1	C	459	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>
1	E	459	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	G	459	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
1	I	459	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	K	459	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	459	 90% 6%
1	O	459	 86% 8% 6%
1	Q	459	 86% 8% 6%
1	S	459	 85% 9% 6%
1	U	459	 86% 8% 6%
1	W	459	 84% 10% 6%
2	B	188	 89% 6% . .
2	D	188	 86% 10% . .
2	F	188	 86% 10% . .
2	H	188	 83% 12% . . .
2	J	188	 84% 12% . .
2	L	188	 82% 13% . .
2	N	188	 81% 14% . .
2	P	188	 85% 11% . .
2	R	188	 84% 12% . .
2	T	188	 88% 8% .
2	V	188	 86% 10% . .
2	X	188	 86% 10% . .

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 59977 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	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	C	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	E	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	G	432	Total	C	N	O	S	0	0	0
			3416	2172	600	621	23			
1	I	432	Total	C	N	O	S	0	0	0
			3416	2172	600	621	23			
1	K	432	Total	C	N	O	S	0	0	0
			3416	2172	600	621	23			
1	M	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	O	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	Q	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	S	432	Total	C	N	O	S	0	0	0
			3417	2172	600	622	23			
1	U	432	Total	C	N	O	S	0	0	0
			3417	2172	600	622	23			
1	W	432	Total	C	N	O	S	0	0	0
			3417	2172	600	622	23			

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

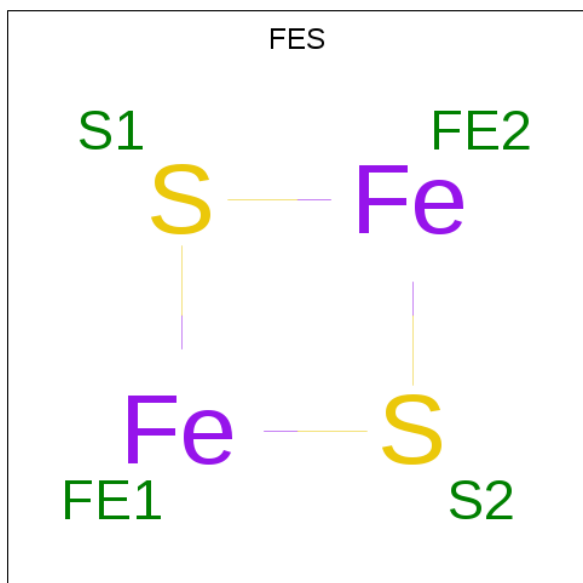
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			
2	D	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			
2	H	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	J	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	L	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	N	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	P	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	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			
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<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).

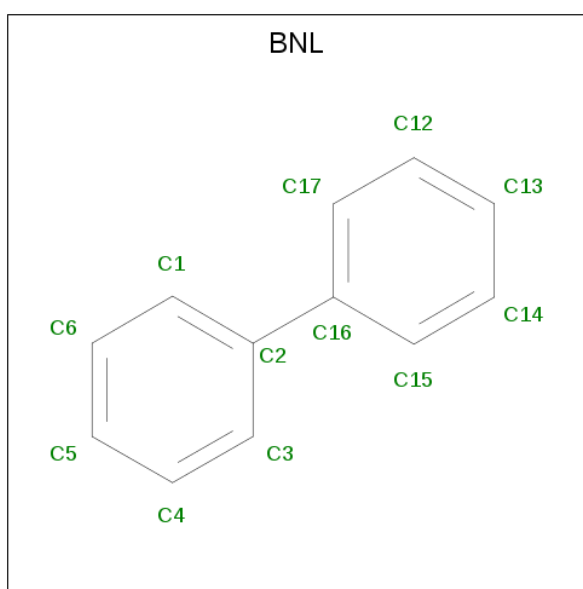
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Fe 1	0	0
4	Q	1	Total 1	Fe 1	0	0
4	K	1	Total 1	Fe 1	0	0
4	E	1	Total 1	Fe 1	0	0
4	I	1	Total 1	Fe 1	0	0
4	C	1	Total 1	Fe 1	0	0
4	W	1	Total 1	Fe 1	0	0
4	A	1	Total 1	Fe 1	0	0

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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 BIPHENYL (three-letter code: BNL) (formula: C<sub>12</sub>H<sub>10</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 12	C 12	0	0
5	C	1	Total 12	C 12	0	0
5	E	1	Total 12	C 12	0	0
5	G	1	Total 12	C 12	0	0
5	I	1	Total 12	C 12	0	0
5	K	1	Total 12	C 12	0	0
5	M	1	Total 12	C 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total C 12 12	0	0
5	Q	1	Total C 12 12	0	0
5	S	1	Total C 12 12	0	0
5	U	1	Total C 12 12	0	0
5	W	1	Total C 12 12	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	44	Total O 44 44	0	0
6	B	19	Total O 19 19	0	0
6	C	31	Total O 31 31	0	0
6	D	21	Total O 21 21	0	0
6	E	50	Total O 50 50	0	0
6	F	35	Total O 35 35	0	0
6	G	24	Total O 24 24	0	0
6	H	12	Total O 12 12	0	0
6	I	25	Total O 25 25	0	0
6	J	7	Total O 7 7	0	0
6	K	16	Total O 16 16	0	0
6	L	12	Total O 12 12	0	0
6	M	38	Total O 38 38	0	0
6	N	25	Total O 25 25	0	0

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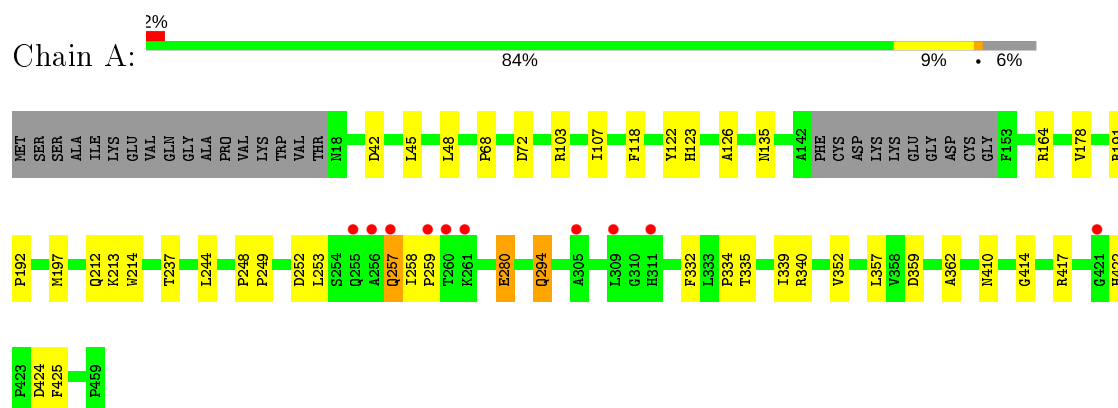
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	O	65	Total 65	O 65	0	0
6	P	26	Total 26	O 26	0	0
6	Q	83	Total 83	O 83	0	0
6	R	30	Total 30	O 30	0	0
6	S	33	Total 33	O 33	0	0
6	T	18	Total 18	O 18	0	0
6	U	25	Total 25	O 25	0	0
6	V	11	Total 11	O 11	0	0
6	W	30	Total 30	O 30	0	0
6	X	14	Total 14	O 14	0	0

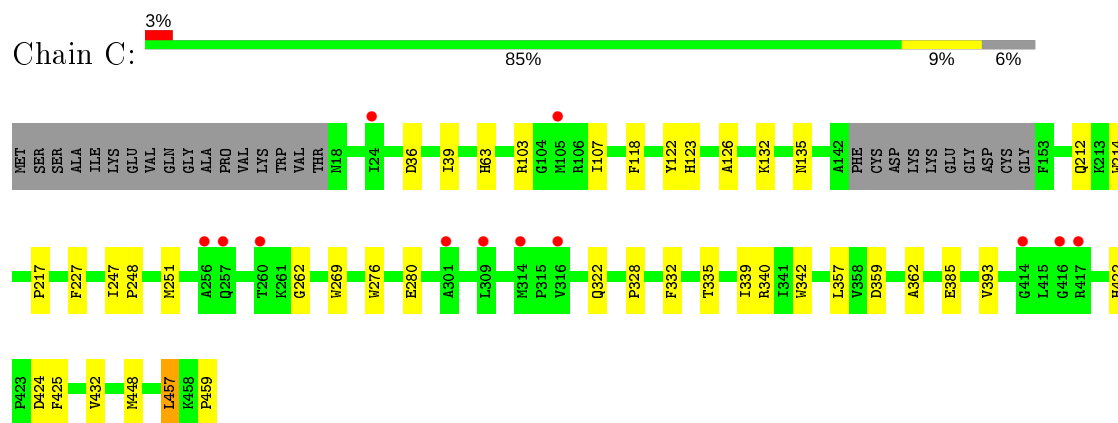
### 3 Residue-property plots [i](#)

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

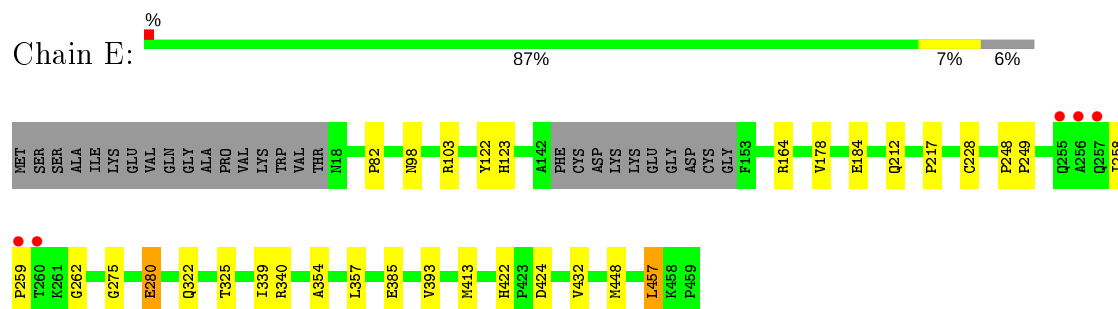
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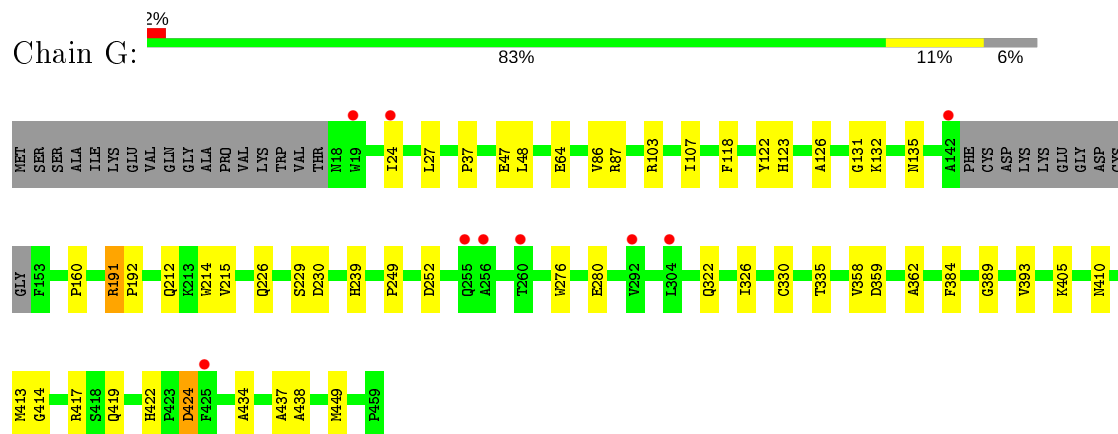
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



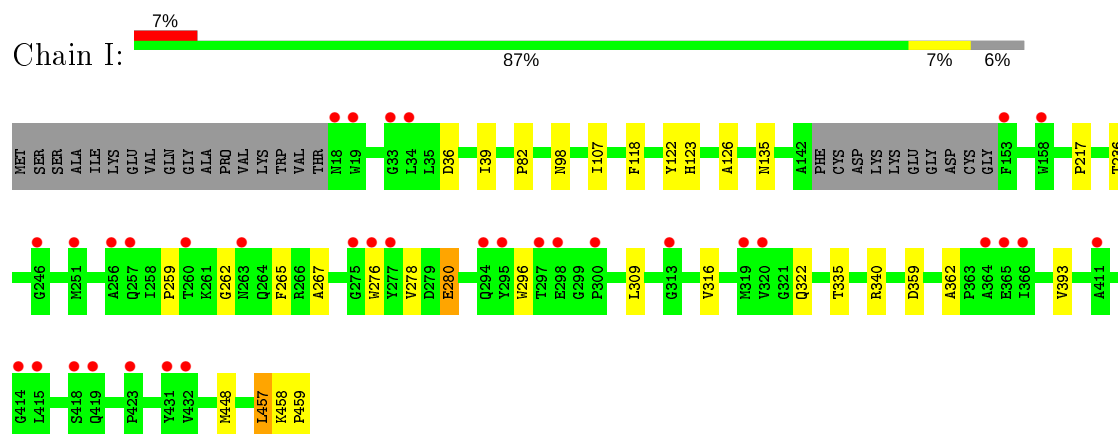
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



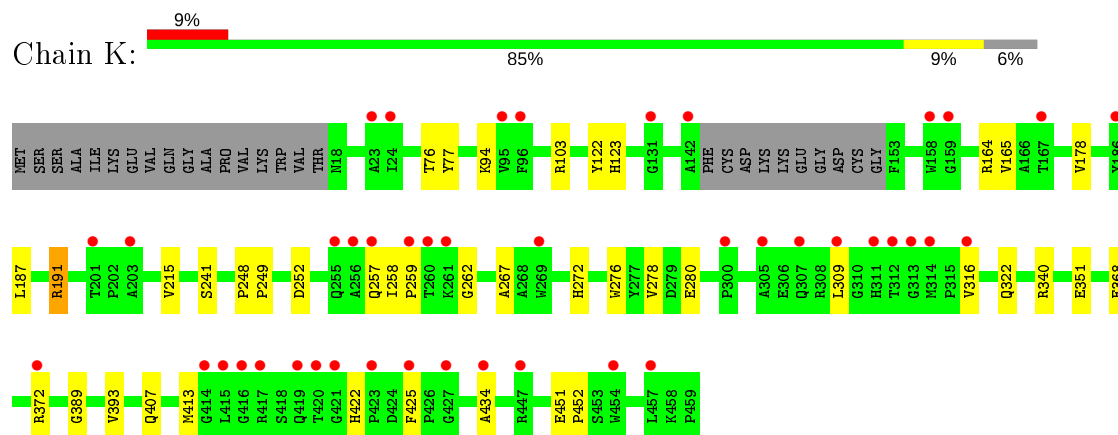
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



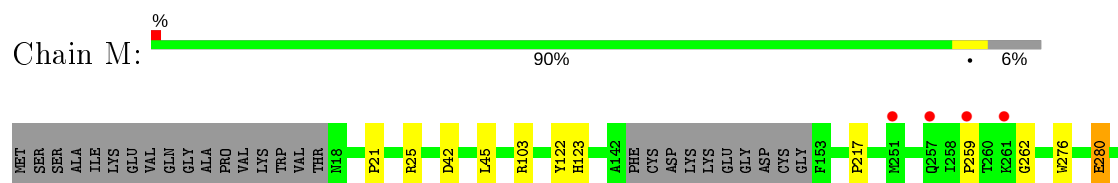
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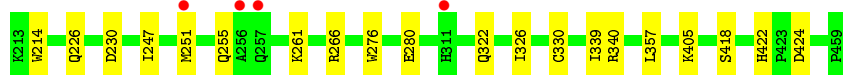
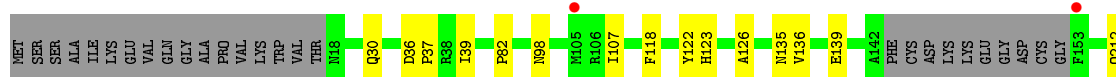
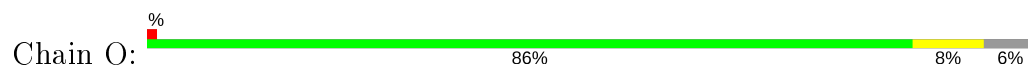


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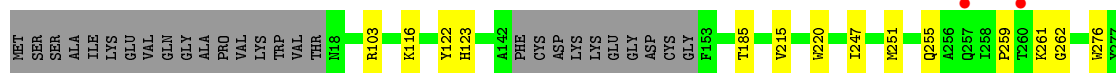
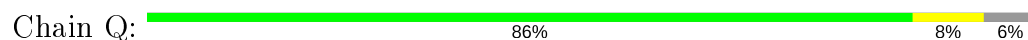




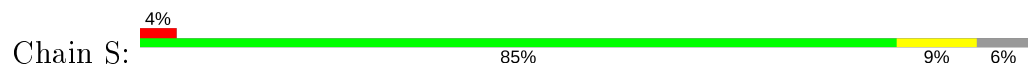
● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



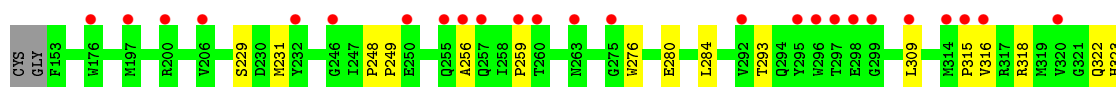
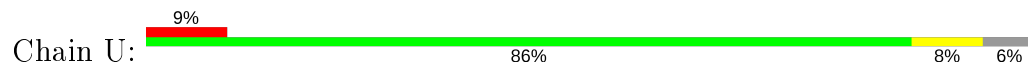
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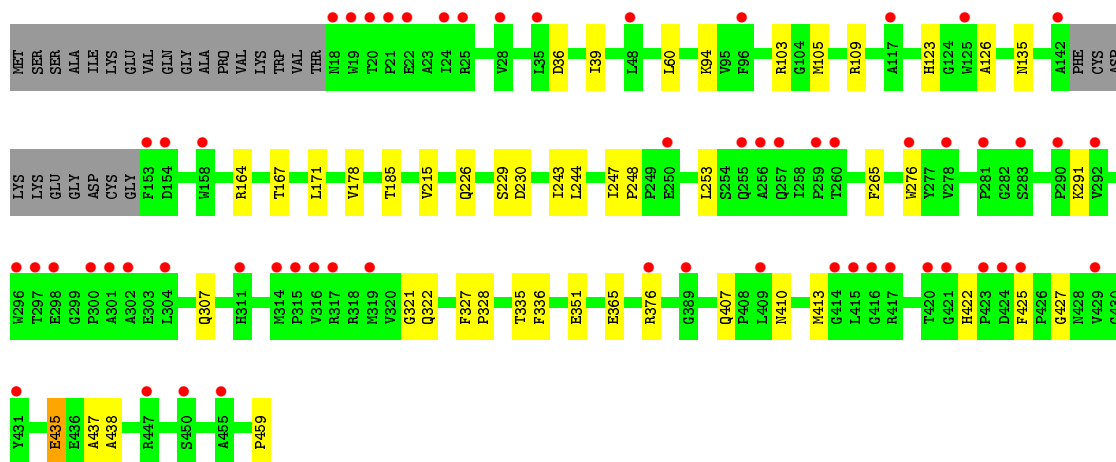
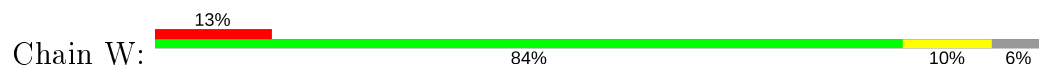


● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

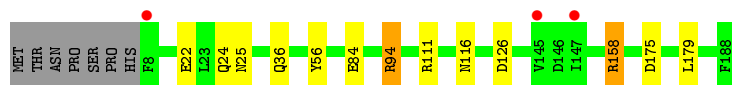
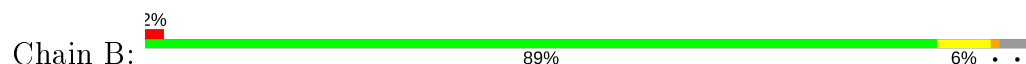




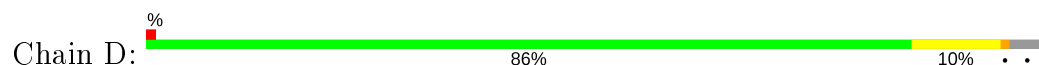
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



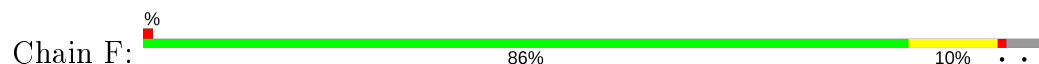
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



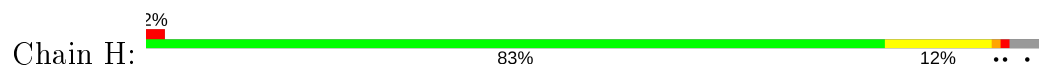
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



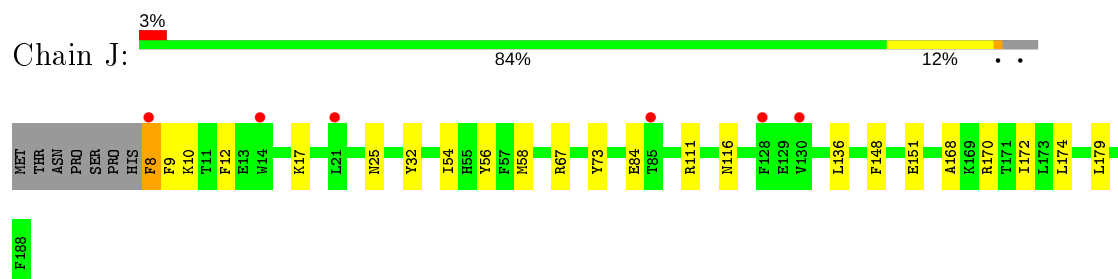
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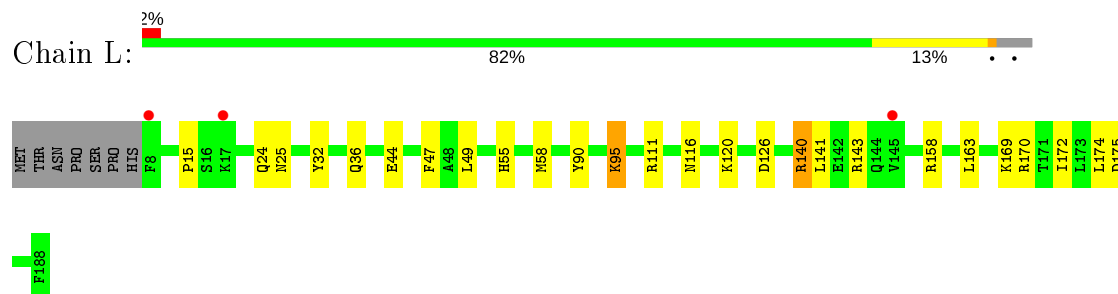
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



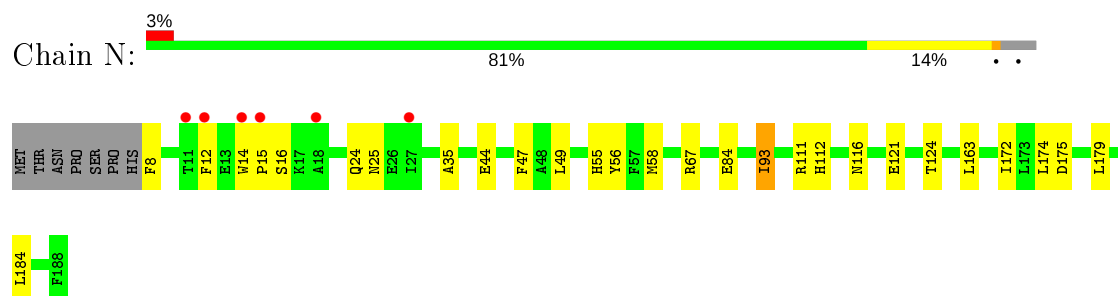
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



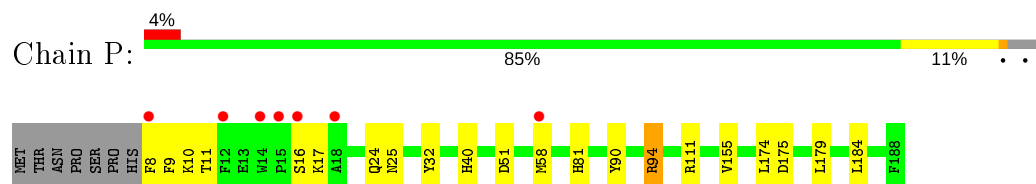
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



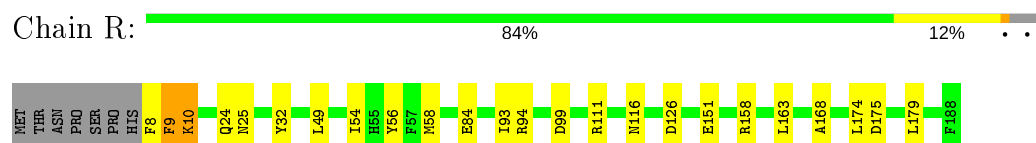
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



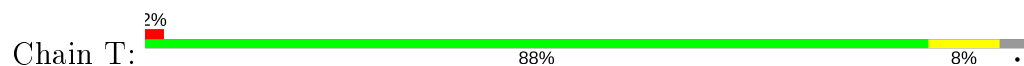
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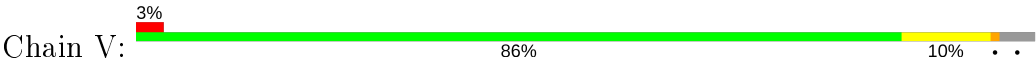


- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

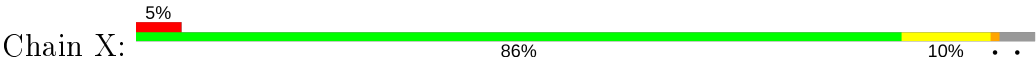




● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.82Å 132.65Å 130.42Å 102.65° 101.11° 105.31°	Depositor
Resolution (Å)	119.52 – 2.42 49.50 – 2.42	Depositor EDS
% Data completeness (in resolution range)	95.0 (119.52-2.42) 82.5 (49.50-2.42)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.233 , 0.270 0.235 , 0.269	Depositor DCC
$R_{free}$ test set	2612 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,h,k 0.007 for k,l,h 0.010 for -h,-l,-k 0.008 for -l,-k,-h 0.010 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	59977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.32	0/3523	0.48	0/4784
1	C	0.32	0/3523	0.47	0/4784
1	E	0.32	0/3523	0.49	0/4784
1	G	0.33	0/3518	0.47	0/4777
1	I	0.33	0/3518	0.47	0/4777
1	K	0.33	0/3518	0.47	0/4777
1	M	0.33	0/3523	0.48	0/4784
1	O	0.32	0/3523	0.48	0/4784
1	Q	0.33	0/3523	0.49	0/4784
1	S	0.32	0/3519	0.47	0/4780
1	U	0.34	0/3519	0.46	0/4780
1	W	0.34	0/3519	0.47	0/4780
2	B	0.34	0/1532	0.51	0/2072
2	D	0.34	0/1532	0.50	0/2072
2	F	0.35	0/1532	0.50	0/2072
2	H	0.34	0/1542	0.51	0/2084
2	J	0.35	0/1542	0.49	0/2084
2	L	0.34	0/1542	0.49	0/2084
2	N	0.35	0/1542	0.52	0/2084
2	P	0.34	0/1542	0.52	0/2084
2	R	0.34	0/1542	0.53	0/2084
2	T	0.34	0/1542	0.49	0/2084
2	V	0.35	0/1542	0.49	0/2084
2	X	0.36	0/1542	0.49	0/2084
All	All	0.33	0/60723	0.48	0/82347

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	3421	0	3269	25	0
1	C	3421	0	3269	21	0
1	E	3421	0	3269	17	0
1	G	3416	0	3262	26	0
1	I	3416	0	3262	16	0
1	K	3416	0	3262	21	0
1	M	3421	0	3269	10	0
1	O	3421	0	3269	15	0
1	Q	3421	0	3269	16	0
1	S	3417	0	3258	22	0
1	U	3417	0	3258	19	0
1	W	3417	0	3258	22	0
2	B	1497	0	1441	13	0
2	D	1497	0	1441	16	0
2	F	1497	0	1441	11	0
2	H	1507	0	1456	20	0
2	J	1507	0	1456	18	0
2	L	1507	0	1456	21	0
2	N	1507	0	1456	17	0
2	P	1507	0	1456	17	0
2	R	1507	0	1456	19	0
2	T	1507	0	1456	11	0
2	V	1507	0	1456	15	0
2	X	1507	0	1456	15	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	12	0	10	0	0
5	C	12	0	10	0	0
5	E	12	0	10	0	0
5	G	12	0	10	0	0
5	I	12	0	10	0	0
5	K	12	0	10	0	0
5	M	12	0	10	1	0
5	O	12	0	10	0	0
5	Q	12	0	10	0	0
5	S	12	0	10	0	0
5	U	12	0	10	0	0
5	W	12	0	10	0	0
6	A	44	0	0	1	0
6	B	19	0	0	0	0
6	C	31	0	0	0	0
6	D	21	0	0	0	0
6	E	50	0	0	1	0
6	F	35	0	0	0	0
6	G	24	0	0	0	0
6	H	12	0	0	0	0
6	I	25	0	0	0	0
6	J	7	0	0	0	0
6	K	16	0	0	0	0
6	L	12	0	0	0	0
6	M	38	0	0	0	0
6	N	25	0	0	1	0
6	O	65	0	0	0	0
6	P	26	0	0	0	0
6	Q	83	0	0	0	0
6	R	30	0	0	0	0
6	S	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	18	0	0	0	0
6	U	25	0	0	0	0
6	V	11	0	0	1	0
6	W	30	0	0	1	0
6	X	14	0	0	0	0
All	All	59977	0	56721	362	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.

The worst 5 of 362 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:8:PHE:HA	2:H:9:PHE:HB2	1.28	1.16
2:X:8:PHE:HD1	2:X:8:PHE:O	1.54	0.90
2:P:94:ARG:HH11	2:P:94:ARG:HG2	1.36	0.89
2:J:8:PHE:HA	2:J:73:TYR:HD2	1.37	0.88
2:R:8:PHE:N	2:R:9:PHE:HB2	1.87	0.88

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	428/459 (93%)	414 (97%)	14 (3%)	0	100	100
1	C	428/459 (93%)	411 (96%)	16 (4%)	1 (0%)	47	61
1	E	428/459 (93%)	413 (96%)	15 (4%)	0	100	100
1	G	428/459 (93%)	413 (96%)	15 (4%)	0	100	100
1	I	428/459 (93%)	412 (96%)	15 (4%)	1 (0%)	47	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	428/459 (93%)	411 (96%)	17 (4%)	0	100	100
1	M	428/459 (93%)	417 (97%)	11 (3%)	0	100	100
1	O	428/459 (93%)	411 (96%)	17 (4%)	0	100	100
1	Q	428/459 (93%)	415 (97%)	13 (3%)	0	100	100
1	S	428/459 (93%)	414 (97%)	14 (3%)	0	100	100
1	U	428/459 (93%)	407 (95%)	20 (5%)	1 (0%)	47	61
1	W	428/459 (93%)	404 (94%)	24 (6%)	0	100	100
2	B	179/188 (95%)	170 (95%)	9 (5%)	0	100	100
2	D	179/188 (95%)	168 (94%)	10 (6%)	1 (1%)	25	35
2	F	179/188 (95%)	171 (96%)	7 (4%)	1 (1%)	25	35
2	H	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	25	35
2	J	179/188 (95%)	168 (94%)	11 (6%)	0	100	100
2	L	179/188 (95%)	171 (96%)	8 (4%)	0	100	100
2	N	179/188 (95%)	170 (95%)	7 (4%)	2 (1%)	14	19
2	P	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	25	35
2	R	179/188 (95%)	170 (95%)	9 (5%)	0	100	100
2	T	179/188 (95%)	172 (96%)	7 (4%)	0	100	100
2	V	179/188 (95%)	171 (96%)	8 (4%)	0	100	100
2	X	179/188 (95%)	171 (96%)	7 (4%)	1 (1%)	25	35
All	All	7284/7764 (94%)	6982 (96%)	292 (4%)	10 (0%)	51	67

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	9	PHE
2	X	10	LYS
2	F	10	LYS
1	U	256	ALA
2	D	10	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/373 (94%)	340 (97%)	10 (3%)	42	61
1	C	350/373 (94%)	345 (99%)	5 (1%)	67	81
1	E	350/373 (94%)	344 (98%)	6 (2%)	60	77
1	G	349/373 (94%)	336 (96%)	13 (4%)	34	51
1	I	349/373 (94%)	345 (99%)	4 (1%)	73	86
1	K	349/373 (94%)	343 (98%)	6 (2%)	60	77
1	M	350/373 (94%)	346 (99%)	4 (1%)	73	86
1	O	350/373 (94%)	344 (98%)	6 (2%)	60	77
1	Q	350/373 (94%)	341 (97%)	9 (3%)	46	64
1	S	349/373 (94%)	345 (99%)	4 (1%)	73	86
1	U	349/373 (94%)	344 (99%)	5 (1%)	67	81
1	W	349/373 (94%)	339 (97%)	10 (3%)	42	61
2	B	158/167 (95%)	154 (98%)	4 (2%)	47	66
2	D	158/167 (95%)	156 (99%)	2 (1%)	69	83
2	F	158/167 (95%)	150 (95%)	8 (5%)	24	37
2	H	160/167 (96%)	155 (97%)	5 (3%)	40	58
2	J	160/167 (96%)	156 (98%)	4 (2%)	47	66
2	L	160/167 (96%)	158 (99%)	2 (1%)	69	83
2	N	160/167 (96%)	154 (96%)	6 (4%)	33	50
2	P	160/167 (96%)	155 (97%)	5 (3%)	40	58
2	R	160/167 (96%)	154 (96%)	6 (4%)	33	50
2	T	160/167 (96%)	158 (99%)	2 (1%)	69	83
2	V	160/167 (96%)	156 (98%)	4 (2%)	47	66
2	X	160/167 (96%)	158 (99%)	2 (1%)	69	83
All	All	6108/6480 (94%)	5976 (98%)	132 (2%)	52	69

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	67	ARG
2	N	14	TRP
1	W	103	ARG

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Mol	Chain	Res	Type
1	K	103	ARG
2	L	95	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	212	GLN
1	M	343	HIS
1	U	422	HIS
1	K	343	HIS
2	L	36	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	S	1460	1	0,4,4	0.00	-	-		
3	FES	C	1460	1	0,4,4	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FES	M	1460	1	0,4,4	0.00	-	-		
3	FES	O	1460	1	0,4,4	0.00	-	-		
3	FES	U	1460	1	0,4,4	0.00	-	-		
5	BNL	W	1462	-	13,13,13	0.55	0	16,16,16	0.55	0
3	FES	Q	1460	1	0,4,4	0.00	-	-		
5	BNL	E	1462	-	13,13,13	0.55	0	16,16,16	0.53	0
3	FES	G	1460	1	0,4,4	0.00	-	-		
5	BNL	A	1462	-	13,13,13	0.54	0	16,16,16	0.57	0
5	BNL	I	1462	-	13,13,13	0.52	0	16,16,16	0.62	0
3	FES	K	1460	1	0,4,4	0.00	-	-		
5	BNL	S	1462	-	13,13,13	0.54	0	16,16,16	0.56	0
5	BNL	C	1462	-	13,13,13	0.54	0	16,16,16	0.46	0
5	BNL	M	1462	-	13,13,13	0.53	0	16,16,16	0.50	0
5	BNL	O	1462	-	13,13,13	0.56	0	16,16,16	0.49	0
5	BNL	U	1462	-	13,13,13	0.52	0	16,16,16	0.54	0
3	FES	W	1460	1	0,4,4	0.00	-	-		
5	BNL	Q	1462	-	13,13,13	0.60	0	16,16,16	0.44	0
3	FES	E	1460	1	0,4,4	0.00	-	-		
5	BNL	G	1462	-	13,13,13	0.53	0	16,16,16	0.50	0
3	FES	A	1460	1	0,4,4	0.00	-	-		
3	FES	I	1460	1	0,4,4	0.00	-	-		
5	BNL	K	1462	-	13,13,13	0.57	0	16,16,16	0.43	0

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	S	1460	1	-	-	0/1/1/1
3	FES	C	1460	1	-	-	0/1/1/1
3	FES	M	1460	1	-	-	0/1/1/1
3	FES	O	1460	1	-	-	0/1/1/1
3	FES	U	1460	1	-	-	0/1/1/1
5	BNL	W	1462	-	-	4/4/4/4	0/2/2/2
3	FES	Q	1460	1	-	-	0/1/1/1
5	BNL	E	1462	-	-	0/4/4/4	0/2/2/2
3	FES	G	1460	1	-	-	0/1/1/1
5	BNL	A	1462	-	-	4/4/4/4	0/2/2/2
5	BNL	I	1462	-	-	4/4/4/4	0/2/2/2
3	FES	K	1460	1	-	-	0/1/1/1
5	BNL	S	1462	-	-	0/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BNL	C	1462	-	-	0/4/4/4	0/2/2/2
5	BNL	M	1462	-	-	0/4/4/4	0/2/2/2
5	BNL	O	1462	-	-	0/4/4/4	0/2/2/2
5	BNL	U	1462	-	-	0/4/4/4	0/2/2/2
3	FES	W	1460	1	-	-	0/1/1/1
5	BNL	Q	1462	-	-	0/4/4/4	0/2/2/2
3	FES	E	1460	1	-	-	0/1/1/1
5	BNL	G	1462	-	-	0/4/4/4	0/2/2/2
3	FES	A	1460	1	-	-	0/1/1/1
3	FES	I	1460	1	-	-	0/1/1/1
5	BNL	K	1462	-	-	0/4/4/4	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1462	BNL	C15-C16-C2-C1
5	I	1462	BNL	C17-C16-C2-C3
5	I	1462	BNL	C17-C16-C2-C1
5	I	1462	BNL	C15-C16-C2-C3
5	A	1462	BNL	C15-C16-C2-C1

There are no ring outliers.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	1460	FES	1	0
3	C	1460	FES	1	0
3	M	1460	FES	1	0
3	O	1460	FES	1	0
3	U	1460	FES	1	0
3	Q	1460	FES	1	0
3	G	1460	FES	1	0
3	K	1460	FES	1	0
5	M	1462	BNL	1	0
3	W	1460	FES	1	0
3	E	1460	FES	1	0
3	A	1460	FES	1	0
3	I	1460	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 i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	432/459 (94%)	-0.06	10 (2%) 60 57	24, 41, 55, 61	17 (3%)
1	C	432/459 (94%)	-0.00	12 (2%) 53 50	30, 44, 54, 58	17 (3%)
1	E	432/459 (94%)	-0.10	5 (1%) 79 76	23, 35, 47, 55	17 (3%)
1	G	432/459 (94%)	0.01	9 (2%) 63 60	35, 47, 60, 66	17 (3%)
1	I	432/459 (94%)	0.32	34 (7%) 12 11	39, 52, 64, 69	17 (3%)
1	K	432/459 (94%)	0.54	43 (9%) 7 6	42, 55, 65, 68	17 (3%)
1	M	432/459 (94%)	-0.06	6 (1%) 75 73	26, 38, 58, 62	17 (3%)
1	O	432/459 (94%)	-0.20	6 (1%) 75 73	20, 34, 49, 57	17 (3%)
1	Q	432/459 (94%)	-0.31	2 (0%) 91 89	22, 31, 44, 61	17 (3%)
1	S	432/459 (94%)	0.23	17 (3%) 39 37	36, 47, 58, 67	17 (3%)
1	U	432/459 (94%)	0.60	42 (9%) 7 6	39, 57, 72, 74	17 (3%)
1	W	432/459 (94%)	0.80	59 (13%) 3 2	46, 59, 70, 74	17 (3%)
2	B	181/188 (96%)	-0.01	3 (1%) 70 67	30, 38, 47, 58	4 (2%)
2	D	181/188 (96%)	-0.07	2 (1%) 80 78	28, 39, 51, 56	4 (2%)
2	F	181/188 (96%)	-0.27	1 (0%) 89 88	28, 33, 47, 60	4 (2%)
2	H	181/188 (96%)	0.17	4 (2%) 62 59	36, 45, 60, 66	4 (2%)
2	J	181/188 (96%)	0.22	6 (3%) 46 44	40, 50, 57, 63	4 (2%)
2	L	181/188 (96%)	0.33	3 (1%) 70 67	39, 48, 63, 70	4 (2%)
2	N	181/188 (96%)	-0.03	6 (3%) 46 44	27, 38, 61, 75	4 (2%)
2	P	181/188 (96%)	-0.05	7 (3%) 39 37	24, 36, 64, 79	4 (2%)
2	R	181/188 (96%)	-0.23	0 100 100	24, 32, 52, 62	4 (2%)
2	T	181/188 (96%)	0.14	4 (2%) 62 59	33, 39, 55, 65	4 (2%)
2	V	181/188 (96%)	0.18	5 (2%) 53 50	45, 53, 59, 64	4 (2%)
2	X	181/188 (96%)	0.50	10 (5%) 25 23	42, 52, 59, 62	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%)	0.12	296 (4%) 38 36	20, 44, 63, 79	252 (3%)

The worst 5 of 296 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	ALA	9.8
1	K	256	ALA	9.2
1	A	257	GLN	7.3
1	S	256	ALA	7.0
1	K	255	GLN	6.8

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	BNL	W	1462	12/12	0.77	0.34	87,87,88,88	0
5	BNL	K	1462	12/12	0.79	0.33	86,86,87,87	0
5	BNL	S	1462	12/12	0.83	0.33	82,82,82,82	0
5	BNL	A	1462	12/12	0.83	0.26	76,76,76,76	0
5	BNL	U	1462	12/12	0.84	0.30	86,86,86,86	0
5	BNL	I	1462	12/12	0.86	0.22	63,63,64,64	0
3	FES	E	1460	4/4	0.90	0.11	44,46,47,50	0
5	BNL	G	1462	12/12	0.90	0.30	63,64,64,64	0
3	FES	W	1460	4/4	0.91	0.09	74,75,76,77	0
3	FES	S	1460	4/4	0.91	0.10	86,86,86,87	0
5	BNL	E	1462	12/12	0.92	0.17	49,49,49,49	0
3	FES	I	1460	4/4	0.92	0.11	45,46,48,50	0
5	BNL	O	1462	12/12	0.93	0.24	44,44,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FES	A	1460	4/4	0.93	0.10	43,44,46,48	0
5	BNL	C	1462	12/12	0.93	0.18	55,56,56,56	0
5	BNL	M	1462	12/12	0.93	0.18	55,56,56,56	0
3	FES	Q	1460	4/4	0.94	0.09	39,39,41,44	0
5	BNL	Q	1462	12/12	0.94	0.18	40,40,41,41	0
4	FE2	W	1461	1/1	0.95	0.09	68,68,68,68	0
3	FES	M	1460	4/4	0.95	0.09	38,38,39,42	0
3	FES	O	1460	4/4	0.95	0.11	44,45,46,48	0
3	FES	K	1460	4/4	0.96	0.07	74,75,75,76	0
3	FES	G	1460	4/4	0.96	0.10	54,54,54,56	0
3	FES	C	1460	4/4	0.96	0.10	43,44,45,46	0
4	FE2	K	1461	1/1	0.97	0.14	59,59,59,59	0
3	FES	U	1460	4/4	0.97	0.08	48,48,49,49	0
4	FE2	S	1461	1/1	0.98	0.14	51,51,51,51	0
4	FE2	U	1461	1/1	0.98	0.08	57,57,57,57	0
4	FE2	E	1461	1/1	0.98	0.15	41,41,41,41	0
4	FE2	I	1461	1/1	0.98	0.14	58,58,58,58	0
4	FE2	Q	1461	1/1	0.99	0.12	37,37,37,37	0
4	FE2	A	1461	1/1	0.99	0.16	53,53,53,53	0
4	FE2	M	1461	1/1	0.99	0.13	43,43,43,43	0
4	FE2	C	1461	1/1	0.99	0.11	44,44,44,44	0
4	FE2	G	1461	1/1	0.99	0.07	52,52,52,52	0
4	FE2	O	1461	1/1	1.00	0.13	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.