



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:52 AM GMT

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

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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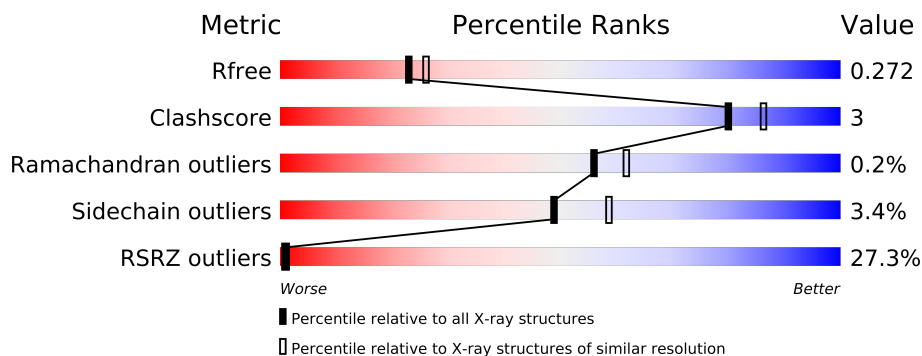
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

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Mol	Chain	Length	Quality of chain
2	F	188	
2	H	188	
2	J	188	
2	L	188	
2	N	188	
2	P	188	
2	R	188	
2	T	188	
2	V	188	
2	X	188	

## 2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BIPHENYL DIOXYGENASE SUBUNIT ALPHA.

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

There are 24 discrepancies between the modelled and reference sequences:

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

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

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

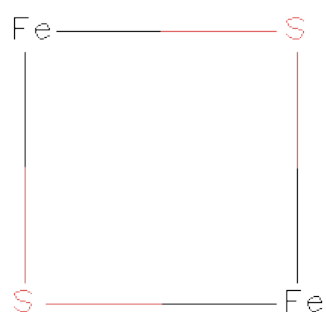
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	D	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	F	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	H	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	J	183	Total	C	N	O	S	0	0	0
			1524	968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

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

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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

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

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

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

- Molecule 5 is water.

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

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

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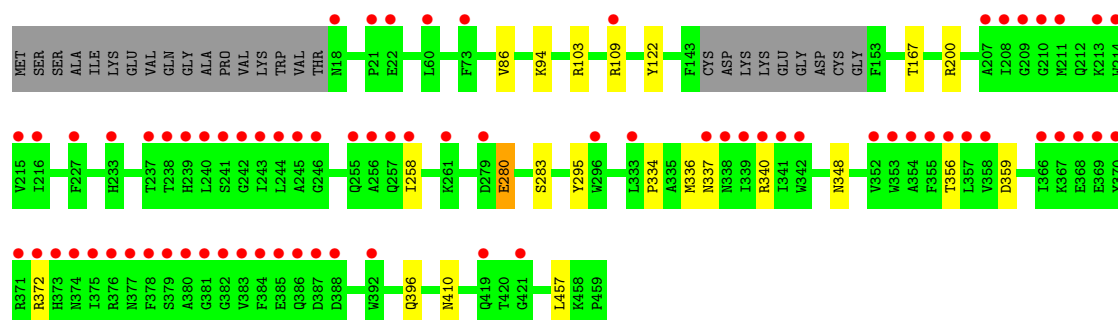
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	37	Total	O	0	0
			37	37		

### 3 Residue-property plots

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

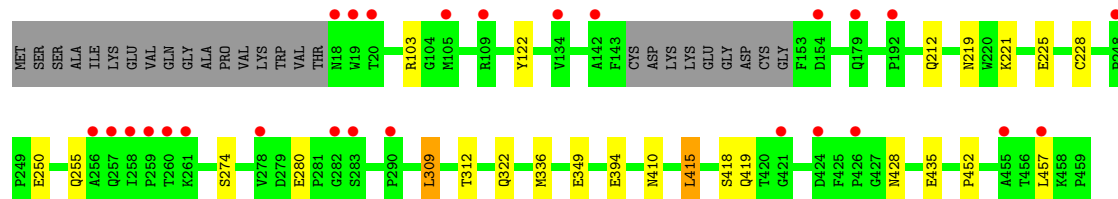
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain A: 



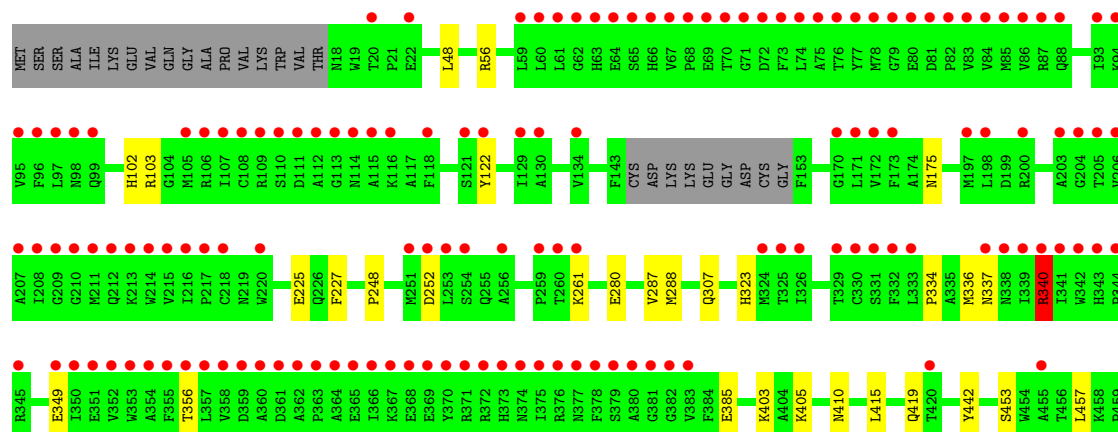
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain C: 

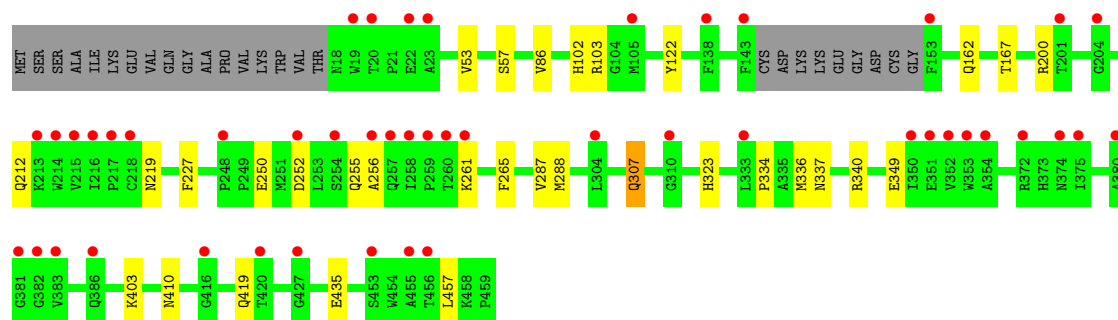


#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

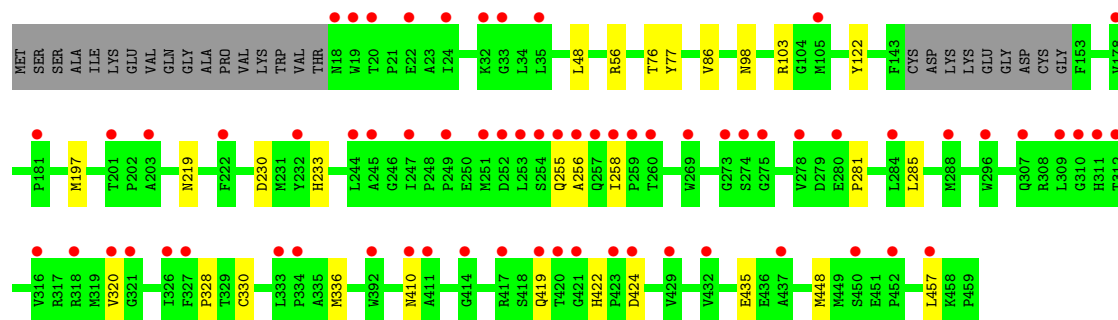
Chain E: 



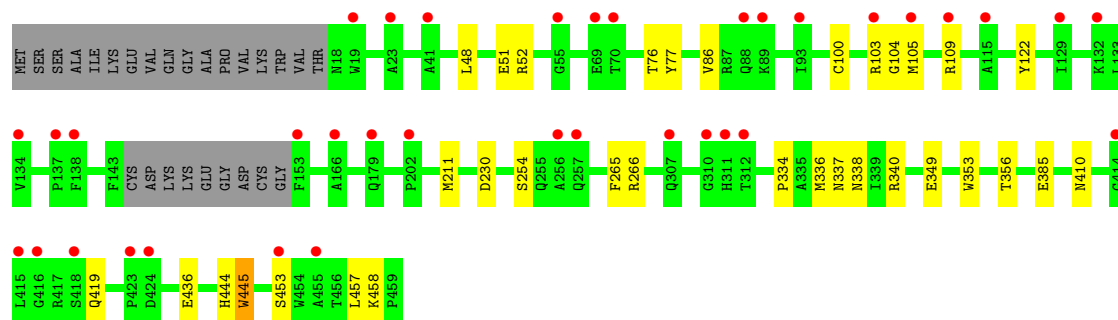
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain G: 

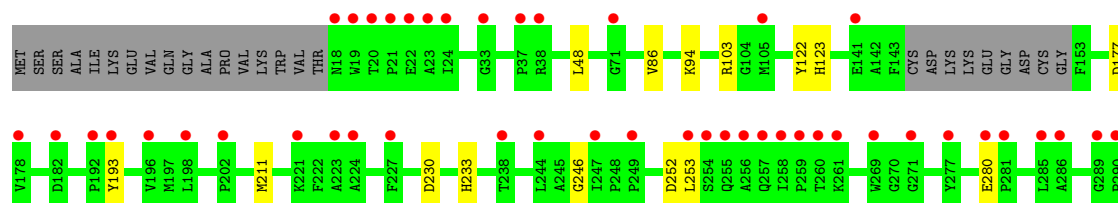
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

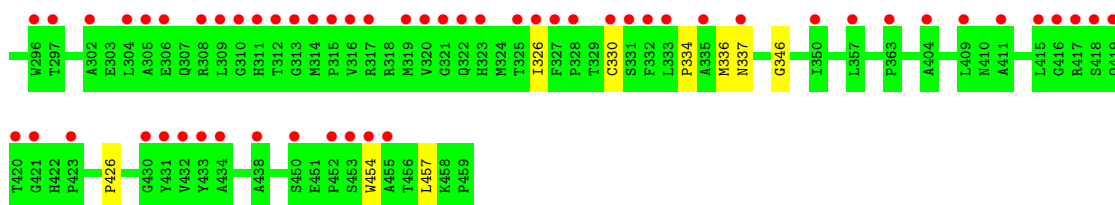
Chain I: 

- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain K: 

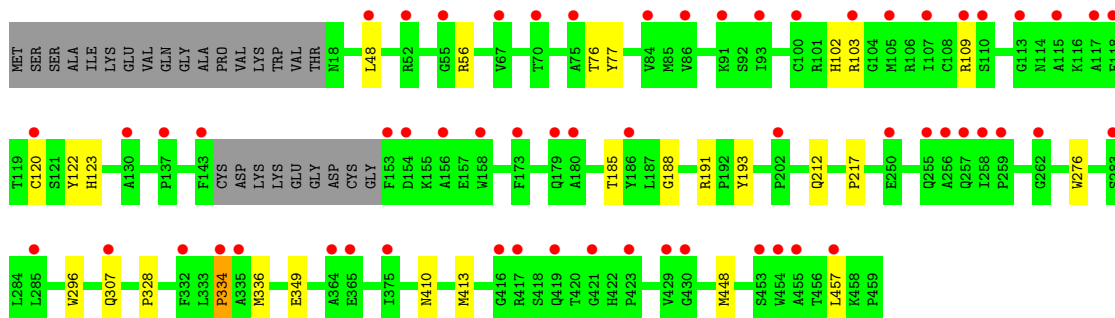
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain M: 



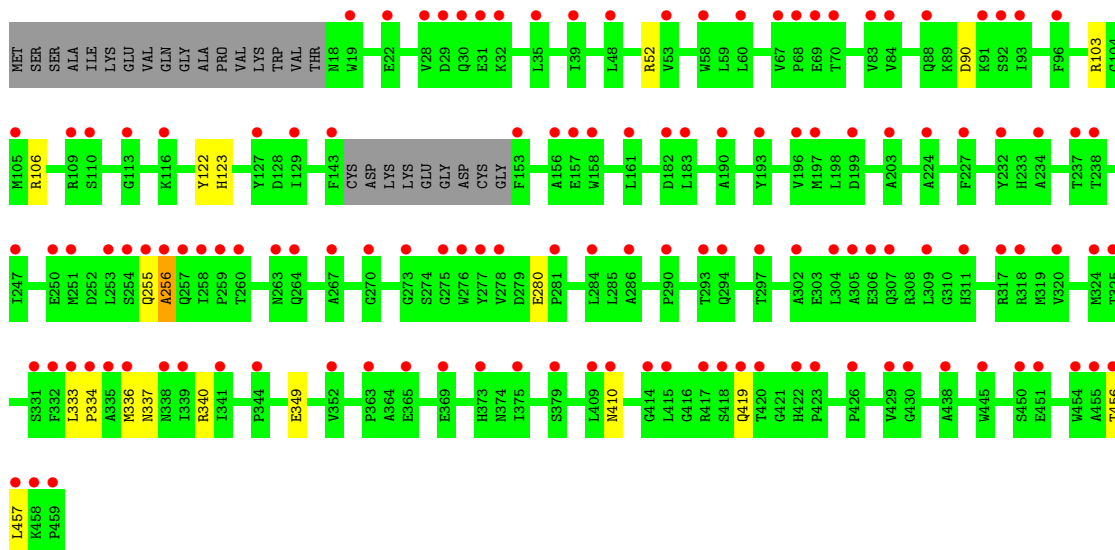
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain O:



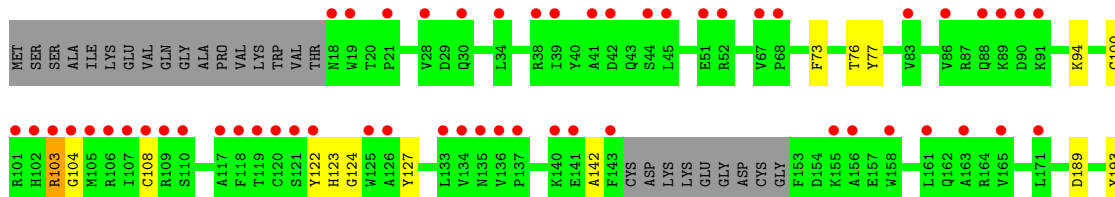
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

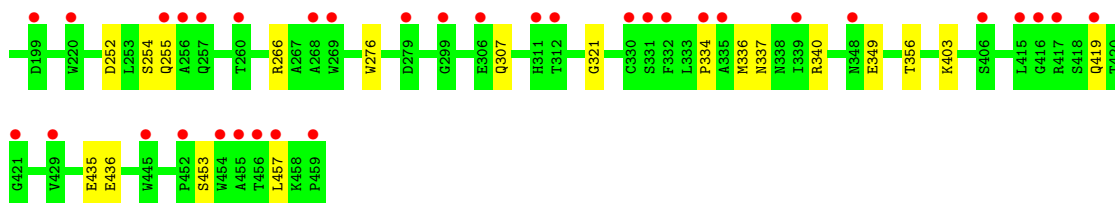
Chain Q:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

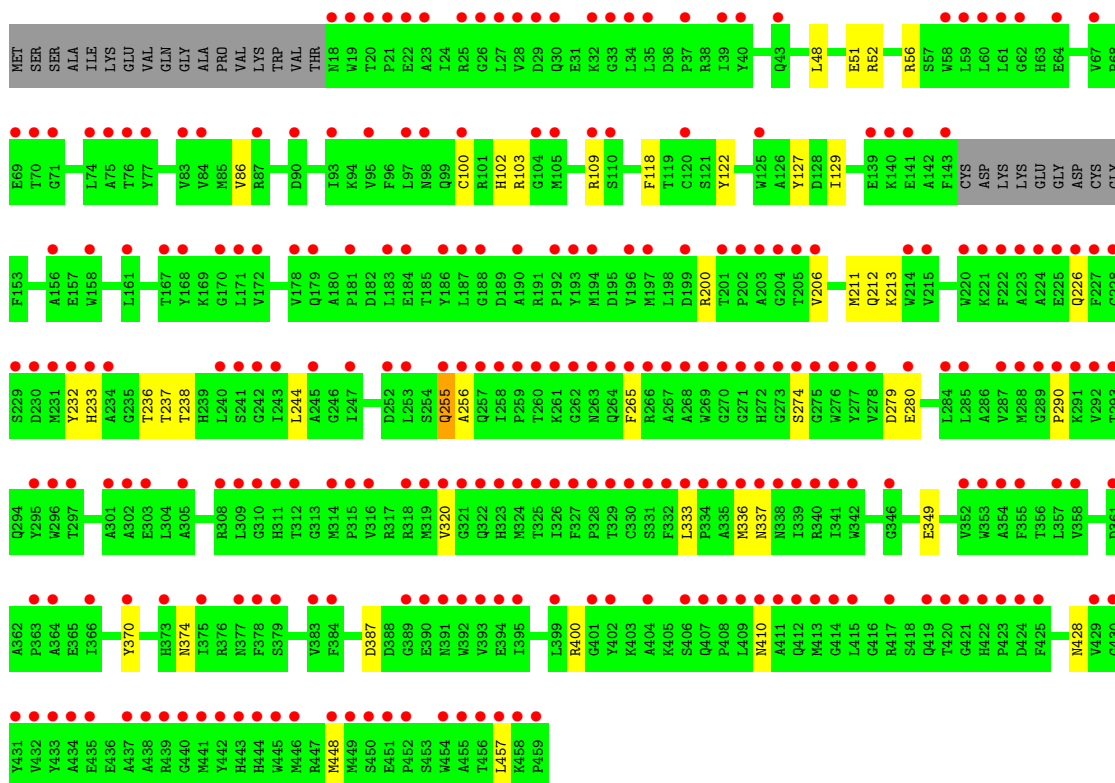
Chain S:





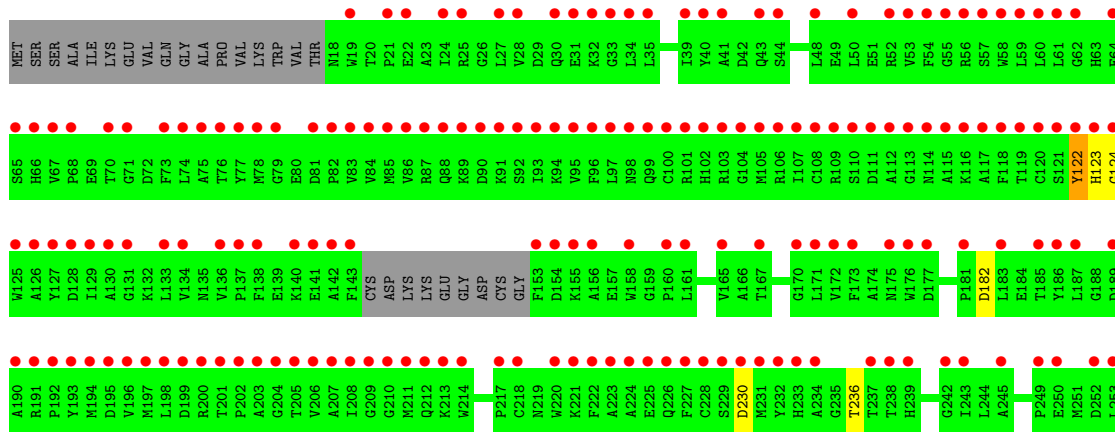
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

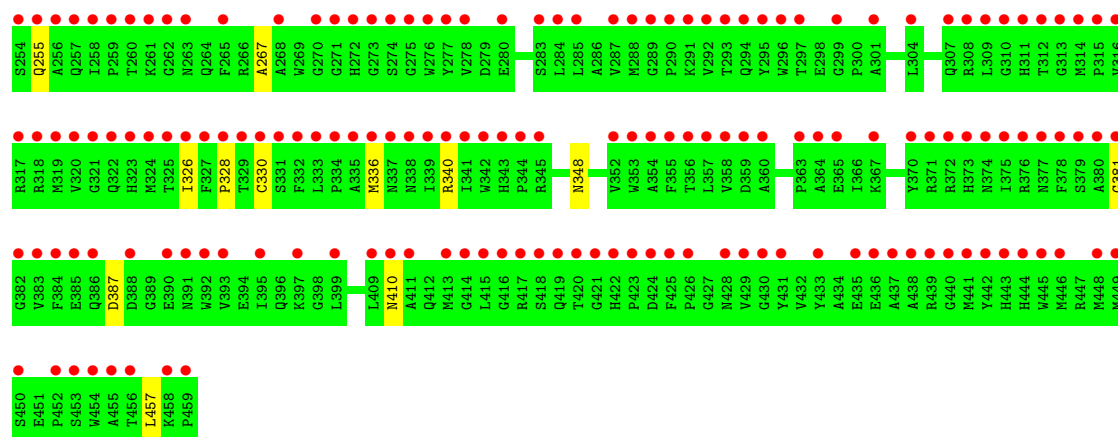
Chain U:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

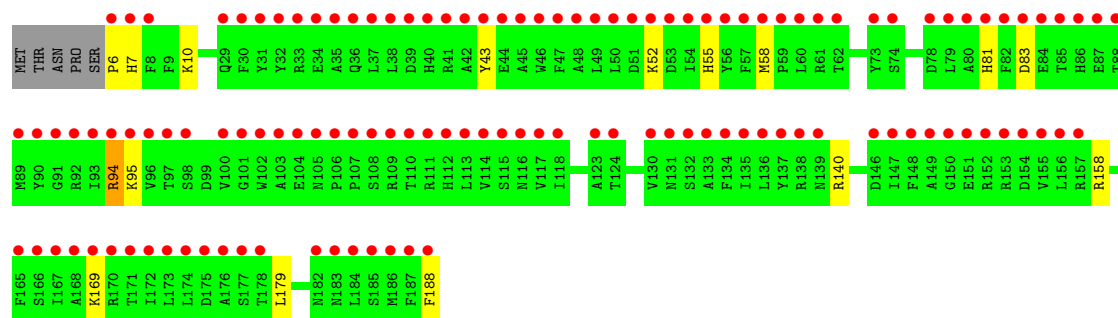
Chain W:





• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain B:



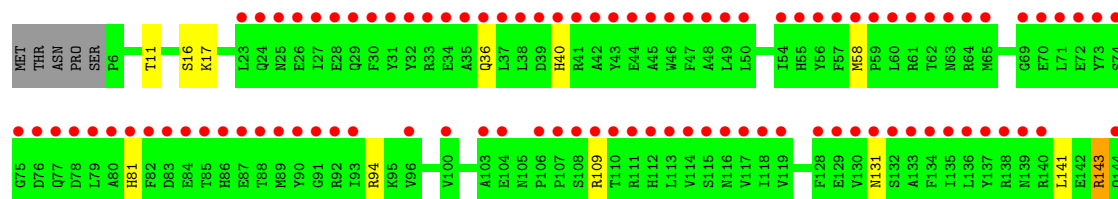
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

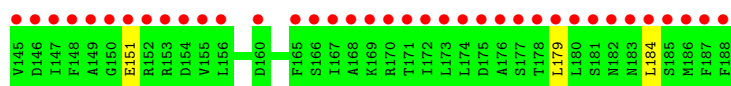
Chain D:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

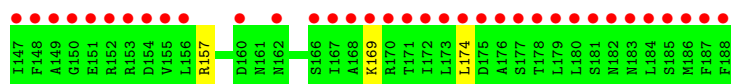
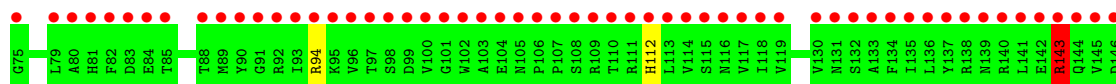
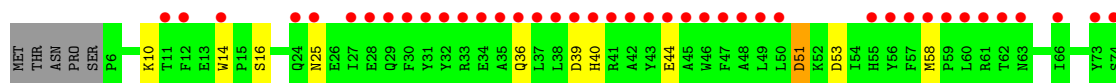
Chain F:





• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain H:



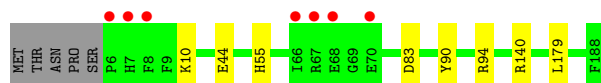
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain J:



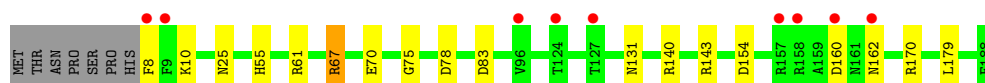
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain L:



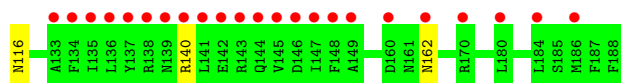
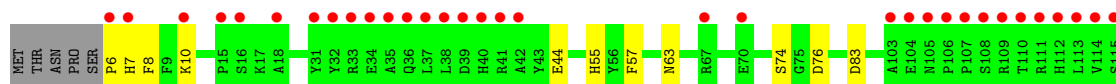
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain N:



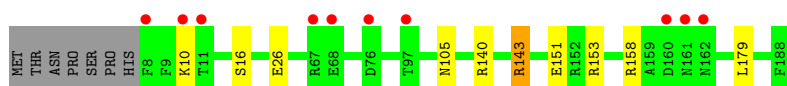
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain P:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain R:



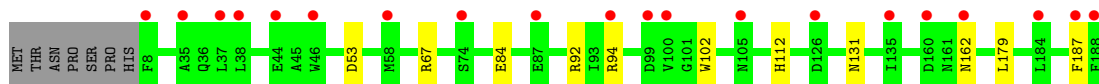
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain T:



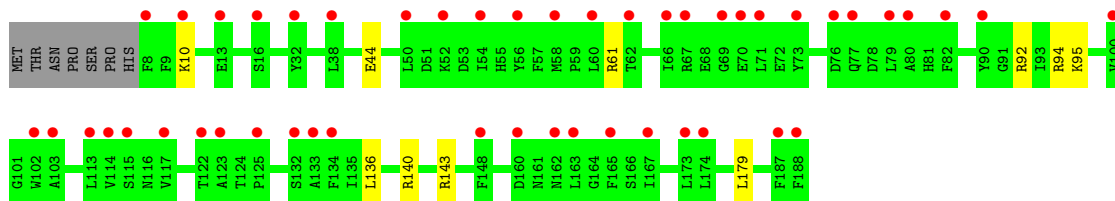
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain V:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain X:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.47Å 133.59Å 133.23Å 102.51° 104.99° 102.75°	Depositor
Resolution (Å)	125.00 – 2.20 28.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.0 (125.00-2.20) 81.0 (28.40-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.266 0.234 , 0.272	Depositor DCC
$R_{free}$ test set	17050 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 20.7	EDS
Estimated twinning fraction	0.080 for k,l,h 0.080 for l,h,k 0.018 for -l,-k,-h 0.022 for -h,-l,-k 0.023 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 339687 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	61911	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.51	0/3529	0.63	0/4791
1	C	0.47	0/3529	0.59	1/4791 (0.0%)
1	E	0.52	0/3529	0.64	1/4791 (0.0%)
1	G	0.52	0/3529	0.64	0/4791
1	I	0.43	0/3529	0.57	0/4791
1	K	0.46	0/3529	0.59	0/4791
1	M	0.44	0/3529	0.57	0/4791
1	O	0.43	0/3529	0.58	0/4791
1	Q	0.43	0/3529	0.56	0/4791
1	S	0.43	0/3529	0.56	0/4791
1	U	0.41	0/3529	0.54	0/4791
1	W	0.39	0/3529	0.52	0/4791
2	B	0.60	0/1561	0.68	0/2110
2	D	0.57	0/1561	0.69	1/2110 (0.0%)
2	F	0.59	0/1561	0.69	0/2110
2	H	0.60	0/1561	0.68	1/2110 (0.0%)
2	J	0.42	0/1561	0.54	0/2110
2	L	0.50	0/1561	0.63	0/2110
2	N	0.49	0/1542	0.60	0/2084
2	P	0.44	0/1561	0.59	0/2110
2	R	0.48	0/1542	0.61	0/2084
2	T	0.49	0/1542	0.60	0/2084
2	V	0.43	0/1542	0.55	0/2084
2	X	0.41	0/1542	0.54	0/2084
All	All	0.47	0/60985	0.59	4/82682 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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

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

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

The worst 5 of 199 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:188:PHE:C	5:B:2106:HOH:O	2.03	0.97
1:I:197:MET:SD	5:I:2068:HOH:O	2.27	0.92
3:O:900:FES:S2	5:O:2036:HOH:O	2.28	0.90
2:D:55:HIS:NE2	2:D:83:ASP:OD2	2.07	0.87
1:S:103:ARG:CB	5:S:2028:HOH:O	2.26	0.83

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/459 (94%)	417 (97%)	12 (3%)	0	100	100
1	C	429/459 (94%)	410 (96%)	19 (4%)	0	100	100
1	E	429/459 (94%)	413 (96%)	15 (4%)	1 (0%)	56	62
1	G	429/459 (94%)	407 (95%)	22 (5%)	0	100	100
1	I	429/459 (94%)	414 (96%)	14 (3%)	1 (0%)	56	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	429/459 (94%)	407 (95%)	21 (5%)	1 (0%)	56	62
1	M	429/459 (94%)	402 (94%)	26 (6%)	1 (0%)	56	62
1	O	429/459 (94%)	407 (95%)	20 (5%)	2 (0%)	38	38
1	Q	429/459 (94%)	405 (94%)	23 (5%)	1 (0%)	56	62
1	S	429/459 (94%)	412 (96%)	15 (4%)	2 (0%)	38	38
1	U	429/459 (94%)	401 (94%)	24 (6%)	4 (1%)	25	21
1	W	429/459 (94%)	396 (92%)	33 (8%)	0	100	100
2	B	181/188 (96%)	172 (95%)	9 (5%)	0	100	100
2	D	181/188 (96%)	174 (96%)	7 (4%)	0	100	100
2	F	181/188 (96%)	174 (96%)	7 (4%)	0	100	100
2	H	181/188 (96%)	174 (96%)	7 (4%)	0	100	100
2	J	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	33	32
2	L	181/188 (96%)	171 (94%)	10 (6%)	0	100	100
2	N	179/188 (95%)	173 (97%)	6 (3%)	0	100	100
2	P	181/188 (96%)	170 (94%)	9 (5%)	2 (1%)	21	16
2	R	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
2	T	179/188 (95%)	172 (96%)	6 (3%)	1 (1%)	33	32
2	V	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
2	X	179/188 (95%)	168 (94%)	11 (6%)	0	100	100
All	All	7310/7764 (94%)	6959 (95%)	334 (5%)	17 (0%)	56	62

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	8	PHE
2	P	8	PHE
1	Q	256	ALA
1	M	253	LEU
1	K	445	TRP

### 5.3.2 Protein sidechains ⓘ

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

conformation was analysed, and the total number of residues.

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

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	86	VAL
1	M	122	TYR
2	V	179	LEU
1	K	103	ARG

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Mol	Chain	Res	Type
1	K	457	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	FES	A	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	C	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	E	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	G	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	I	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	K	900	1,5	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	M	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	O	900	1,5	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	Q	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	S	900	1,5	0,4,4	0.00	-	0,4,4	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FES	U	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	W	900	1,5	0,4,4	0.00	-	0,4,4	0.00	-

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	2.35	74 (17%) 2 2	-7, 10, 35, 51	18 (4%)
1	C	433/459 (94%)	0.46	26 (6%) 21 21	3, 29, 56, 66	18 (4%)
1	E	433/459 (94%)	5.48	143 (33%) 1 1	-11, 7, 33, 47	18 (4%)
1	G	433/459 (94%)	1.15	47 (10%) 6 6	-3, 17, 42, 60	18 (4%)
1	I	433/459 (94%)	0.95	67 (15%) 3 3	7, 50, 89, 101	18 (4%)
1	K	433/459 (94%)	0.55	36 (8%) 11 11	12, 29, 54, 99	18 (4%)
1	M	433/459 (94%)	1.25	102 (23%) 1 1	17, 47, 83, 92	18 (4%)
1	O	433/459 (94%)	0.88	60 (13%) 4 3	20, 49, 71, 100	18 (4%)
1	Q	433/459 (94%)	1.57	130 (30%) 1 1	37, 64, 92, 108	18 (4%)
1	S	433/459 (94%)	1.13	89 (20%) 1 1	15, 48, 80, 113	18 (4%)
1	U	433/459 (94%)	2.81	257 (59%) 0 0	43, 88, 126, 135	18 (4%)
1	W	433/459 (94%)	3.66	339 (78%) 0 0	71, 111, 142, 155	18 (4%)
2	B	183/188 (97%)	10.66	124 (67%) 0 0	-12, -2, 16, 28	4 (2%)
2	D	183/188 (97%)	7.43	88 (48%) 1 0	-12, 2, 28, 40	4 (2%)
2	F	183/188 (97%)	11.98	134 (73%) 0 0	-16, -5, 19, 32	4 (2%)
2	H	183/188 (97%)	11.64	133 (72%) 0 0	-15, -4, 33, 48	4 (2%)
2	J	183/188 (97%)	0.46	16 (8%) 10 10	1, 22, 47, 58	4 (2%)
2	L	183/188 (97%)	-0.03	7 (3%) 38 39	3, 12, 33, 52	4 (2%)
2	N	181/188 (96%)	0.30	9 (4%) 28 27	8, 25, 40, 46	4 (2%)
2	P	183/188 (97%)	5.57	56 (30%) 1 1	-11, 12, 45, 67	4 (2%)
2	R	181/188 (96%)	0.19	10 (5%) 24 24	7, 22, 41, 53	4 (2%)
2	T	181/188 (96%)	0.17	7 (3%) 37 38	5, 20, 49, 75	4 (2%)
2	V	181/188 (96%)	0.96	20 (11%) 6 6	25, 50, 81, 99	4 (2%)
2	X	181/188 (96%)	1.53	48 (26%) 1 1	42, 69, 103, 117	4 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	7382/7764 (95%)	2.56	2022 (27%) <b>1</b> <b>1</b>	-16, 33, 105, 155	264 (3%)

The worst 5 of 2022 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	PHE	41.3
1	E	325	THR	40.1
1	A	353	TRP	39.3
2	D	46	TRP	38.9
2	P	134	PHE	38.8

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	FE2	G	901	1/1	0.11	-0.49	14,14,14,14	0
3	FES	E	900	4/4	0.05	-0.60	13,13,14,15	0
3	FES	I	900	4/4	0.07	-0.85	14,15,15,17	0
3	FES	C	900	4/4	0.07	-0.86	17,18,19,19	0
4	FE2	A	901	1/1	0.10	-1.01	13,13,13,13	0
3	FES	G	900	4/4	0.09	-1.47	25,26,26,27	0
4	FE2	O	901	1/1	0.09	-1.53	32,32,32,32	0
3	FES	A	900	4/4	0.07	-1.59	19,20,22,22	0
4	FE2	C	901	1/1	0.08	-1.68	29,29,29,29	0
4	FE2	U	901	1/1	0.19	-1.83	67,67,67,67	0
4	FE2	E	901	1/1	0.05	-2.00	20,20,20,20	0

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

## 6.5 Other polymers ⓘ

There are no such residues in this entry.