



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 5, 2016 – 02:42 PM EDT

PDB ID : 5AEU  
Title : Crystal structure of II9 variant of Biphenyl dioxygenase from Burkholderia xenovorans LB400  
Authors : Dhindwal, S.; Gomez-Gil, L.; Sylvestre, M.; Eltis, L.D.; Bolin, J.T.; Kumar, P.  
Deposited on : 2015-01-10  
Resolution : 2.49 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  
<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027457  
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) : rb-20027457

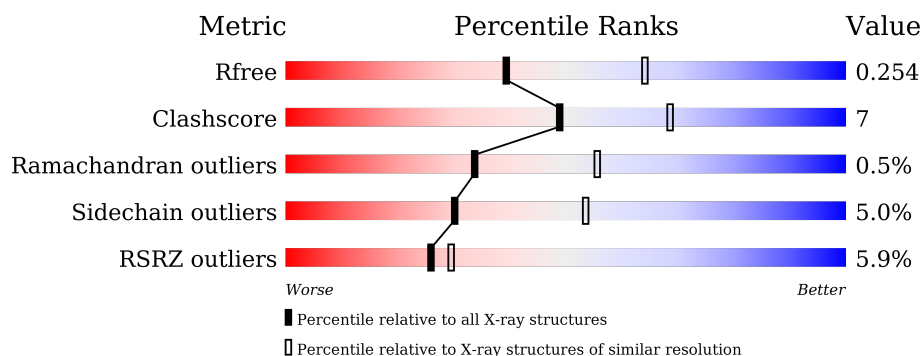
# 1 Overall quality at a glance

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>81% 12% • 6%</div> </div>
1	C	459	<div> <div>3%</div> <div>77% 15% • 6%</div> </div>
1	E	459	<div> <div>11%</div> <div>73% 20% • 6%</div> </div>
1	G	459	<div> <div>14%</div> <div>71% 20% • 6%</div> </div>
2	B	188	<div> <div>86% 11% • •</div> </div>
2	D	188	<div> <div>85% 11% • •</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	188	<div><div><div>2%</div><div></div><div>76%</div><div>20%</div><div></div><div>• •</div></div></div>
2	H	188	<div><div><div>2%</div><div></div><div>76%</div><div>21%</div><div></div><div>• •</div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20136 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
			3428	2180	602	623	23			
1	C	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	E	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	G	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			

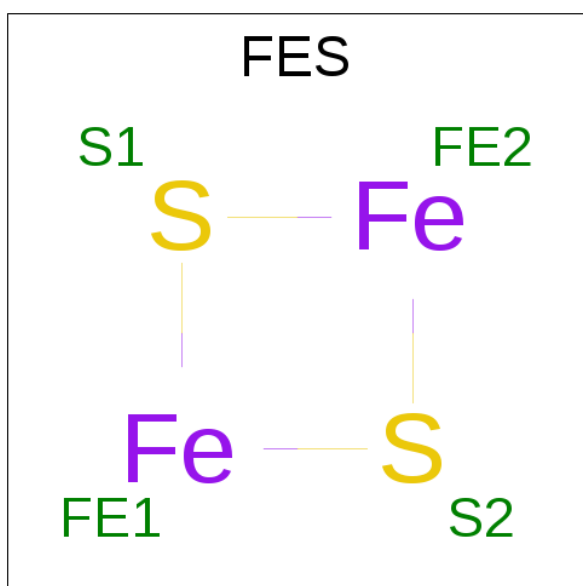
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
A	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
A	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
A	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
C	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
C	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
C	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
C	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
E	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
E	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
E	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
E	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
G	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
G	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
G	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
G	341	THR	ILE	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	182	Total	C	N	O	S	0	0	0
			1517	963	269	281	4			
2	F	182	Total	C	N	O	S	0	0	0
			1517	963	269	281	4			
2	H	182	Total	C	N	O	S	0	0	0
			1517	963	269	281	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		
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		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Fe	0	0
			1	1		
4	A	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Fe 1	0	0
4	E	1	Total 1	Fe 1	0	0

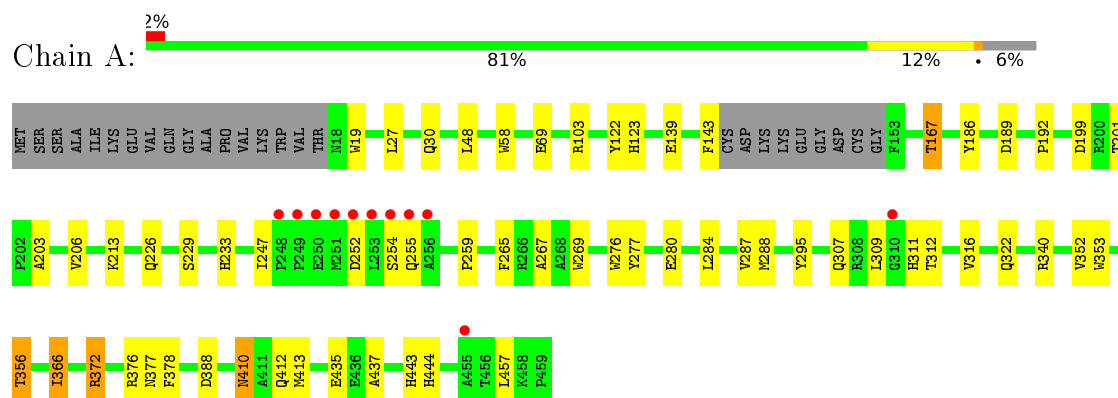
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total 105	O 105	0	0
5	B	56	Total 56	O 56	0	0
5	C	46	Total 46	O 46	0	0
5	D	50	Total 50	O 50	0	0
5	E	20	Total 20	O 20	0	0
5	F	26	Total 26	O 26	0	0
5	G	14	Total 14	O 14	0	0
5	H	12	Total 12	O 12	0	0

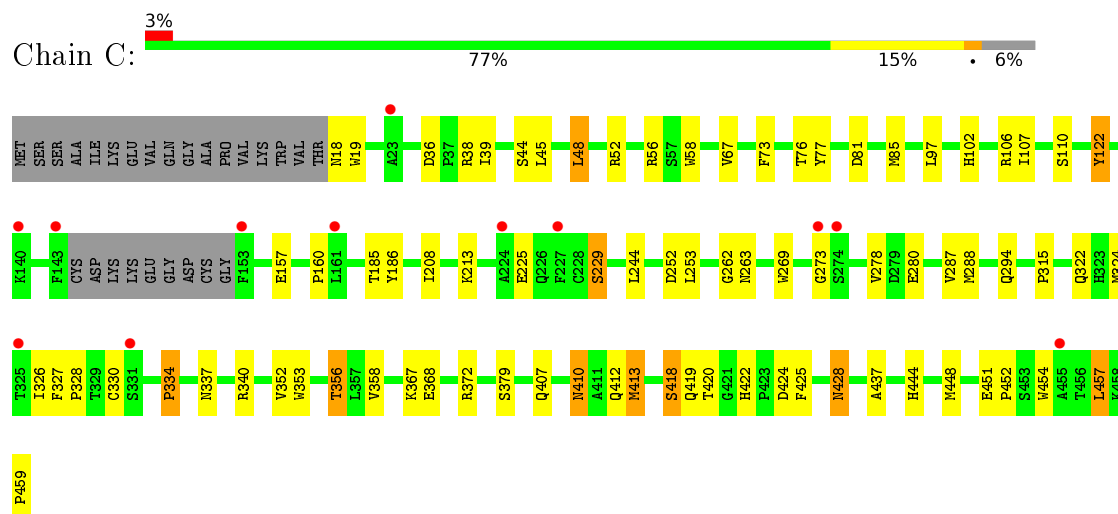
### 3 Residue-property plots

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.

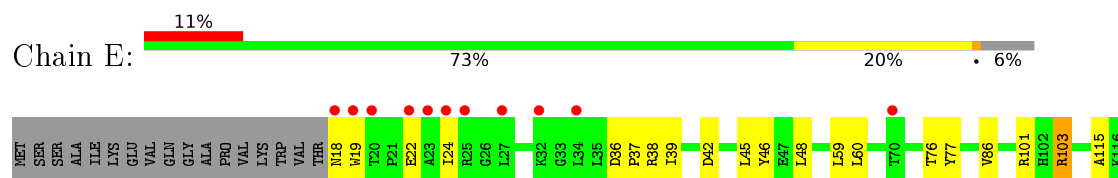
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

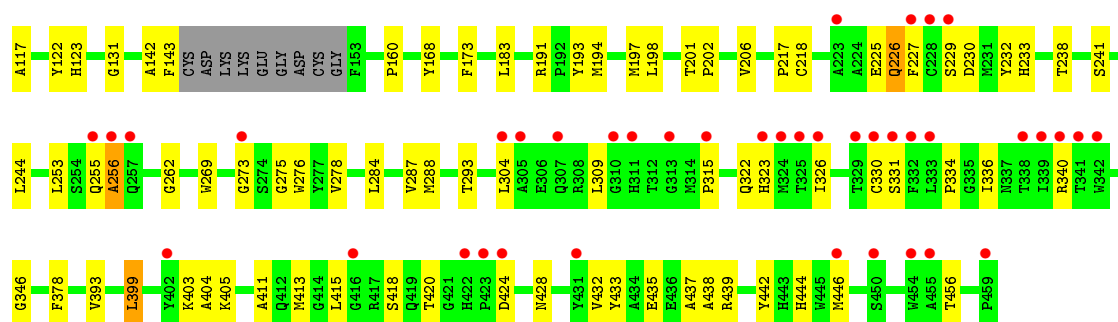


#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

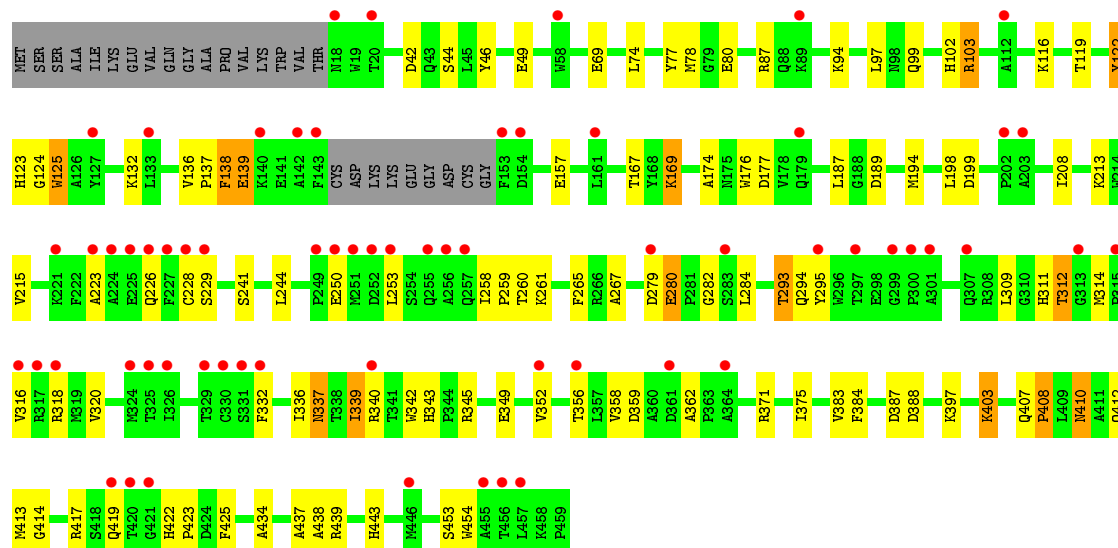


#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

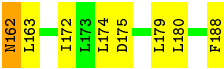




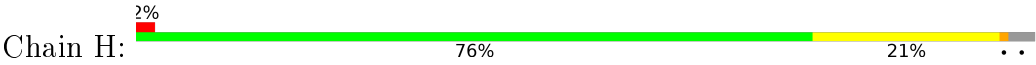
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA







● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.89Å 211.89Å 168.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.56 – 2.49 38.53 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.56-2.49) 99.3 (38.53-2.49)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.193 , 0.254 0.192 , 0.254	Depositor DCC
$R_{free}$ test set	4865 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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	0.48	0/3530	0.67	0/4792
1	C	0.45	0/3530	0.61	0/4792
1	E	0.40	0/3530	0.59	0/4792
1	G	0.42	0/3530	0.59	0/4792
2	B	0.55	0/1561	0.74	0/2110
2	D	0.49	0/1553	0.68	0/2099
2	F	0.47	0/1553	0.66	0/2099
2	H	0.46	0/1553	0.66	0/2099
All	All	0.45	0/20340	0.64	0/27575

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	PHE	Peptide

## 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	3428	0	3284	38	0
1	C	3428	0	3284	50	0
1	E	3428	0	3284	61	0
1	G	3428	0	3284	64	0
2	B	1524	0	1471	16	0
2	D	1517	0	1463	34	0
2	F	1517	0	1463	30	0
2	H	1517	0	1463	32	0
3	A	4	0	0	1	0
3	C	4	0	0	0	0
3	E	4	0	0	1	0
3	G	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
5	A	105	0	0	8	0
5	B	56	0	0	2	1
5	C	46	0	0	3	0
5	D	50	0	0	2	0
5	E	20	0	0	0	0
5	F	26	0	0	3	0
5	G	14	0	0	2	0
5	H	12	0	0	0	0
All	All	20136	0	18996	280	1

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 7.

The worst 5 of 280 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:A:259:PRO:HB3	1:A:280:GLU:HG2	1.50	0.94
2:B:140:ARG:HH11	2:B:140:ARG:HG2	1.39	0.87
1:G:123:HIS:HB2	3:G:500:FES:S1	2.15	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:162:ASN:H	2:F:162:ASN:ND2	1.76	0.83
2:D:36:GLN:HE21	2:F:12:PHE:H	1.32	0.77

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2008:HOH:O	5:B:2008:HOH:O[3_565]	1.90	0.30

## 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%)	406 (95%)	22 (5%)	1 (0%)	52	75
1	C	429/459 (94%)	406 (95%)	21 (5%)	2 (0%)	34	55
1	E	429/459 (94%)	397 (92%)	30 (7%)	2 (0%)	34	55
1	G	429/459 (94%)	382 (89%)	42 (10%)	5 (1%)	16	29
2	B	181/188 (96%)	174 (96%)	7 (4%)	0	100	100
2	D	180/188 (96%)	171 (95%)	9 (5%)	0	100	100
2	F	180/188 (96%)	168 (93%)	11 (6%)	1 (1%)	30	50
2	H	180/188 (96%)	168 (93%)	11 (6%)	1 (1%)	30	50
All	All	2437/2588 (94%)	2272 (93%)	153 (6%)	12 (0%)	34	55

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	E	256	ALA
2	F	8	PHE

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Mol	Chain	Res	Type
2	H	99	ASP
1	C	122	TYR

### 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	351/372 (94%)	336 (96%)	15 (4%)	35	61
1	C	351/372 (94%)	332 (95%)	19 (5%)	27	49
1	E	351/372 (94%)	336 (96%)	15 (4%)	35	61
1	G	351/372 (94%)	325 (93%)	26 (7%)	17	31
2	B	162/167 (97%)	155 (96%)	7 (4%)	35	61
2	D	161/167 (96%)	156 (97%)	5 (3%)	47	75
2	F	161/167 (96%)	153 (95%)	8 (5%)	30	53
2	H	161/167 (96%)	153 (95%)	8 (5%)	30	53
All	All	2049/2156 (95%)	1946 (95%)	103 (5%)	30	53

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	18	ASN
1	E	415	LEU
2	H	22	GLU
1	E	22	GLU
1	E	206	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	25	ASN
2	F	25	ASN
2	H	25	ASN

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Mol	Chain	Res	Type
1	E	263	ASN
2	B	77	GLN

### 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	500	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	C	500	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	E	500	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	G	500	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	500	1	-	0/0/4/4	0/1/1/1
3	FES	C	500	1	-	0/0/4/4	0/1/1/1
3	FES	E	500	1	-	0/0/4/4	0/1/1/1
3	FES	G	500	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	FES	1	0
3	E	500	FES	1	0
3	G	500	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	433/459 (94%)	-0.13	11 (2%) 61 65	31, 44, 67, 178	5 (1%)
1	C	433/459 (94%)	-0.01	12 (2%) 56 61	35, 55, 78, 108	2 (0%)
1	E	433/459 (94%)	0.55	51 (11%) 6 6	43, 71, 107, 129	10 (2%)
1	G	433/459 (94%)	0.76	64 (14%) 3 3	49, 79, 109, 139	10 (2%)
2	B	183/188 (97%)	-0.65	0 100 100	27, 35, 63, 85	1 (0%)
2	D	182/188 (96%)	-0.49	0 100 100	32, 42, 63, 94	2 (1%)
2	F	182/188 (96%)	-0.42	3 (1%) 74 78	35, 50, 72, 124	1 (0%)
2	H	182/188 (96%)	-0.21	3 (1%) 74 78	39, 55, 82, 119	0
All	All	2461/2588 (95%)	0.07	144 (5%) 26 29	27, 56, 97, 178	31 (1%)

The worst 5 of 144 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	PRO	9.0
1	A	251	MET	7.8
1	E	256	ALA	6.6
1	A	252	ASP	5.9
1	A	255	GLN	5.9

### 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

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	E	500	4/4	0.99	0.10	-0.75	42,45,46,47	0
3	FES	G	500	4/4	0.99	0.09	-0.98	70,73,75,78	0
3	FES	C	500	4/4	0.98	0.09	-1.57	62,68,68,78	0
3	FES	A	500	4/4	0.99	0.08	-1.88	40,41,42,46	0
4	FE2	G	501	1/1	0.99	0.15	-	69,69,69,69	0
4	FE2	C	501	1/1	1.00	0.15	-	43,43,43,43	0
4	FE2	A	501	1/1	1.00	0.12	-	39,39,39,39	0
4	FE2	E	501	1/1	1.00	0.20	-	71,71,71,71	0

## 6.5 Other polymers

There are no such residues in this entry.