



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:38 am GMT

PDB ID : 2YFL  
Title : Crystal Structure of Biphenyl dioxygenase variant RR41 with 2-chloro dibenzofuran  
Authors : Kumar, P.; Bolin, J.T.  
Deposited on : 2011-04-06  
Resolution : 2.60 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

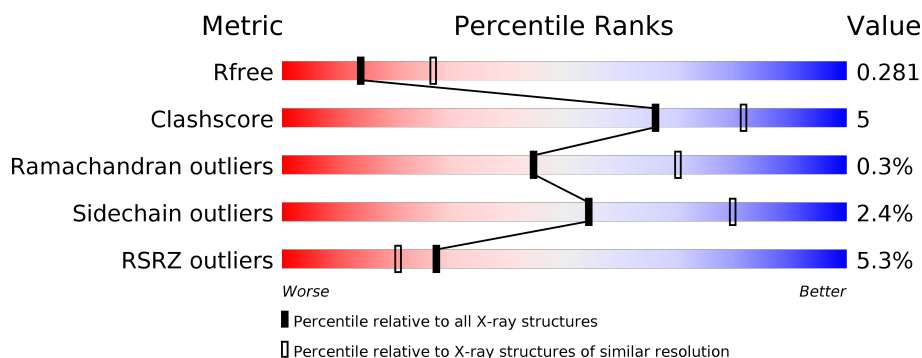
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



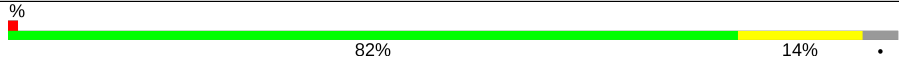
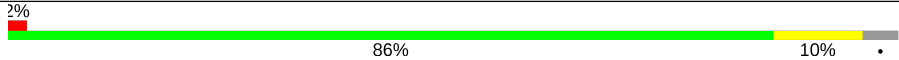
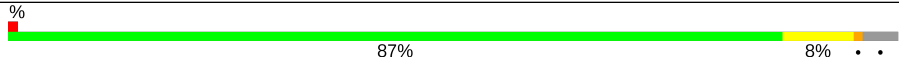
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
1	C	459	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
1	E	459	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>
1	G	459	<div> <div>12%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	I	459	<div> <div>10%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
1	K	459	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	188	
2	D	188	
2	F	188	
2	H	188	
2	J	188	
2	L	188	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	G	900	-	-	X	-
5	DC4	A	1460	-	-	-	X
5	DC4	C	1460	-	-	X	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29968 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
			3430	2182	602	622	24			
1	C	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	E	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	G	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	I	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			
1	K	433	Total	C	N	O	S	0	0	0
			3430	2182	602	622	24			

There are 30 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
A	338	GLN	ASN	ENGINEERED MUTATION	UNP P37333
A	341	VAL	ILE	ENGINEERED MUTATION	UNP P37333
A	409	PHE	LEU	ENGINEERED MUTATION	UNP P37333
C	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
C	336	MET	PHE	ENGINEERED MUTATION	UNP P37333
C	338	GLN	ASN	ENGINEERED MUTATION	UNP P37333
C	341	VAL	ILE	ENGINEERED MUTATION	UNP P37333
C	409	PHE	LEU	ENGINEERED MUTATION	UNP P37333
E	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
E	336	MET	PHE	ENGINEERED MUTATION	UNP P37333
E	338	GLN	ASN	ENGINEERED MUTATION	UNP P37333
E	341	VAL	ILE	ENGINEERED MUTATION	UNP P37333
E	409	PHE	LEU	ENGINEERED MUTATION	UNP P37333
G	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
G	336	MET	PHE	ENGINEERED MUTATION	UNP P37333

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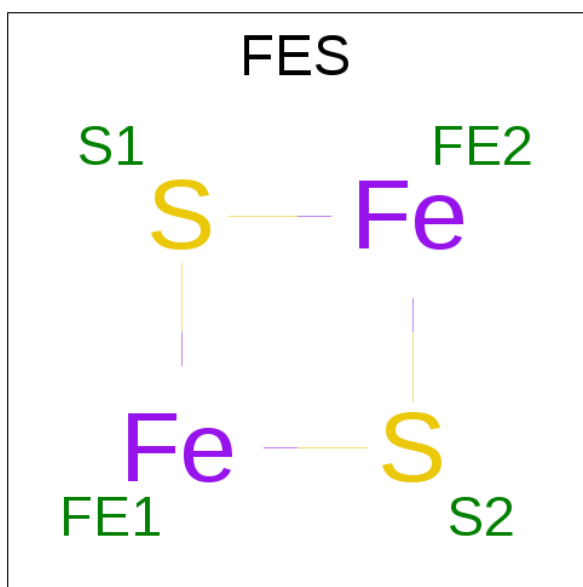
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Chain	Residue	Modelled	Actual	Comment	Reference
G	338	GLN	ASN	ENGINEERED MUTATION	UNP P37333
G	341	VAL	ILE	ENGINEERED MUTATION	UNP P37333
G	409	PHE	LEU	ENGINEERED MUTATION	UNP P37333
I	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
I	336	MET	PHE	ENGINEERED MUTATION	UNP P37333
I	338	GLN	ASN	ENGINEERED MUTATION	UNP P37333
I	341	VAL	ILE	ENGINEERED MUTATION	UNP P37333
I	409	PHE	LEU	ENGINEERED MUTATION	UNP P37333
K	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
K	336	MET	PHE	ENGINEERED MUTATION	UNP P37333
K	338	GLN	ASN	ENGINEERED MUTATION	UNP P37333
K	341	VAL	ILE	ENGINEERED MUTATION	UNP P37333
K	409	PHE	LEU	ENGINEERED MUTATION	UNP P37333

- 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			
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			

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

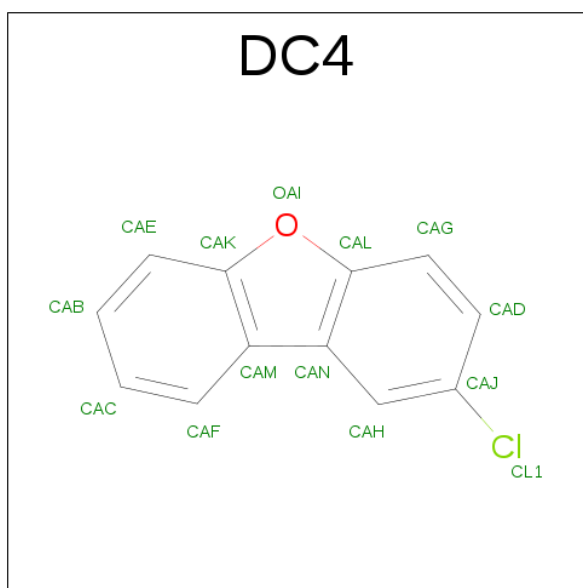


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		

- 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	K	1	Total	Fe	0	0
			1	1		
4	E	1	Total	Fe	0	0
			1	1		
4	I	1	Total	Fe	0	0
			1	1		
4	C	1	Total	Fe	0	0
			1	1		
4	A	1	Total	Fe	0	0
			1	1		

- Molecule 5 is 2-CHLORODIBENZOFURAN (three-letter code: DC4) (formula: C<sub>12</sub>H<sub>7</sub>ClO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Cl	O	0	0
			14	12	1	1		
5	C	1	Total	C	Cl	O	0	0
			14	12	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	50	Total	O	0	0
			50	50		
6	B	26	Total	O	0	0
			26	26		
6	C	41	Total	O	0	0
			41	41		
6	D	24	Total	O	0	0
			24	24		
6	E	62	Total	O	0	0
			62	62		
6	F	21	Total	O	0	0
			21	21		
6	G	30	Total	O	0	0
			30	30		
6	H	19	Total	O	0	0
			19	19		
6	I	35	Total	O	0	0
			35	35		

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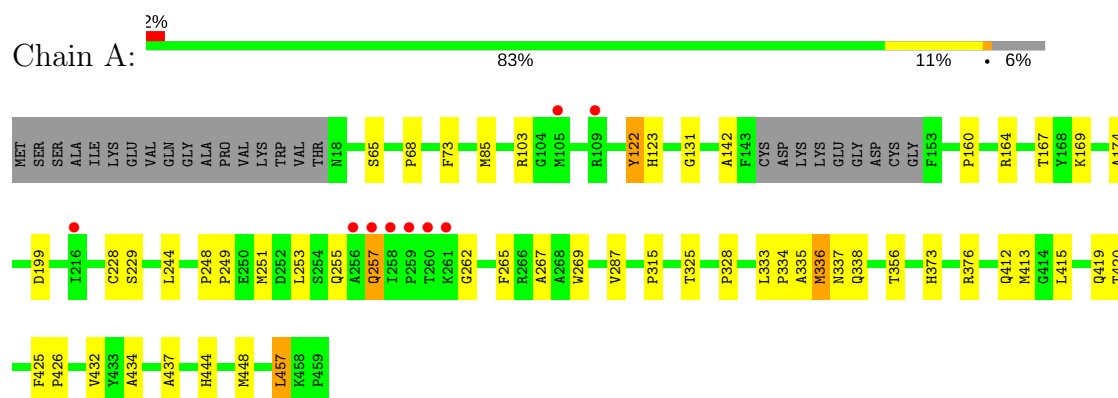
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	11	Total 11	O 11	0	0
6	K	20	Total 20	O 20	0	0
6	L	15	Total 15	O 15	0	0



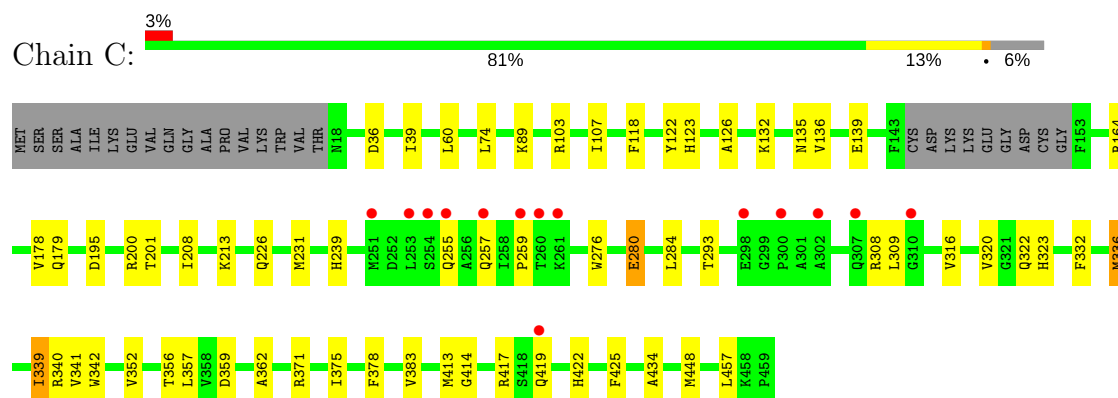
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

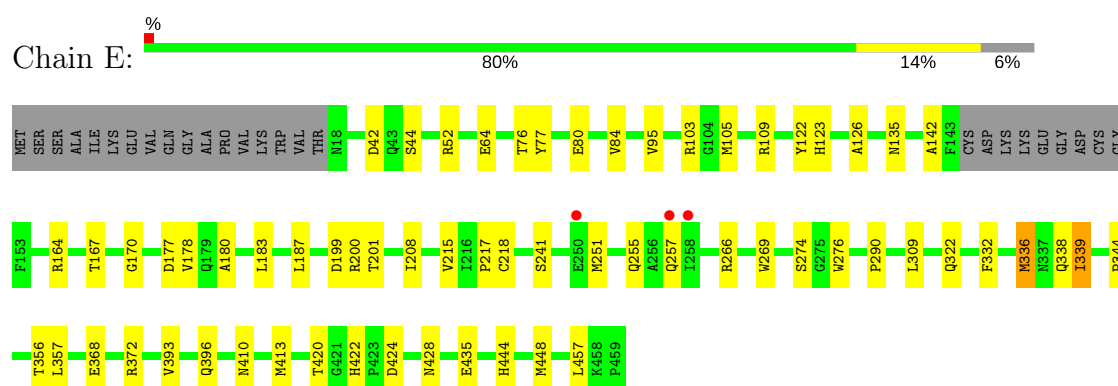
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



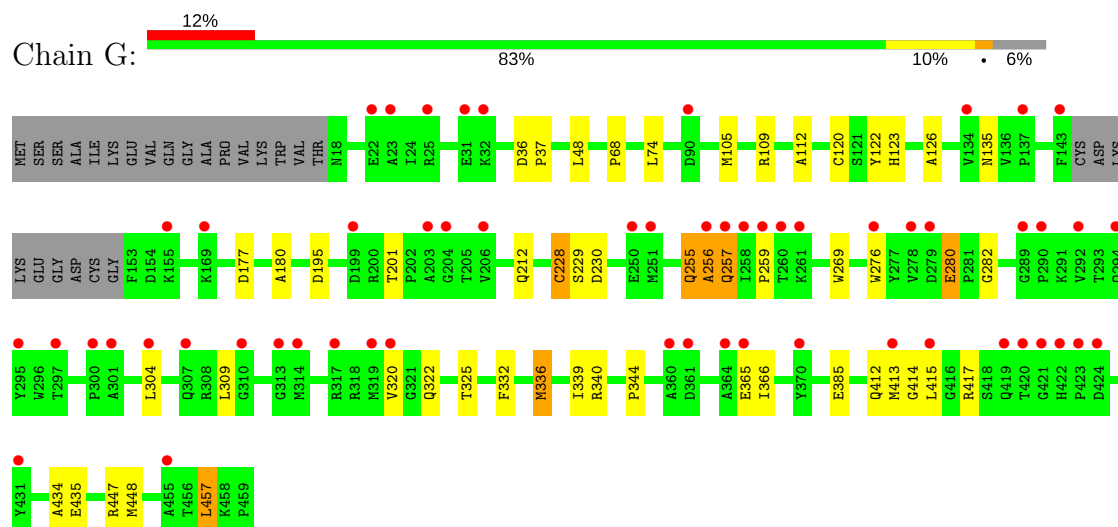
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



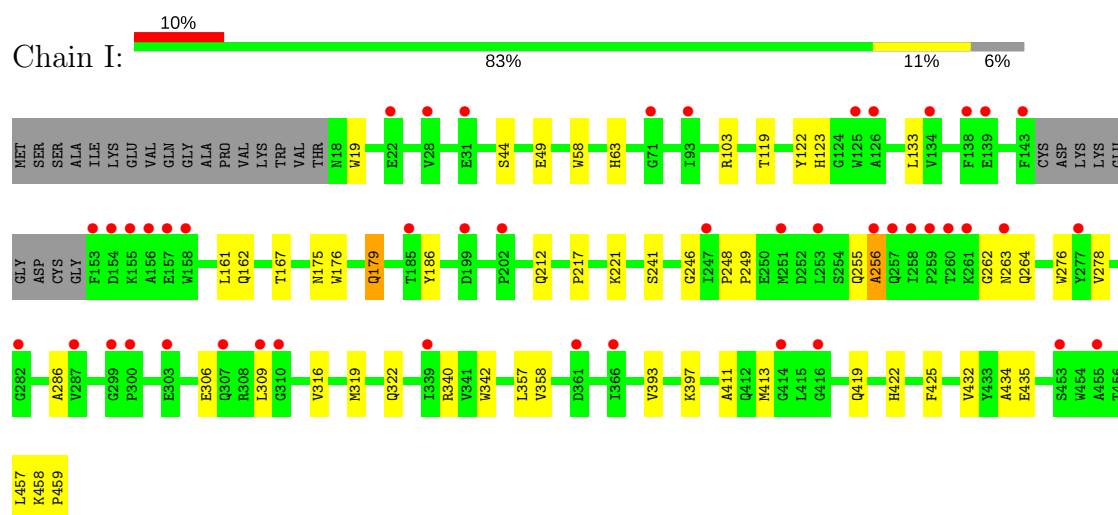
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



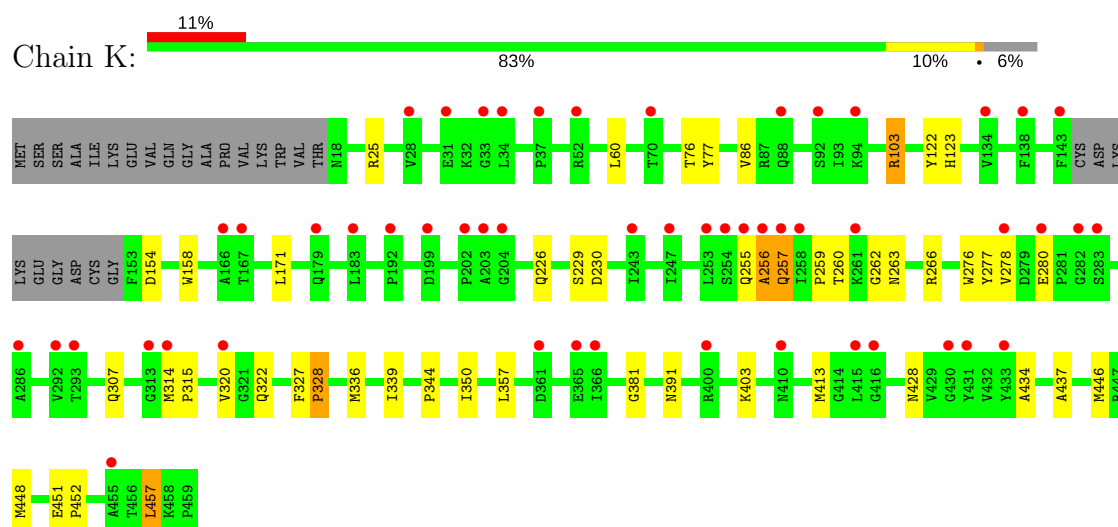
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



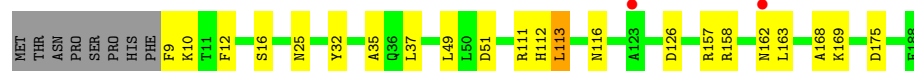
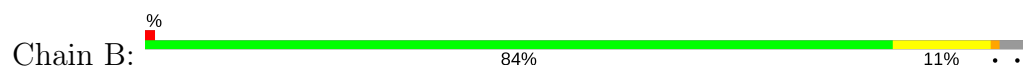
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



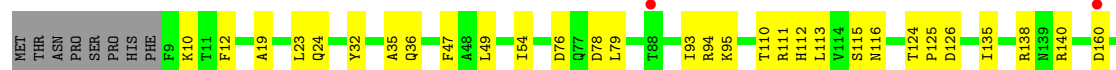
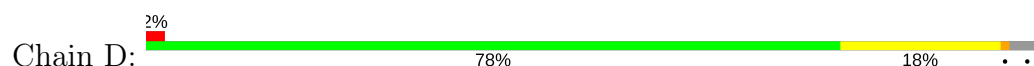
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



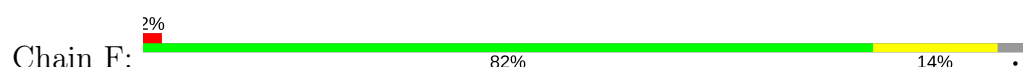
## ● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



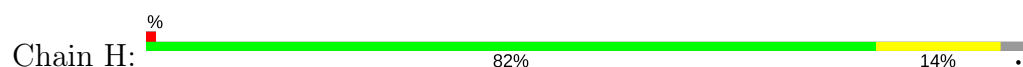
## ● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



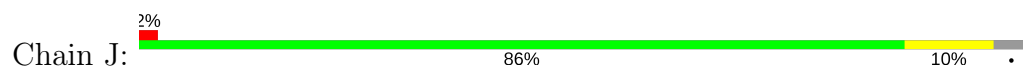
## ● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



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## ● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.56Å 275.98Å 92.06Å 90.00° 117.46° 90.00°	Depositor
Resolution (Å)	137.36 – 2.60 44.82 – 2.54	Depositor EDS
% Data completeness (in resolution range)	77.7 (137.36-2.60) 77.7 (44.82-2.54)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.280 0.217 , 0.281	Depositor DCC
$R_{free}$ test set	4854 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	29968	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: DC4, 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	0.35	0/3533	0.49	0/4796
1	C	0.34	0/3533	0.49	0/4796
1	E	0.36	0/3533	0.49	0/4796
1	G	0.33	0/3533	0.47	0/4796
1	I	0.32	0/3533	0.47	0/4796
1	K	0.33	0/3533	0.46	0/4796
2	B	0.36	0/1530	0.51	0/2068
2	D	0.35	0/1530	0.51	0/2068
2	F	0.37	0/1530	0.51	0/2068
2	H	0.34	0/1530	0.49	0/2068
2	J	0.33	0/1530	0.47	0/2068
2	L	0.34	0/1530	0.48	0/2068
All	All	0.34	0/30378	0.48	0/41184

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	3430	0	3274	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3430	0	3274	42	0
1	E	3430	0	3274	34	0
1	G	3430	0	3274	32	0
1	I	3430	0	3274	33	0
1	K	3430	0	3274	33	0
2	B	1496	0	1447	16	0
2	D	1496	0	1447	21	0
2	F	1496	0	1447	22	0
2	H	1496	0	1447	18	0
2	J	1496	0	1447	16	0
2	L	1496	0	1447	13	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	2	0
3	I	4	0	0	1	0
3	K	4	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	1	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
5	A	14	0	7	1	0
5	C	14	0	7	8	0
6	A	50	0	0	1	0
6	B	26	0	0	3	0
6	C	41	0	0	4	0
6	D	24	0	0	0	0
6	E	62	0	0	3	0
6	F	21	0	0	1	0
6	G	30	0	0	4	0
6	H	19	0	0	1	0
6	I	35	0	0	9	0
6	J	11	0	0	0	0
6	K	20	0	0	2	0
6	L	15	0	0	0	0
All	All	29968	0	28340	268	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 5.

All (268) 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:K:255:GLN:O	1:K:257:GLN:N	1.70	1.24
1:I:58:TRP:HA	6:I:2007:HOH:O	1.44	1.14
1:K:263:ASN:HA	6:K:2019:HOH:O	1.49	1.13
1:K:256:ALA:O	1:K:257:GLN:O	1.77	1.02
1:K:255:GLN:C	1:K:257:GLN:H	1.65	1.00
1:I:255:GLN:O	1:I:256:ALA:O	1.89	0.91
1:A:142:ALA:HB1	1:C:413:MET:HG3	1.53	0.90
1:C:378:PHE:HE1	5:C:1460:DC4:HAD	1.35	0.90
1:A:413:MET:HG3	1:E:142:ALA:HB1	1.57	0.85
1:G:259:PRO:HA	1:G:280:GLU:HG2	1.59	0.82
1:G:255:GLN:O	1:G:257:GLN:N	2.12	0.82
1:C:378:PHE:CE1	5:C:1460:DC4:HAD	2.15	0.80
1:I:264:GLN:HA	6:I:2021:HOH:O	1.85	0.77
2:J:180:LEU:HD11	2:L:145:VAL:HG21	1.67	0.76
1:K:255:GLN:C	1:K:257:GLN:N	2.30	0.74
1:G:126:ALA:HB3	1:G:135:ASN:HB3	1.69	0.74
1:G:255:GLN:C	1:G:257:GLN:H	1.92	0.73
1:C:226:GLN:O	5:C:1460:DC4:HAC	1.88	0.73
1:C:239:HIS:NE2	6:C:2027:HOH:O	2.22	0.72
3:G:900:FES:S2	6:G:2004:HOH:O	2.50	0.70
1:E:339:ILE:HD11	1:E:357:LEU:HG	1.76	0.68
1:G:256:ALA:O	1:G:257:GLN:O	2.13	0.67
1:I:123:HIS:HB2	3:I:900:FES:S2	2.35	0.67
1:G:414:GLY:HA2	1:G:417:ARG:HD2	1.76	0.66
1:A:413:MET:HG2	1:A:434:ALA:HA	1.77	0.66
1:G:413:MET:HG2	1:G:434:ALA:HA	1.79	0.65
1:G:123:HIS:HB2	3:G:900:FES:S2	2.35	0.65
1:C:339:ILE:HD11	1:C:357:LEU:HG	1.78	0.65
1:G:276:TRP:HB3	1:G:322:GLN:HG3	1.78	0.65
2:D:180:LEU:HD11	2:F:145:VAL:HG21	1.79	0.65
1:G:255:GLN:C	1:G:257:GLN:N	2.50	0.64
1:K:256:ALA:O	1:K:257:GLN:C	2.36	0.64
4:C:901:FE2:FE	6:C:2027:HOH:O	1.49	0.64
2:B:175:ASP:OD2	2:D:111:ARG:HB2	1.97	0.64
1:E:251:MET:HG3	1:E:255:GLN:HB2	1.80	0.64
2:J:49:LEU:HD21	2:J:163:LEU:HD13	1.79	0.63
1:I:413:MET:HG2	1:I:434:ALA:HA	1.79	0.63
1:G:366:ILE:HB	6:G:2021:HOH:O	1.98	0.62
1:E:266:ARG:HB3	1:E:428:ASN:ND2	2.14	0.62
1:A:287:VAL:HG21	5:A:1460:DC4:HAD	1.82	0.62
2:J:60:LEU:HD23	2:J:81:HIS:CE1	2.37	0.59
1:E:199:ASP:HB3	1:E:309:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:133:LEU:HG	6:I:2014:HOH:O	2.02	0.59
1:A:265:PHE:CZ	1:A:267:ALA:HA	2.38	0.59
1:G:448:MET:HA	1:G:457:LEU:HD11	1.85	0.58
1:G:195:ASP:HB3	1:G:309:LEU:HD22	1.84	0.58
1:A:123:HIS:HB2	3:A:900:FES:S2	2.44	0.58
2:H:49:LEU:HD21	2:H:163:LEU:HD13	1.84	0.58
2:B:113:LEU:HD13	2:F:135:ILE:HG13	1.85	0.58
1:I:309:LEU:HD13	1:I:316:VAL:HG11	1.84	0.58
1:C:309:LEU:HD13	1:C:316:VAL:HG11	1.87	0.57
1:G:447:ARG:HH21	1:G:457:LEU:HA	1.69	0.57
1:I:319:MET:HG2	6:I:2022:HOH:O	2.05	0.57
1:C:123:HIS:HB2	3:C:900:FES:S2	2.45	0.57
1:C:339:ILE:CD1	1:C:357:LEU:HG	2.34	0.57
1:G:120:CYS:SG	6:G:2004:HOH:O	2.58	0.56
2:H:25:ASN:HD21	2:L:24:GLN:HG2	1.71	0.56
1:C:413:MET:HG2	1:C:434:ALA:HA	1.88	0.56
1:I:262:GLY:HA2	1:I:278:VAL:HG23	1.87	0.55
1:G:212:GLN:HG2	2:H:60:LEU:HD21	1.88	0.55
2:H:12:PHE:H	2:J:36:GLN:HE21	1.55	0.55
2:D:54:ILE:HA	2:D:168:ALA:O	2.05	0.55
1:A:373:HIS:HD2	1:A:376:ARG:HE	1.54	0.55
2:H:116:ASN:HA	2:J:32:TYR:CD1	2.42	0.55
1:E:332:PHE:HB3	1:E:339:ILE:HG23	1.89	0.55
2:H:135:ILE:HD12	2:J:113:LEU:HD22	1.89	0.54
1:C:378:PHE:HE1	5:C:1460:DC4:CAD	2.15	0.54
1:K:123:HIS:HB2	3:K:900:FES:S2	2.48	0.54
2:H:68:GLU:HB3	2:H:71:LEU:HD12	1.89	0.54
1:C:448:MET:HG2	1:C:457:LEU:HD21	1.89	0.54
1:E:266:ARG:HB3	1:E:428:ASN:HD22	1.73	0.54
1:K:255:GLN:O	1:K:256:ALA:C	2.45	0.54
1:I:422:HIS:HB2	6:I:2033:HOH:O	2.09	0.53
1:C:414:GLY:HA2	1:C:417:ARG:HD2	1.90	0.53
1:C:231:MET:SD	5:C:1460:DC4:HAE	2.50	0.52
2:J:126:ASP:HB3	2:J:158:ARG:HB2	1.90	0.52
1:K:448:MET:HA	1:K:457:LEU:HD11	1.91	0.52
1:E:241:SER:HB2	2:F:95:LYS:HG3	1.92	0.52
2:D:24:GLN:HG2	2:F:25:ASN:HD21	1.75	0.52
1:I:241:SER:HB2	2:J:95:LYS:HG3	1.91	0.52
1:G:412:GLN:O	1:G:415:LEU:HB2	2.10	0.51
1:E:123:HIS:HB2	3:E:900:FES:S2	2.51	0.51
2:L:22:GLU:O	2:L:26:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:PHE:CE1	5:C:1460:DC4:CAD	2.90	0.51
2:D:12:PHE:H	2:F:36:GLN:NE2	2.08	0.51
2:H:126:ASP:O	2:H:157:ARG:HA	2.10	0.51
2:B:162:ASN:HB3	6:B:2020:HOH:O	2.10	0.51
1:G:201:THR:HG22	1:G:304:LEU:HD23	1.93	0.51
1:C:60:LEU:HD23	1:C:341:VAL:HG22	1.92	0.50
2:F:126:ASP:HB3	2:F:158:ARG:HB2	1.92	0.50
2:D:110:THR:HG22	2:D:138:ARG:HG2	1.92	0.50
2:F:110:THR:HA	2:F:137:TYR:O	2.11	0.50
1:A:122:TYR:OH	1:C:226:GLN:NE2	2.44	0.50
1:K:60:LEU:HD11	1:K:171:LEU:HD22	1.94	0.50
2:B:116:ASN:HA	2:D:32:TYR:CD1	2.47	0.49
1:C:422:HIS:HD2	1:C:425:PHE:H	1.59	0.49
1:C:340:ARG:HD2	1:C:342:TRP:CH2	2.48	0.49
2:J:180:LEU:HD11	2:L:145:VAL:CG2	2.42	0.49
1:C:276:TRP:HB3	1:C:322:GLN:HG3	1.94	0.49
1:E:126:ALA:HB3	1:E:135:ASN:HB3	1.94	0.49
1:C:257:GLN:HE21	1:C:259:PRO:N	2.10	0.48
1:A:169:LYS:HD3	1:A:199:ASP:HB2	1.95	0.48
2:H:150:GLY:HA2	2:H:175:ASP:OD2	2.13	0.48
1:G:228:CYS:HB2	1:G:325:THR:HB	1.95	0.48
1:E:52:ARG:HB3	1:E:448:MET:O	2.13	0.48
1:C:164:ARG:HD2	1:C:178:VAL:HA	1.94	0.48
1:K:344:PRO:HA	1:K:350:ILE:HG22	1.95	0.48
2:B:9:PHE:N	6:B:2001:HOH:O	2.45	0.48
1:E:200:ARG:HB2	6:E:2049:HOH:O	2.14	0.48
2:J:120:LYS:HB3	2:J:129:GLU:HB2	1.96	0.48
1:C:36:ASP:O	1:C:39:ILE:HG12	2.12	0.48
1:C:126:ALA:HB3	1:C:135:ASN:HB3	1.96	0.48
1:I:411:ALA:HA	1:I:435:GLU:OE1	2.14	0.48
2:J:81:HIS:CE1	2:J:179:LEU:HD11	2.49	0.48
1:G:344:PRO:HD3	6:G:2019:HOH:O	2.14	0.47
2:H:36:GLN:HE21	2:L:12:PHE:H	1.62	0.47
1:G:435:GLU:OE2	1:K:103:ARG:NH2	2.44	0.47
1:I:276:TRP:HB3	1:I:322:GLN:HG3	1.97	0.47
1:A:262:GLY:C	1:A:432:VAL:HB	2.33	0.47
1:C:419:GLN:HB2	6:C:2038:HOH:O	2.13	0.47
2:J:135:ILE:HD12	2:L:113:LEU:HD22	1.96	0.47
2:L:54:ILE:HA	2:L:168:ALA:O	2.15	0.47
1:C:359:ASP:HB2	1:C:362:ALA:HB2	1.95	0.47
2:J:118:ILE:HB	2:J:131:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:VAL:O	1:E:95:VAL:HA	2.15	0.47
1:G:177:ASP:HB3	1:G:180:ALA:HB2	1.96	0.47
1:E:164:ARG:HD2	1:E:178:VAL:HA	1.97	0.47
1:C:208:ILE:HD12	1:C:356:THR:OG1	2.15	0.47
1:I:58:TRP:HD1	1:I:186:TYR:CG	2.33	0.47
1:E:80:GLU:HG2	1:E:344:PRO:O	2.15	0.46
2:H:59:PRO:HD2	2:H:172:ILE:O	2.14	0.46
1:E:183:LEU:O	1:E:187:LEU:HG	2.15	0.46
2:B:25:ASN:HD21	2:F:24:GLN:HG2	1.81	0.46
2:L:31:TYR:HE2	2:L:130:VAL:HG11	1.80	0.46
1:E:208:ILE:HD12	1:E:356:THR:OG1	2.16	0.46
2:F:85:THR:O	2:F:89:MET:HG2	2.16	0.46
2:D:175:ASP:OD2	2:F:111:ARG:HB2	2.16	0.46
1:I:263:ASN:HB2	1:I:276:TRP:NE1	2.31	0.46
2:L:19:ALA:HB1	2:L:23:LEU:HD23	1.97	0.46
1:K:413:MET:HG2	1:K:434:ALA:HA	1.98	0.46
2:D:35:ALA:HB1	2:D:112:HIS:HB2	1.97	0.46
1:I:176:TRP:HB3	1:K:403:LYS:HE3	1.97	0.46
1:I:19:TRP:HE1	1:I:44:SER:HB2	1.81	0.46
2:L:179:LEU:HD21	2:L:184:LEU:HD11	1.98	0.46
2:B:35:ALA:HB1	2:B:112:HIS:HB2	1.97	0.46
1:C:371:ARG:HD2	2:D:78:ASP:O	2.15	0.46
1:I:49:GLU:OE2	1:I:221:LYS:NZ	2.44	0.46
1:I:217:PRO:HG2	1:I:393:VAL:HG22	1.98	0.45
1:K:229:SER:HB2	1:K:437:ALA:HB3	1.98	0.45
1:K:277:TYR:HB2	1:K:320:VAL:O	2.16	0.45
2:D:116:ASN:HA	2:F:32:TYR:CD1	2.52	0.45
1:A:131:GLY:O	1:A:160:PRO:HD2	2.16	0.45
1:C:332:PHE:HB3	1:C:339:ILE:HG23	1.98	0.45
2:D:116:ASN:HA	2:F:32:TYR:CG	2.51	0.45
1:C:195:ASP:HB3	1:C:309:LEU:HD21	1.99	0.45
1:E:290:PRO:HD2	6:E:2052:HOH:O	2.16	0.45
2:B:37:LEU:HD23	2:F:11:THR:HG21	1.99	0.45
1:E:215:VAL:O	2:F:182:ASN:HA	2.16	0.45
1:E:76:THR:OG1	1:E:77:TYR:N	2.49	0.45
1:I:422:HIS:HD2	1:I:425:PHE:H	1.65	0.45
2:D:49:LEU:HD21	2:D:163:LEU:HD13	1.98	0.45
2:H:36:GLN:NE2	2:L:12:PHE:H	2.15	0.45
2:B:49:LEU:HD21	2:B:163:LEU:HD13	1.99	0.45
1:E:217:PRO:HG2	1:E:393:VAL:HG22	1.99	0.45
2:F:138:ARG:NH2	2:F:181:SER:OG	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:246:GLY:HA3	1:I:286:ALA:O	2.17	0.45
2:J:116:ASN:HA	2:L:32:TYR:CD1	2.52	0.45
1:A:229:SER:HB2	1:A:437:ALA:HB3	1.99	0.45
1:K:262:GLY:HA2	1:K:278:VAL:HG23	1.98	0.45
1:G:280:GLU:H	1:G:320:VAL:HG21	1.82	0.44
1:E:422:HIS:CD2	1:E:424:ASP:H	2.36	0.44
1:A:164:ARG:O	1:A:174:ALA:HA	2.18	0.44
1:I:162:GLN:HG2	6:I:2018:HOH:O	2.18	0.44
2:B:12:PHE:H	2:D:36:GLN:NE2	2.16	0.44
2:D:19:ALA:HB1	2:D:23:LEU:HD23	1.99	0.44
2:D:135:ILE:HD12	2:F:113:LEU:HD22	2.00	0.44
2:B:126:ASP:HB3	2:B:158:ARG:HB2	1.99	0.43
1:E:339:ILE:CD1	1:E:357:LEU:HG	2.45	0.43
1:I:179:GLN:HA	1:I:179:GLN:HE21	1.82	0.43
1:C:257:GLN:HE21	1:C:259:PRO:CA	2.31	0.43
1:K:154:ASP:O	1:K:158:TRP:HD1	2.01	0.43
2:B:32:TYR:CD1	2:F:116:ASN:HA	2.54	0.43
1:C:213:LYS:HA	1:C:352:VAL:O	2.18	0.43
1:G:336:MET:H	1:G:336:MET:HG2	1.56	0.43
2:H:12:PHE:H	2:J:36:GLN:NE2	2.16	0.43
1:K:381:GLY:HA3	2:L:184:LEU:HB2	2.00	0.43
1:K:259:PRO:HA	1:K:280:GLU:HG2	2.01	0.43
1:K:76:THR:OG1	1:K:77:TYR:N	2.51	0.43
1:A:425:PHE:HA	1:A:426:PRO:HD3	1.86	0.43
1:C:280:GLU:H	1:C:320:VAL:HG21	1.84	0.43
2:D:47:PHE:HB2	2:D:93:ILE:HG13	2.00	0.43
1:G:269:TRP:HZ2	1:G:457:LEU:HD22	1.84	0.43
1:I:262:GLY:C	1:I:432:VAL:HB	2.39	0.43
1:A:335:ALA:HB3	1:A:336:MET:HE1	2.00	0.43
1:E:368:GLU:HG3	1:E:372:ARG:HE	1.84	0.43
2:H:116:ASN:HA	2:J:32:TYR:CG	2.54	0.42
1:K:266:ARG:HB3	1:K:428:ASN:HB3	2.00	0.42
1:K:339:ILE:HD13	1:K:357:LEU:HG	2.01	0.42
1:A:228:CYS:HB2	1:A:325:THR:HB	2.00	0.42
1:A:73:PHE:HA	1:A:85:MET:O	2.19	0.42
1:A:373:HIS:CD2	1:A:376:ARG:HE	2.37	0.42
2:B:16:SER:HA	6:B:2003:HOH:O	2.19	0.42
2:D:113:LEU:HD23	2:F:113:LEU:CD2	2.49	0.42
1:I:248:PRO:HA	1:I:249:PRO:HD3	1.85	0.42
1:C:383:VAL:HB	2:D:95:LYS:HD3	2.01	0.42
1:G:332:PHE:HB3	1:G:339:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:161:LEU:HD21	1:K:403:LYS:HD2	2.01	0.42
1:A:251:MET:HG3	1:A:255:GLN:HB2	2.01	0.42
1:A:412:GLN:O	1:A:415:LEU:HB2	2.18	0.42
1:K:451:GLU:HA	1:K:452:PRO:HD3	1.88	0.42
1:G:340:ARG:HH12	1:G:385:GLU:CD	2.23	0.42
2:H:60:LEU:HG	2:H:80:ALA:HA	2.02	0.42
2:H:104:GLU:HG2	2:H:185:SER:HB2	2.01	0.42
1:A:269:TRP:CZ2	1:A:444:HIS:HE1	2.37	0.42
1:A:333:LEU:HD12	1:A:338:GLN:HB3	2.02	0.42
1:E:276:TRP:HB3	1:E:322:GLN:HG3	2.01	0.42
2:F:58:MET:HG3	2:F:172:ILE:HB	2.01	0.42
1:I:340:ARG:HD3	1:I:342:TRP:CH2	2.55	0.42
1:A:334:PRO:O	1:A:337:ASN:OD1	2.37	0.41
1:K:391:ASN:HD22	1:K:391:ASN:HA	1.64	0.41
1:C:323:HIS:CD2	5:C:1460:DC4:HAB	2.55	0.41
2:F:161:ASN:HB2	6:F:2018:HOH:O	2.19	0.41
1:G:105:MET:HE2	1:G:109:ARG:HD2	2.01	0.41
2:B:168:ALA:O	2:B:169:LYS:HG2	2.21	0.41
1:E:336:MET:H	1:E:336:MET:HG2	1.60	0.41
1:G:36:ASP:HA	1:G:37:PRO:HD3	1.89	0.41
1:E:177:ASP:HB3	1:E:180:ALA:HB2	2.02	0.41
1:I:306:GLU:C	6:I:2025:HOH:O	2.58	0.41
2:B:111:ARG:HB2	2:F:175:ASP:OD2	2.21	0.41
2:B:51:ASP:OD2	2:B:157:ARG:NH1	2.53	0.41
2:H:54:ILE:HA	2:H:168:ALA:O	2.20	0.41
1:I:212:GLN:HB2	1:I:212:GLN:HE21	1.62	0.41
1:I:397:LYS:NZ	6:I:2031:HOH:O	2.51	0.41
1:I:458:LYS:HA	1:I:459:PRO:HD3	1.92	0.41
1:C:257:GLN:HE21	1:C:259:PRO:HA	1.85	0.41
1:C:284:LEU:HD23	1:C:293:THR:HG23	2.02	0.41
1:E:257:GLN:HG2	6:E:2040:HOH:O	2.20	0.41
1:G:230:ASP:OD2	1:K:123:HIS:NE2	2.45	0.41
1:K:314:MET:HA	1:K:315:PRO:HD3	1.92	0.41
1:A:244:LEU:HD13	1:A:253:LEU:HG	2.03	0.41
1:I:175:ASN:HB2	6:I:2007:HOH:O	2.21	0.41
1:K:307:GLN:HB3	6:K:2014:HOH:O	2.20	0.41
1:A:248:PRO:HA	1:A:249:PRO:HD2	1.86	0.41
5:C:1460:DC4:CAH	6:C:2027:HOH:O	2.69	0.41
1:C:375:ILE:HD11	2:D:79:LEU:HA	2.02	0.41
2:D:125:PRO:O	2:D:126:ASP:HB2	2.20	0.41
1:E:218:CYS:HA	1:E:396:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:VAL:O	1:C:139:GLU:HB2	2.21	0.41
1:C:336:MET:HG2	1:C:336:MET:H	1.56	0.41
1:E:413:MET:HB2	1:E:435:GLU:OE1	2.21	0.41
1:E:42:ASP:OD2	1:E:44:SER:HB2	2.21	0.41
1:I:63:HIS:CD2	1:I:357:LEU:HD21	2.56	0.41
1:E:269:TRP:CZ2	1:E:444:HIS:HE1	2.40	0.40
1:G:105:MET:CE	1:G:109:ARG:HD2	2.50	0.40
1:K:276:TRP:HB3	1:K:322:GLN:HG3	2.02	0.40
1:C:107:ILE:HG22	1:C:118:PHE:HB3	2.03	0.40
1:E:105:MET:CE	1:E:109:ARG:HD2	2.51	0.40
2:F:58:MET:HA	2:F:59:PRO:HD2	1.98	0.40
1:A:257:GLN:HG2	6:A:2034:HOH:O	2.21	0.40
1:A:65:SER:O	1:A:68:PRO:HG3	2.22	0.40
2:H:161:ASN:HB3	6:H:2018:HOH:O	2.21	0.40
1:K:226:GLN:HA	1:K:230:ASP:CB	2.52	0.40
1:K:25:ARG:HG2	1:K:446:MET:SD	2.61	0.40
1:A:448:MET:HA	1:A:457:LEU:HD11	2.04	0.40
1:K:327:PHE:HA	1:K:328:PRO:HA	1.92	0.40
1:C:200:ARG:O	1:C:308:ARG:HD3	2.21	0.40
1:E:64:GLU:HG3	1:E:170:GLY:O	2.21	0.40
1:G:74:LEU:HD12	1:G:112:ALA:HB2	2.03	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%)	405 (94%)	23 (5%)	1 (0%)	51	76
1	C	429/459 (94%)	404 (94%)	25 (6%)	0	100	100
1	E	429/459 (94%)	409 (95%)	20 (5%)	0	100	100
1	G	429/459 (94%)	399 (93%)	25 (6%)	5 (1%)	15	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	429/459 (94%)	400 (93%)	28 (6%)	1 (0%)	51	76
1	K	429/459 (94%)	394 (92%)	32 (8%)	3 (1%)	25	49
2	B	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
2	D	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
2	F	178/188 (95%)	168 (94%)	10 (6%)	0	100	100
2	H	178/188 (95%)	168 (94%)	10 (6%)	0	100	100
2	J	178/188 (95%)	169 (95%)	9 (5%)	0	100	100
2	L	178/188 (95%)	167 (94%)	11 (6%)	0	100	100
All	All	3642/3882 (94%)	3425 (94%)	207 (6%)	10 (0%)	44	70

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	256	ALA
1	G	257	GLN
1	I	256	ALA
1	K	256	ALA
1	K	257	GLN
1	G	255	GLN
1	G	68	PRO
1	G	282	GLY
1	A	328	PRO
1	K	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	350/372 (94%)	340 (97%)	10 (3%)	48	75
1	C	350/372 (94%)	339 (97%)	11 (3%)	45	73
1	E	350/372 (94%)	339 (97%)	11 (3%)	45	73
1	G	350/372 (94%)	342 (98%)	8 (2%)	56	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	350/372 (94%)	342 (98%)	8 (2%)	56	81
1	K	350/372 (94%)	344 (98%)	6 (2%)	66	86
2	B	159/167 (95%)	157 (99%)	2 (1%)	73	90
2	D	159/167 (95%)	151 (95%)	8 (5%)	28	53
2	F	159/167 (95%)	158 (99%)	1 (1%)	89	96
2	H	159/167 (95%)	155 (98%)	4 (2%)	53	79
2	J	159/167 (95%)	158 (99%)	1 (1%)	89	96
2	L	159/167 (95%)	157 (99%)	2 (1%)	73	90
All	All	3054/3234 (94%)	2982 (98%)	72 (2%)	54	80

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	122	TYR
1	A	167	THR
1	A	257	GLN
1	A	315	PRO
1	A	336	MET
1	A	356	THR
1	A	419	GLN
1	A	420	THR
1	A	457	LEU
2	B	10	LYS
2	B	113	LEU
1	C	74	LEU
1	C	89	LYS
1	C	103	ARG
1	C	122	TYR
1	C	132	LYS
1	C	179	GLN
1	C	201	THR
1	C	255	GLN
1	C	280	GLU
1	C	336	MET
1	C	339	ILE
2	D	10	LYS
2	D	76	ASP
2	D	94	ARG

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Mol	Chain	Res	Type
2	D	115	SER
2	D	124	THR
2	D	140	ARG
2	D	160	ASP
2	D	180	LEU
1	E	103	ARG
1	E	122	TYR
1	E	167	THR
1	E	201	THR
1	E	274	SER
1	E	336	MET
1	E	338	GLN
1	E	339	ILE
1	E	410	ASN
1	E	420	THR
1	E	457	LEU
2	F	140	ARG
1	G	48	LEU
1	G	122	TYR
1	G	228	CYS
1	G	229	SER
1	G	280	GLU
1	G	336	MET
1	G	365	GLU
1	G	457	LEU
2	H	10	LYS
2	H	70	GLU
2	H	140	ARG
2	H	179	LEU
1	I	103	ARG
1	I	119	THR
1	I	122	TYR
1	I	167	THR
1	I	179	GLN
1	I	358	VAL
1	I	419	GLN
1	I	457	LEU
2	J	10	LYS
1	K	86	VAL
1	K	103	ARG
1	K	122	TYR
1	K	260	THR

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Mol	Chain	Res	Type
1	K	336	MET
1	K	457	LEU
2	L	67	ARG
2	L	113	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	226	GLN
1	A	263	ASN
1	A	373	HIS
1	A	391	ASN
1	A	410	ASN
1	A	444	HIS
2	B	25	ASN
2	B	36	GLN
2	B	77	GLN
2	B	131	ASN
1	C	179	GLN
1	C	212	GLN
1	C	226	GLN
1	C	257	GLN
1	C	373	HIS
1	C	391	ASN
1	C	410	ASN
1	C	422	HIS
2	D	25	ASN
2	D	36	GLN
2	D	81	HIS
2	D	131	ASN
1	E	179	GLN
1	E	212	GLN
1	E	226	GLN
1	E	338	GLN
1	E	373	HIS
1	E	391	ASN
1	E	410	ASN
1	E	422	HIS
1	E	428	ASN
1	E	444	HIS
2	F	25	ASN

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Mol	Chain	Res	Type
2	F	36	GLN
2	F	131	ASN
1	G	212	GLN
1	G	226	GLN
1	G	419	GLN
1	G	444	HIS
2	H	25	ASN
2	H	36	GLN
2	H	131	ASN
1	I	179	GLN
1	I	212	GLN
1	I	419	GLN
1	I	422	HIS
1	I	444	HIS
2	J	25	ASN
2	J	36	GLN
2	J	131	ASN
1	K	307	GLN
1	K	343	HIS
1	K	348	ASN
1	K	391	ASN
1	K	396	GLN
1	K	410	ASN
2	L	25	ASN
2	L	36	GLN
2	L	131	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\# Z  > 2$
5	DC4	A	1460	-	10,16,16	1.24	1 (10%)	13,23,23	0.70	0
3	FES	A	900	1	0,4,4	0.00	-	0,4,4	0.00	-
5	DC4	C	1460	-	10,16,16	1.26	1 (10%)	13,23,23	1.00	0
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	1,6	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	-

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
5	DC4	A	1460	-	-	0/0/0/0	0/2/3/3
3	FES	A	900	1	-	0/0/4/4	0/1/1/1
5	DC4	C	1460	-	-	0/0/0/0	0/2/3/3
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	1,6	-	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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1460	DC4	CAM-CAN	-2.47	1.38	1.45
5	A	1460	DC4	CAM-CAN	-2.09	1.39	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1460	DC4	1	0
3	A	900	FES	1	0
5	C	1460	DC4	8	0
3	C	900	FES	1	0
3	E	900	FES	1	0
3	G	900	FES	2	0
3	I	900	FES	1	0
3	K	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%)	-0.17	9 (2%) 64 58	35, 49, 66, 74	18 (4%)
1	C	433/459 (94%)	-0.08	14 (3%) 48 40	37, 56, 79, 88	18 (4%)
1	E	433/459 (94%)	-0.10	3 (0%) 87 85	36, 52, 72, 81	18 (4%)
1	G	433/459 (94%)	0.65	57 (13%) 4 2	50, 94, 141, 163	18 (4%)
1	I	433/459 (94%)	0.63	46 (10%) 7 4	53, 94, 140, 162	18 (4%)
1	K	433/459 (94%)	0.71	52 (12%) 5 3	56, 95, 137, 156	18 (4%)
2	B	180/188 (95%)	-0.20	2 (1%) 80 77	32, 46, 61, 68	4 (2%)
2	D	180/188 (95%)	-0.15	3 (1%) 70 65	34, 49, 62, 70	4 (2%)
2	F	180/188 (95%)	-0.09	3 (1%) 70 65	35, 48, 67, 74	4 (2%)
2	H	180/188 (95%)	-0.11	1 (0%) 89 88	43, 62, 84, 95	4 (2%)
2	J	180/188 (95%)	0.02	4 (2%) 62 56	40, 64, 84, 94	4 (2%)
2	L	180/188 (95%)	-0.09	2 (1%) 80 77	41, 61, 81, 91	4 (2%)
All	All	3678/3882 (94%)	0.16	196 (5%) 27 20	32, 62, 121, 163	132 (3%)

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	361	ASP	8.9
1	K	258	ILE	8.4
1	G	292	VAL	6.5
1	K	199	ASP	6.0
1	K	34	LEU	5.5
1	I	157	GLU	5.5
1	G	259	PRO	5.4
1	G	256	ALA	5.4
1	I	300	PRO	5.2
1	K	257	GLN	5.2
1	G	143	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	I	257	GLN	5.0
1	K	243	ILE	4.9
1	K	320	VAL	4.8
1	I	158	TRP	4.8
1	I	251	MET	4.7
1	G	257	GLN	4.7
1	G	31	GLU	4.5
1	G	422	HIS	4.4
1	G	423	PRO	4.3
1	I	253	LEU	4.3
1	I	416	GLY	4.2
1	G	260	THR	4.2
1	G	22	GLU	4.2
1	K	94	LYS	4.2
1	I	455	ALA	4.1
1	C	260	THR	4.0
1	G	294	GLN	4.0
1	K	416	GLY	3.8
1	G	300	PRO	3.8
1	I	282	GLY	3.8
1	K	433	TYR	3.7
1	I	143	PHE	3.7
1	I	154	ASP	3.6
1	I	153	PHE	3.6
1	K	202	PRO	3.6
1	K	361	ASP	3.5
1	K	31	GLU	3.5
1	K	192	PRO	3.5
1	E	250	GLU	3.5
1	K	278	VAL	3.5
1	G	415	LEU	3.5
1	K	286	ALA	3.4
1	G	314	MET	3.4
1	G	370	TYR	3.4
2	B	123	ALA	3.4
1	I	93	ILE	3.4
1	G	364	ALA	3.3
1	I	155	LYS	3.3
1	E	257	GLN	3.3
1	G	251	MET	3.3
1	G	455	ALA	3.2
1	K	283	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	289	GLY	3.2
2	J	16	SER	3.2
1	K	256	ALA	3.2
1	I	256	ALA	3.1
1	A	105	MET	3.1
1	E	258	ILE	3.1
1	I	258	ILE	3.1
1	K	415	LEU	3.0
1	G	313	GLY	3.0
1	G	278	VAL	3.0
1	G	250	GLU	3.0
1	I	366	ILE	3.0
1	G	261	LYS	3.0
1	G	204	GLY	3.0
1	K	410	ASN	3.0
1	I	125	TRP	2.9
1	K	255	GLN	2.9
2	F	52	LYS	2.9
1	G	420	THR	2.9
1	K	293	THR	2.9
1	G	25	ARG	2.9
1	G	295	TYR	2.9
1	K	431	TYR	2.9
2	D	160	ASP	2.9
1	G	424	ASP	2.9
1	G	307	GLN	2.9
1	I	261	LYS	2.8
1	K	203	ALA	2.8
1	C	259	PRO	2.8
1	I	310	GLY	2.8
1	G	360	ALA	2.8
1	C	298	GLU	2.8
1	K	88	GLN	2.7
1	G	290	PRO	2.7
1	C	254	SER	2.7
1	K	166	ALA	2.7
1	C	310	GLY	2.7
2	L	67	ARG	2.7
1	C	300	PRO	2.7
1	G	320	VAL	2.7
1	G	32	LYS	2.7
1	K	261	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	261	LYS	2.7
1	K	313	GLY	2.7
1	G	206	VAL	2.6
2	D	188	PHE	2.6
1	A	259	PRO	2.6
2	L	52	LYS	2.6
1	G	419	GLN	2.6
1	G	297	THR	2.6
1	K	455	ALA	2.6
1	I	134	VAL	2.6
1	G	199	ASP	2.5
1	G	319	MET	2.5
1	G	134	VAL	2.5
1	I	202	PRO	2.5
1	G	304	LEU	2.5
1	G	317	ARG	2.5
1	G	421	GLY	2.5
1	K	430	GLY	2.5
1	G	279	ASP	2.5
1	I	339	ILE	2.5
1	K	292	VAL	2.5
1	I	277	TYR	2.5
1	I	71	GLY	2.5
1	G	169	LYS	2.5
1	G	276	TRP	2.5
1	C	257	GLN	2.4
1	C	302	ALA	2.4
1	G	203	ALA	2.4
1	C	251	MET	2.4
1	K	280	GLU	2.4
1	I	263	ASN	2.4
1	K	204	GLY	2.4
1	K	282	GLY	2.4
2	J	71	LEU	2.4
1	G	365	GLU	2.4
1	I	22	GLU	2.4
1	I	361	ASP	2.4
2	B	162	ASN	2.4
1	I	259	PRO	2.4
1	A	258	ILE	2.4
1	K	254	SER	2.4
1	K	138	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	310	GLY	2.4
1	G	258	ILE	2.4
1	I	303	GLU	2.4
1	K	143	PHE	2.3
1	I	31	GLU	2.3
2	D	88	THR	2.3
1	G	431	TYR	2.3
1	I	156	ALA	2.3
1	K	366	ILE	2.3
1	G	301	ALA	2.3
2	F	123	ALA	2.3
1	I	126	ALA	2.3
1	K	365	GLU	2.3
1	G	155	LYS	2.3
1	I	138	PHE	2.3
1	I	247	ILE	2.3
1	C	255	GLN	2.2
1	K	400	ARG	2.2
2	J	123	ALA	2.2
1	K	183	LEU	2.2
1	K	33	GLY	2.2
1	I	28	VAL	2.2
1	K	52	ARG	2.2
1	I	309	LEU	2.2
1	I	199	ASP	2.2
1	I	260	THR	2.2
1	K	247	ILE	2.2
1	G	137	PRO	2.2
2	J	51	ASP	2.2
1	I	307	GLN	2.2
1	A	260	THR	2.2
1	I	453	SER	2.1
1	K	28	VAL	2.1
1	I	414	GLY	2.1
1	C	419	GLN	2.1
1	G	90	ASP	2.1
1	A	256	ALA	2.1
1	G	23	ALA	2.1
1	K	70	THR	2.1
1	K	167	THR	2.1
1	K	179	GLN	2.1
1	I	299	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	287	VAL	2.1
1	K	134	VAL	2.1
1	G	413	MET	2.1
1	C	261	LYS	2.1
1	A	109	ARG	2.1
2	H	67	ARG	2.0
1	K	314	MET	2.0
2	F	122	THR	2.0
1	C	307	GLN	2.0
1	K	253	LEU	2.0
1	K	92	SER	2.0
1	A	257	GLN	2.0
1	C	253	LEU	2.0
1	K	37	PRO	2.0
1	A	216	ILE	2.0
1	I	185	THR	2.0
1	I	139	GLU	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
5	DC4	C	1460	14/14	0.72	0.61	16.84	53,53,53,53	14
5	DC4	A	1460	14/14	0.86	0.40	6.17	49,49,49,49	14
3	FES	E	900	4/4	0.97	0.12	-0.39	40,40,41,41	0
3	FES	A	900	4/4	0.98	0.13	-0.49	46,46,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FE2	I	901	1/1	0.97	0.13	-0.93	67,67,67,67	0
3	FES	C	900	4/4	0.98	0.11	-0.98	46,49,49,50	0
3	FES	K	900	4/4	0.96	0.12	-1.04	71,72,72,72	0
4	FE2	E	901	1/1	1.00	0.14	-1.14	41,41,41,41	0
3	FES	I	900	4/4	0.96	0.10	-1.63	76,76,76,77	0
3	FES	G	900	4/4	0.98	0.07	-2.03	65,67,68,68	0
4	FE2	A	901	1/1	0.99	0.13	-	40,40,40,40	0
4	FE2	K	901	1/1	0.97	0.12	-	76,76,76,76	0
4	FE2	G	901	1/1	0.99	0.15	-	89,89,89,89	0
4	FE2	C	901	1/1	0.99	0.16	-	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.