



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:38 am GMT

PDB ID : 2YFJ  
Title : CRYSTAL STRUCTURE OF BIPHENYL DIOXYGENASE VARIANT RR41  
WITH DIBENZOFURAN  
Authors : Kumar, P.; Sylvestre, M.; Bolin, J.T.  
Deposited on : 2011-04-06  
Resolution : 2.15 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

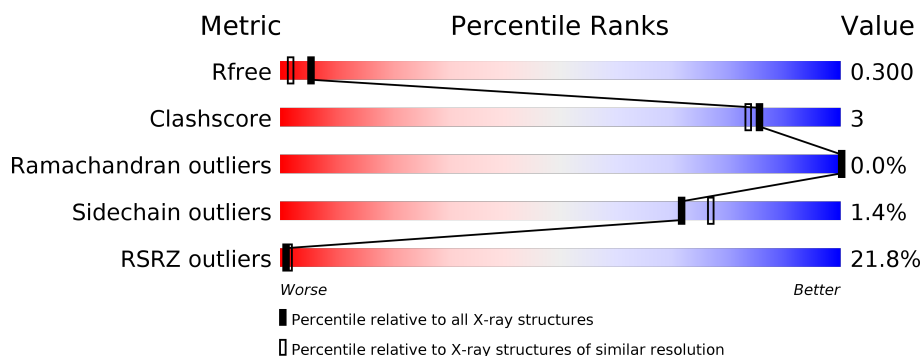
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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>19%</div> <div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>
1	C	459	<div> <div>15%</div> <div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>
1	E	459	<div> <div>13%</div> <div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	G	459	<div> <div>32%</div> <div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	I	459	<div> <div>31%</div> <div> <div>87%</div> <div>8%</div> <div>6%</div> </div> </div>
1	K	459	<div> <div>36%</div> <div> <div>89%</div> <div>5%</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
5	1IT	E	1451	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30277 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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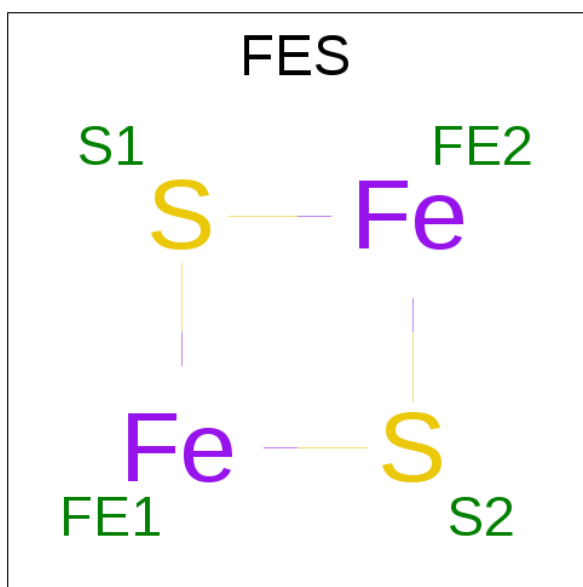
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Chain	Residue	Modelled	Actual	Comment	Reference
G	338	GLN	ASN	ENGINEERED MUTATION	UNP P37333
G	341	VAL	ILE	ENGINEERED MUTATION	UNP P37333
G	409	PHE	LEU	ENGINEERED MUTATION	UNP P37333
I	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
I	336	MET	PHE	ENGINEERED 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>).

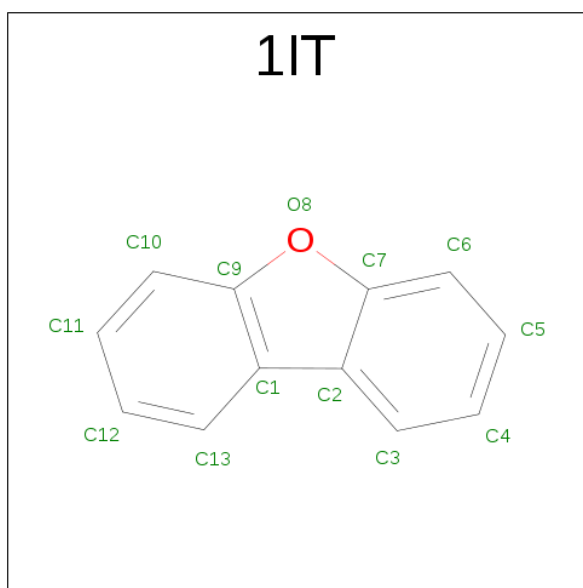


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		

- 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 DIBENZOFURAN (three-letter code: 1IT) (formula: C<sub>12</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	12	1		
5	C	1	Total	C	O	0	0
			13	12	1		
5	E	1	Total	C	O	0	0
			13	12	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	53	Total	O	0	0
			53	53		
6	C	129	Total	O	0	0
			129	129		
6	D	66	Total	O	0	0
			66	66		
6	E	88	Total	O	0	0
			88	88		
6	F	46	Total	O	0	0
			46	46		
6	G	23	Total	O	0	0
			23	23		
6	H	19	Total	O	0	0
			19	19		

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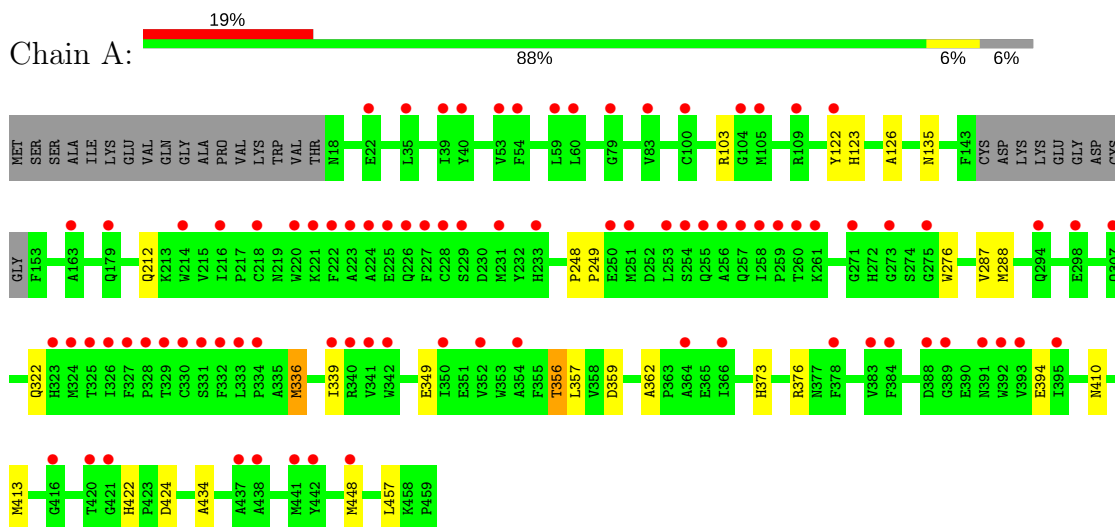
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	29	Total 29	O 29	0	0
6	J	31	Total 31	O 31	0	0
6	K	23	Total 23	O 23	0	0
6	L	17	Total 17	O 17	0	0



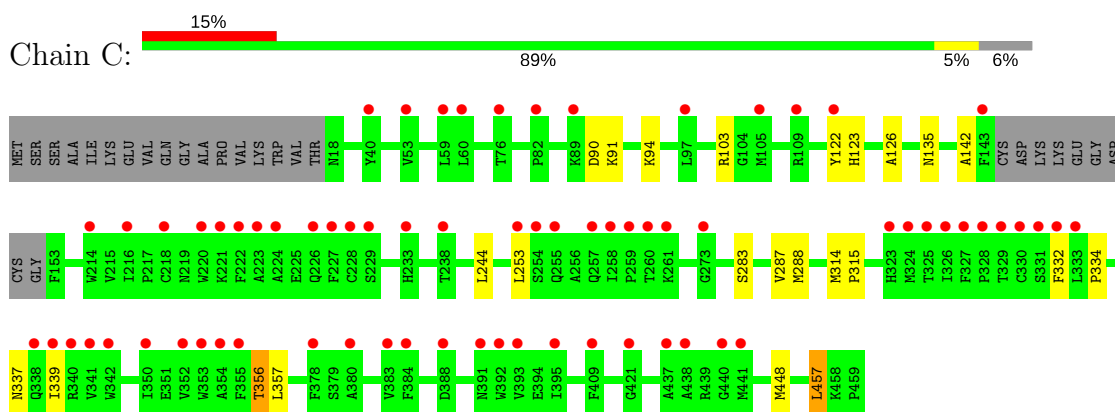
### 3 Residue-property plots

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

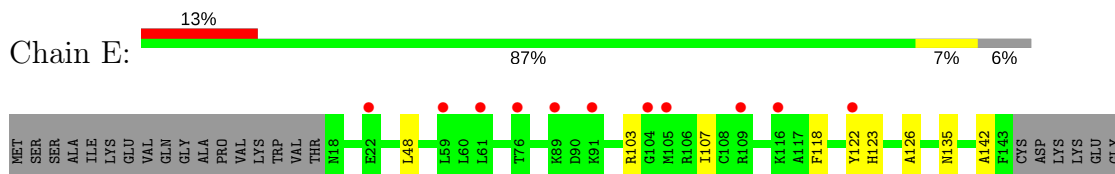
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

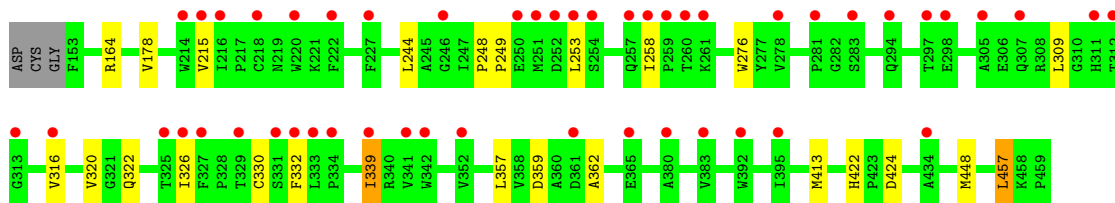


#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



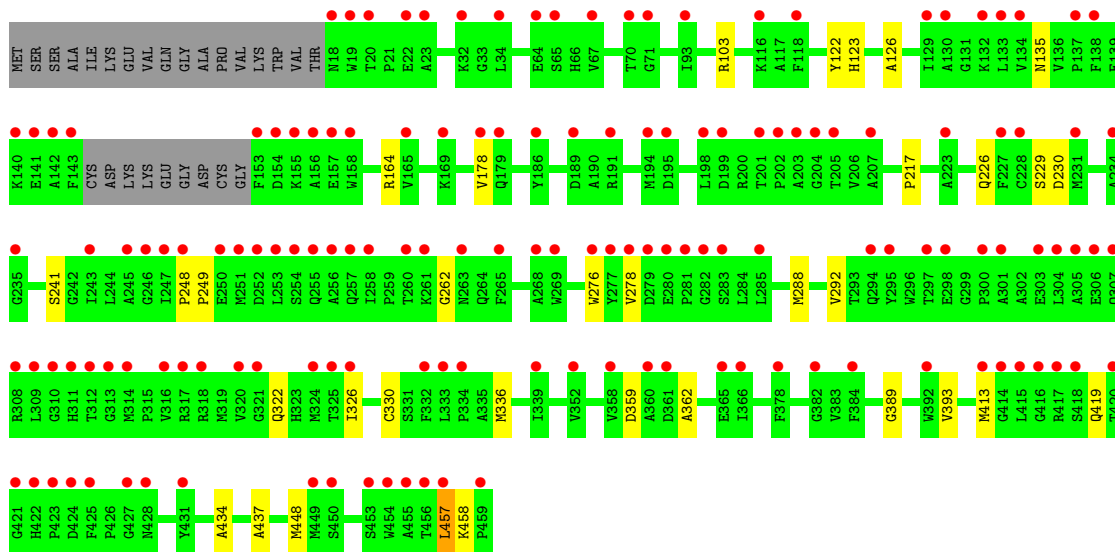
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA





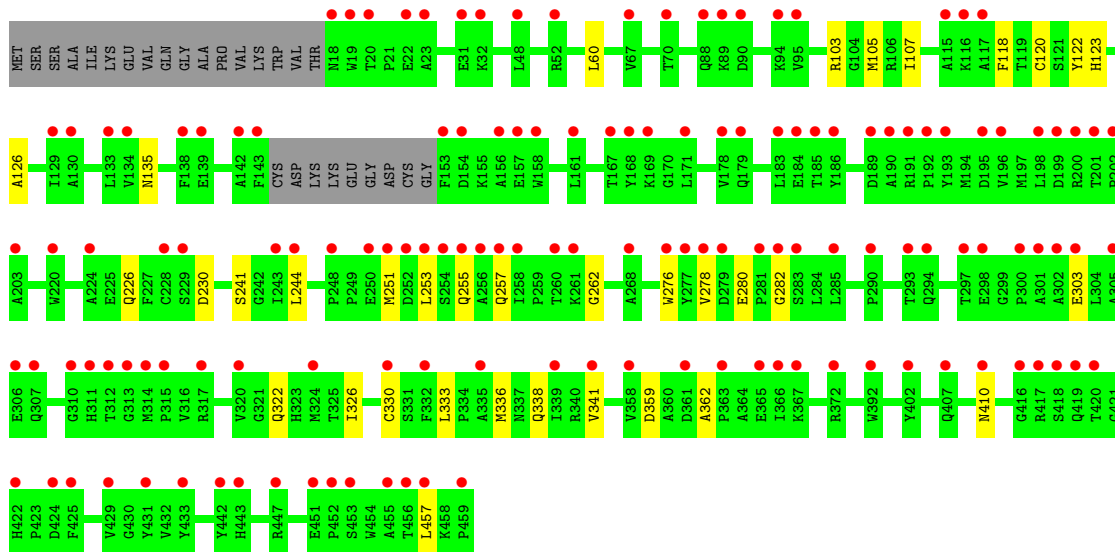
● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain G: 32% 87% 7% 6%



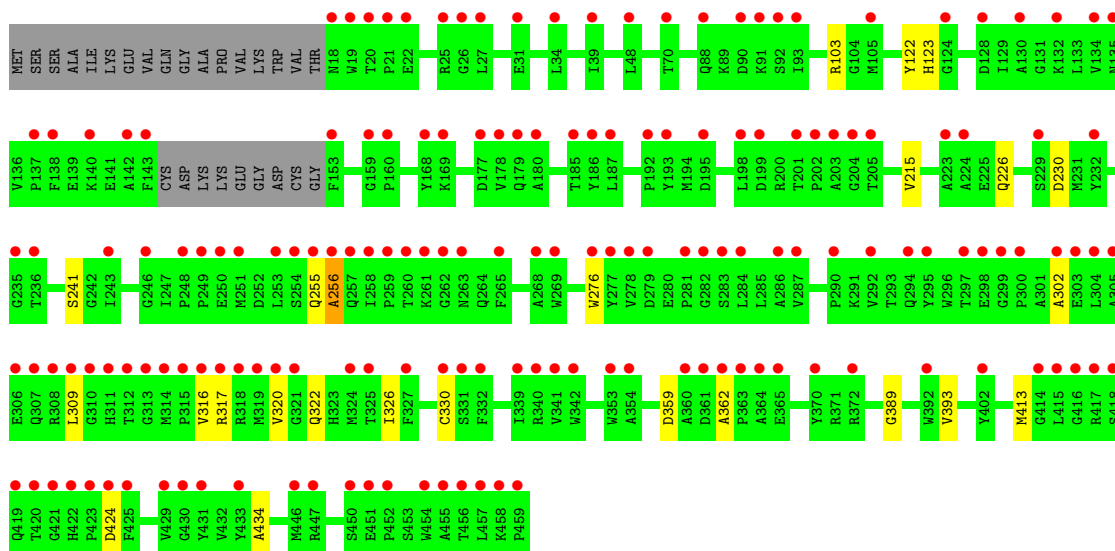
● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain I: 31% 87% 8% 6%

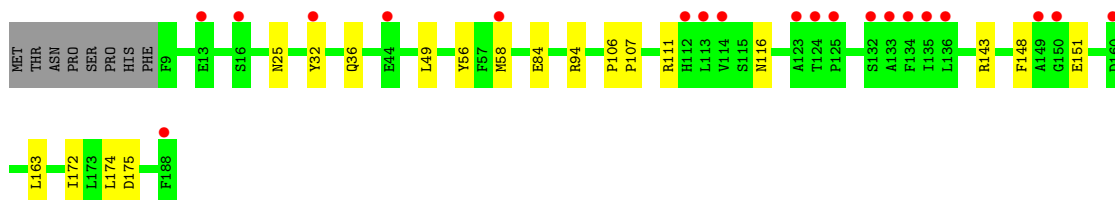
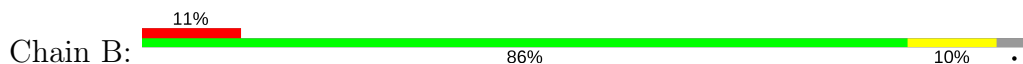


● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

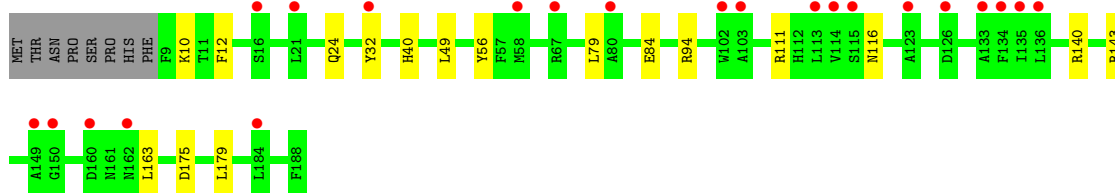
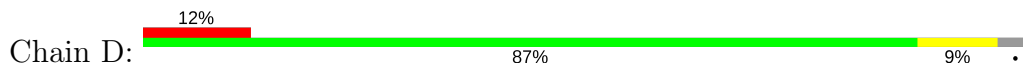
Chain K: 36% 89% 5% 6%



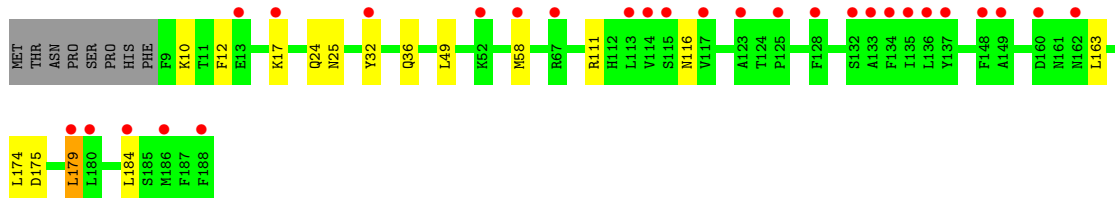
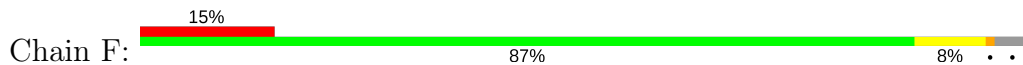
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



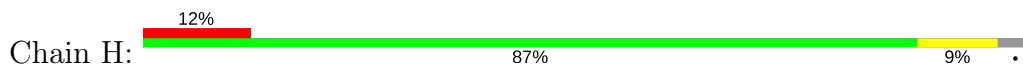
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

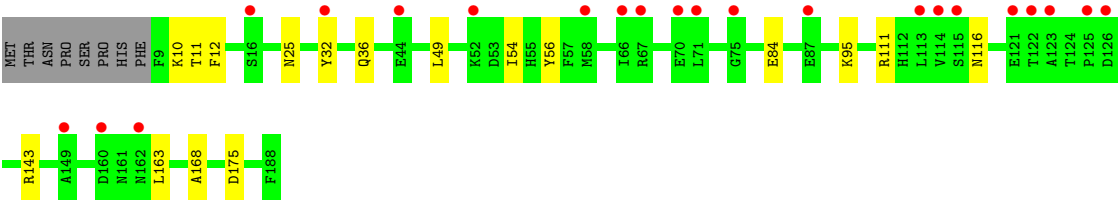


- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

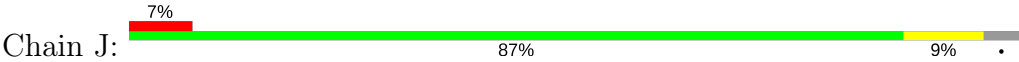


- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

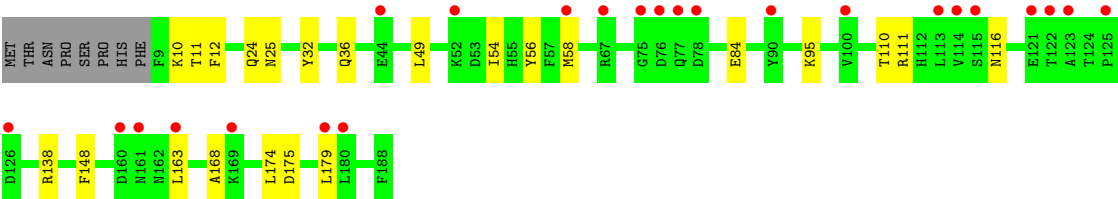
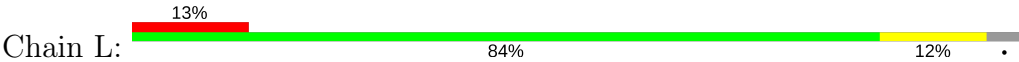




• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.98Å 278.12Å 92.96Å 90.00° 117.65° 90.00°	Depositor
Resolution (Å)	138.68 – 2.15 35.60 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.9 (138.68-2.15) 93.0 (35.60-2.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.204 , 0.233 0.281 , 0.300	Depositor DCC
$R_{free}$ test set	9870 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	30277	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1IT, FE2, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/3533	0.48	0/4796
1	C	0.33	0/3533	0.47	0/4796
1	E	0.32	0/3533	0.47	0/4796
1	G	0.31	0/3533	0.45	0/4796
1	I	0.31	0/3533	0.45	0/4796
1	K	0.31	0/3533	0.45	0/4796
2	B	0.33	0/1530	0.48	0/2068
2	D	0.34	0/1530	0.49	0/2068
2	F	0.33	0/1530	0.49	0/2068
2	H	0.31	0/1530	0.46	0/2068
2	J	0.32	0/1530	0.47	0/2068
2	L	0.31	0/1530	0.47	0/2068
All	All	0.32	0/30378	0.47	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 [i](#)

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	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3430	0	3274	17	0
1	E	3430	0	3274	19	0
1	G	3430	0	3274	16	0
1	I	3430	0	3274	15	0
1	K	3430	0	3274	12	0
2	B	1496	0	1447	16	0
2	D	1496	0	1447	12	0
2	F	1496	0	1447	12	0
2	H	1496	0	1447	14	0
2	J	1496	0	1447	14	0
2	L	1496	0	1447	19	0
3	A	4	0	0	1	0
3	C	4	0	0	1	0
3	E	4	0	0	1	0
3	G	4	0	0	1	0
3	I	4	0	0	1	0
3	K	4	0	0	1	0
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
5	A	13	0	8	0	0
5	C	13	0	8	0	0
5	E	13	0	8	0	0
6	A	128	0	0	0	0
6	B	53	0	0	0	0
6	C	129	0	0	0	0
6	D	66	0	0	0	0
6	E	88	0	0	0	0
6	F	46	0	0	0	0
6	G	23	0	0	0	0
6	H	19	0	0	0	0
6	I	29	0	0	0	0
6	J	31	0	0	0	0
6	K	23	0	0	0	0
6	L	17	0	0	0	0
All	All	30277	0	28350	150	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (150) 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:413:MET:HG3	1:E:142:ALA:HB1	1.59	0.84
1:C:339:ILE:HD11	1:C:357:LEU:HG	1.72	0.72
2:F:58:MET:HE1	2:F:174:LEU:HD22	1.76	0.68
1:I:262:GLY:HA2	1:I:278:VAL:HG23	1.75	0.67
1:A:123:HIS:HB2	3:A:900:FES:S2	2.35	0.66
1:C:339:ILE:CD1	1:C:357:LEU:HG	2.25	0.66
1:A:422:HIS:HD2	1:A:424:ASP:H	1.44	0.63
2:L:58:MET:HE1	2:L:174:LEU:HD22	1.80	0.62
1:K:123:HIS:HB2	3:K:900:FES:S2	2.40	0.61
1:C:123:HIS:HB2	3:C:900:FES:S2	2.41	0.61
1:G:123:HIS:HB2	3:G:900:FES:S2	2.40	0.61
2:B:58:MET:HE3	2:B:174:LEU:HD22	1.83	0.60
1:A:339:ILE:HD11	1:A:357:LEU:HG	1.83	0.59
1:G:217:PRO:HD2	1:G:393:VAL:HG22	1.83	0.59
1:A:373:HIS:HD2	1:A:376:ARG:HE	1.49	0.59
1:C:287:VAL:HG12	1:C:288:MET:CE	2.33	0.58
1:E:123:HIS:HB2	3:E:900:FES:S2	2.43	0.58
1:I:123:HIS:HB2	3:I:900:FES:S2	2.44	0.58
2:B:36:GLN:HE21	2:F:12:PHE:H	1.53	0.57
1:K:255:GLN:O	1:K:256:ALA:C	2.43	0.57
1:A:413:MET:HG2	1:A:434:ALA:HA	1.88	0.56
1:E:164:ARG:HD2	1:E:178:VAL:HA	1.88	0.55
1:I:276:TRP:HB3	1:I:322:GLN:HG3	1.87	0.55
2:H:10:LYS:HG3	2:H:11:THR:H	1.70	0.55
1:A:287:VAL:HG12	1:A:288:MET:CE	2.37	0.55
1:E:332:PHE:HB3	1:E:339:ILE:HG23	1.90	0.54
2:J:56:TYR:HB3	2:J:84:GLU:HB2	1.89	0.54
1:C:356:THR:CG2	2:D:79:LEU:HD21	2.38	0.54
2:F:49:LEU:HD21	2:F:163:LEU:HD13	1.91	0.53
1:E:339:ILE:HD11	1:E:357:LEU:HG	1.90	0.53
2:B:56:TYR:HB3	2:B:84:GLU:HB2	1.90	0.53
1:K:276:TRP:HB3	1:K:322:GLN:HG3	1.91	0.52
1:C:334:PRO:O	1:C:337:ASN:OD1	2.28	0.52
2:J:49:LEU:HD21	2:J:163:LEU:HD13	1.92	0.52
1:C:332:PHE:HB3	1:C:339:ILE:HG23	1.92	0.51
1:G:276:TRP:HB3	1:G:322:GLN:HG3	1.92	0.51
1:K:241:SER:HB2	2:L:95:LYS:HG3	1.93	0.51
1:I:244:LEU:HD13	1:I:253:LEU:HG	1.93	0.51
1:E:126:ALA:HB3	1:E:135:ASN:HB3	1.92	0.50
1:E:448:MET:HA	1:E:457:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASP:OD2	2:D:111:ARG:HB2	2.11	0.50
2:H:116:ASN:HA	2:J:32:TYR:CD1	2.47	0.50
1:A:287:VAL:HG12	1:A:288:MET:HE2	1.93	0.49
2:B:32:TYR:CD1	2:F:116:ASN:HA	2.47	0.49
1:K:309:LEU:HD13	1:K:316:VAL:HG11	1.94	0.49
1:K:359:ASP:HB2	1:K:362:ALA:HB2	1.95	0.49
2:J:10:LYS:HG3	2:J:11:THR:H	1.76	0.49
1:E:309:LEU:HD13	1:E:316:VAL:HG11	1.93	0.49
1:C:287:VAL:HG12	1:C:288:MET:HE2	1.94	0.49
2:D:12:PHE:H	2:F:36:GLN:HE21	1.60	0.48
2:B:143:ARG:HD3	1:E:215:VAL:HG21	1.94	0.48
1:A:339:ILE:CD1	1:A:357:LEU:HG	2.43	0.48
1:G:413:MET:HG2	1:G:434:ALA:HA	1.95	0.48
1:A:349:GLU:OE2	2:D:143:ARG:NH2	2.42	0.48
2:D:24:GLN:HG2	2:F:25:ASN:HD21	1.78	0.48
2:B:116:ASN:HA	2:D:32:TYR:CD1	2.48	0.48
2:J:175:ASP:OD2	2:L:111:ARG:HB2	2.12	0.48
2:H:36:GLN:HE21	2:L:12:PHE:H	1.61	0.48
1:G:359:ASP:HB2	1:G:362:ALA:HB2	1.96	0.48
1:G:448:MET:HA	1:G:457:LEU:HD11	1.95	0.47
2:D:175:ASP:OD2	2:F:111:ARG:HB2	2.14	0.47
1:I:126:ALA:HB3	1:I:135:ASN:HB3	1.96	0.47
1:I:257:GLN:HB3	1:I:282:GLY:HA3	1.97	0.47
2:H:49:LEU:HD21	2:H:163:LEU:HD13	1.96	0.47
1:C:287:VAL:HG12	1:C:288:MET:HE3	1.96	0.47
2:H:175:ASP:OD2	2:J:111:ARG:HB2	2.15	0.47
2:J:10:LYS:HG3	2:J:11:THR:N	2.30	0.46
2:L:56:TYR:HB3	2:L:84:GLU:HB2	1.96	0.46
2:D:56:TYR:HB3	2:D:84:GLU:HB2	1.97	0.46
1:K:226:GLN:HA	1:K:230:ASP:HB3	1.97	0.46
2:B:58:MET:HG3	2:B:172:ILE:HB	1.96	0.46
2:H:32:TYR:CD1	2:L:116:ASN:HA	2.50	0.46
2:J:12:PHE:H	2:L:36:GLN:HE21	1.64	0.46
1:A:336:MET:HG2	1:A:336:MET:H	1.53	0.46
1:A:422:HIS:CD2	1:A:424:ASP:H	2.31	0.45
1:I:226:GLN:HA	1:I:230:ASP:HB3	1.96	0.45
2:D:49:LEU:HD21	2:D:163:LEU:HD13	1.98	0.45
1:E:244:LEU:HD13	1:E:253:LEU:HG	1.99	0.45
1:E:339:ILE:CD1	1:E:357:LEU:HG	2.47	0.45
1:K:413:MET:HG2	1:K:434:ALA:HA	1.99	0.45
1:A:448:MET:HA	1:A:457:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:54:ILE:HA	2:L:168:ALA:O	2.17	0.45
2:B:111:ARG:HB2	2:F:175:ASP:OD2	2.17	0.45
2:B:32:TYR:CG	2:F:116:ASN:HA	2.52	0.44
1:A:212:GLN:HB2	1:A:212:GLN:HE21	1.63	0.44
1:G:241:SER:HB2	2:H:95:LYS:HG3	1.98	0.44
2:B:25:ASN:HD21	2:F:24:GLN:HG2	1.82	0.44
2:B:148:PHE:HB3	2:B:174:LEU:HD11	1.99	0.44
1:G:126:ALA:HB3	1:G:135:ASN:HB3	1.99	0.44
1:G:226:GLN:HA	1:G:230:ASP:HB3	2.00	0.44
2:D:116:ASN:HA	2:F:32:TYR:CD1	2.53	0.44
1:I:107:ILE:HG22	1:I:118:PHE:HB3	1.99	0.44
2:H:25:ASN:HD21	2:L:24:GLN:HG2	1.82	0.44
2:J:116:ASN:HA	2:L:32:TYR:CD1	2.52	0.44
2:L:10:LYS:HG3	2:L:11:THR:N	2.32	0.44
1:E:359:ASP:HB2	1:E:362:ALA:HB2	2.00	0.43
2:B:116:ASN:HA	2:D:32:TYR:CG	2.53	0.43
1:G:288:MET:HB3	1:G:292:VAL:HB	2.00	0.43
1:A:248:PRO:HA	1:A:249:PRO:HD3	1.93	0.43
1:C:448:MET:HA	1:C:457:LEU:HD11	1.98	0.43
1:I:251:MET:HG3	1:I:255:GLN:HB3	2.00	0.43
2:L:148:PHE:HB3	2:L:174:LEU:HD11	2.01	0.43
1:G:262:GLY:HA2	1:G:278:VAL:HG23	2.00	0.43
2:H:111:ARG:HB2	2:L:175:ASP:OD2	2.18	0.43
1:C:283:SER:O	1:C:287:VAL:HG23	2.17	0.43
1:G:248:PRO:HA	1:G:249:PRO:HD3	1.91	0.43
2:H:36:GLN:NE2	2:L:12:PHE:H	2.17	0.43
1:I:359:ASP:HB2	1:I:362:ALA:HB2	2.01	0.43
1:A:126:ALA:HB3	1:A:135:ASN:HB3	2.00	0.43
1:E:326:ILE:HB	1:E:330:CYS:HB3	2.00	0.43
2:H:54:ILE:HA	2:H:168:ALA:O	2.19	0.43
1:C:142:ALA:HB1	1:E:413:MET:HG3	2.01	0.42
2:L:10:LYS:HG3	2:L:11:THR:H	1.83	0.42
2:B:106:PRO:HA	2:B:107:PRO:HD3	1.87	0.42
1:G:229:SER:HB2	1:G:437:ALA:HB3	2.02	0.42
2:J:24:GLN:HG2	2:L:25:ASN:HD21	1.84	0.42
1:A:413:MET:CG	1:E:142:ALA:HB1	2.41	0.42
2:J:54:ILE:HA	2:J:168:ALA:O	2.19	0.42
1:K:302:ALA:HB1	1:K:317:ARG:HG2	2.02	0.42
2:B:151:GLU:OE2	2:D:40:HIS:NE2	2.52	0.42
1:I:241:SER:HB2	2:J:95:LYS:HG3	2.00	0.42
1:I:326:ILE:HB	1:I:330:CYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:110:THR:HG22	2:L:138:ARG:HG2	2.00	0.42
1:A:359:ASP:HB2	1:A:362:ALA:HB2	2.02	0.42
1:E:276:TRP:HB3	1:E:322:GLN:HG3	2.02	0.42
2:H:56:TYR:HB3	2:H:84:GLU:HB2	2.01	0.42
1:A:276:TRP:HB3	1:A:322:GLN:HG3	2.01	0.42
1:C:126:ALA:HB3	1:C:135:ASN:HB3	2.02	0.42
2:F:179:LEU:HD21	2:F:184:LEU:HD11	2.02	0.42
2:B:49:LEU:HD21	2:B:163:LEU:HD13	2.01	0.41
1:A:339:ILE:HD12	1:A:356:THR:HA	2.02	0.41
1:E:248:PRO:HA	1:E:249:PRO:HD3	1.96	0.41
1:I:60:LEU:HD23	1:I:341:VAL:HG22	2.02	0.41
1:G:326:ILE:HB	1:G:330:CYS:HB3	2.01	0.41
2:H:12:PHE:H	2:J:36:GLN:NE2	2.19	0.41
1:E:422:HIS:CD2	1:E:424:ASP:H	2.39	0.41
1:G:389:GLY:O	1:G:393:VAL:HG23	2.19	0.41
2:H:143:ARG:HD3	1:K:215:VAL:HG21	2.03	0.41
2:J:116:ASN:HA	2:L:32:TYR:CG	2.56	0.41
1:K:326:ILE:HB	1:K:330:CYS:HB3	2.02	0.41
1:K:389:GLY:O	1:K:393:VAL:HG23	2.21	0.41
1:C:314:MET:HA	1:C:315:PRO:HD3	1.89	0.40
1:C:339:ILE:HD13	1:C:357:LEU:HG	2.02	0.40
1:C:90:ASP:O	1:C:91:LYS:HB2	2.20	0.40
1:C:244:LEU:HD13	1:C:253:LEU:HG	2.02	0.40
1:G:164:ARG:HD2	1:G:178:VAL:HA	2.02	0.40
1:I:105:MET:HB3	1:I:120:CYS:SG	2.62	0.40
1:I:333:LEU:HD12	1:I:338:GLN:HB3	2.04	0.40
2:L:49:LEU:HD21	2:L:163:LEU:HD13	2.03	0.40
1:E:107:ILE:HG22	1:E:118:PHE:HB3	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%)	415 (97%)	14 (3%)	0	100	100
1	C	429/459 (94%)	409 (95%)	20 (5%)	0	100	100
1	E	429/459 (94%)	416 (97%)	13 (3%)	0	100	100
1	G	429/459 (94%)	416 (97%)	13 (3%)	0	100	100
1	I	429/459 (94%)	408 (95%)	21 (5%)	0	100	100
1	K	429/459 (94%)	410 (96%)	18 (4%)	1 (0%)	51	50
2	B	178/188 (95%)	174 (98%)	4 (2%)	0	100	100
2	D	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	F	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	H	178/188 (95%)	174 (98%)	4 (2%)	0	100	100
2	J	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	L	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
All	All	3642/3882 (94%)	3511 (96%)	130 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	256	ALA

### 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%)	344 (98%)	6 (2%)	66	71
1	C	350/372 (94%)	345 (99%)	5 (1%)	71	77
1	E	350/372 (94%)	343 (98%)	7 (2%)	60	64
1	G	350/372 (94%)	344 (98%)	6 (2%)	66	71
1	I	350/372 (94%)	343 (98%)	7 (2%)	60	64
1	K	350/372 (94%)	346 (99%)	4 (1%)	78	82
2	B	159/167 (95%)	158 (99%)	1 (1%)	89	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	159/167 (95%)	155 (98%)	4 (2%)	53	55
2	F	159/167 (95%)	156 (98%)	3 (2%)	62	66
2	H	159/167 (95%)	159 (100%)	0	100	100
2	J	159/167 (95%)	159 (100%)	0	100	100
2	L	159/167 (95%)	158 (99%)	1 (1%)	89	92
All	All	3054/3234 (94%)	3010 (99%)	44 (1%)	71	77

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	122	TYR
1	A	336	MET
1	A	356	THR
1	A	394	GLU
1	A	410	ASN
2	B	94	ARG
1	C	94	LYS
1	C	103	ARG
1	C	122	TYR
1	C	356	THR
1	C	457	LEU
2	D	10	LYS
2	D	94	ARG
2	D	140	ARG
2	D	179	LEU
1	E	48	LEU
1	E	103	ARG
1	E	122	TYR
1	E	258	ILE
1	E	320	VAL
1	E	339	ILE
1	E	457	LEU
2	F	10	LYS
2	F	17	LYS
2	F	179	LEU
1	G	103	ARG
1	G	122	TYR
1	G	336	MET
1	G	419	GLN

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Mol	Chain	Res	Type
1	G	457	LEU
1	G	458	LYS
1	I	103	ARG
1	I	122	TYR
1	I	280	GLU
1	I	303	GLU
1	I	336	MET
1	I	410	ASN
1	I	457	LEU
1	K	103	ARG
1	K	122	TYR
1	K	320	VAL
1	K	424	ASP
2	L	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	373	HIS
1	A	391	ASN
1	A	410	ASN
1	A	419	GLN
1	A	422	HIS
1	A	444	HIS
2	B	25	ASN
2	B	36	GLN
1	C	212	GLN
1	C	373	HIS
1	C	391	ASN
1	C	410	ASN
1	C	422	HIS
1	C	444	HIS
2	D	25	ASN
2	D	36	GLN
2	D	131	ASN
1	E	212	GLN
1	E	391	ASN
1	E	410	ASN
1	E	422	HIS
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	391	ASN
1	G	410	ASN
1	G	422	HIS
1	G	444	HIS
2	H	25	ASN
2	H	36	GLN
2	H	131	ASN
1	I	212	GLN
1	I	264	GLN
1	I	343	HIS
1	I	391	ASN
1	I	410	ASN
1	I	419	GLN
1	I	444	HIS
2	J	25	ASN
2	J	36	GLN
2	J	131	ASN
1	K	212	GLN
1	K	255	GLN
1	K	343	HIS
1	K	410	ASN
1	K	444	HIS
2	L	25	ASN
2	L	36	GLN
2	L	162	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	1IT	A	1460	-	9,15,15	1.30	0	12,21,21	1.83	4 (33%)
3	FES	A	900	1	0,4,4	0.00	-	0,4,4	0.00	-
5	1IT	C	1451	-	9,15,15	1.28	0	12,21,21	1.87	4 (33%)
3	FES	C	900	1	0,4,4	0.00	-	0,4,4	0.00	-
5	1IT	E	1451	-	9,15,15	1.28	0	12,21,21	1.83	4 (33%)
3	FES	E	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	G	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	I	900	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	K	900	1	0,4,4	0.00	-	0,4,4	0.00	-

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	1IT	A	1460	-	-	0/0/0/0	0/2/3/3
3	FES	A	900	1	-	0/0/4/4	0/1/1/1
5	1IT	C	1451	-	-	0/0/0/0	0/2/3/3
3	FES	C	900	1	-	0/0/4/4	0/1/1/1
5	1IT	E	1451	-	-	0/0/0/0	0/2/3/3
3	FES	E	900	1	-	0/0/4/4	0/1/1/1
3	FES	G	900	1	-	0/0/4/4	0/1/1/1
3	FES	I	900	1	-	0/0/4/4	0/1/1/1
3	FES	K	900	1	-	0/0/4/4	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1451	1IT	C12-C13-C1	-2.56	116.48	120.81
5	E	1451	1IT	C4-C3-C2	-2.53	116.54	120.81
5	A	1460	1IT	C4-C3-C2	-2.50	116.58	120.81
5	E	1451	1IT	C12-C13-C1	-2.43	116.70	120.81
5	A	1460	1IT	C12-C13-C1	-2.41	116.74	120.81
5	C	1451	1IT	C4-C3-C2	-2.40	116.76	120.81
5	E	1451	1IT	C3-C2-C7	3.40	122.53	120.38
5	A	1460	1IT	C13-C1-C9	3.44	122.56	120.38
5	A	1460	1IT	C3-C2-C7	3.45	122.56	120.38
5	E	1451	1IT	C13-C1-C9	3.46	122.56	120.38
5	C	1451	1IT	C13-C1-C9	3.50	122.59	120.38
5	C	1451	1IT	C3-C2-C7	3.61	122.66	120.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FES	1	0
3	C	900	FES	1	0
3	E	900	FES	1	0
3	G	900	FES	1	0
3	I	900	FES	1	0
3	K	900	FES	1	0

## 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%)	1.09	87 (20%) 1 2	37, 42, 48, 56	18 (4%)
1	C	433/459 (94%)	1.05	71 (16%) 2 3	37, 42, 48, 55	18 (4%)
1	E	433/459 (94%)	0.94	60 (13%) 3 4	36, 42, 50, 58	18 (4%)
1	G	433/459 (94%)	1.69	147 (33%) 0 1	37, 42, 48, 54	18 (4%)
1	I	433/459 (94%)	1.60	141 (32%) 0 1	38, 43, 47, 53	18 (4%)
1	K	433/459 (94%)	1.81	165 (38%) 0 1	38, 42, 48, 53	18 (4%)
2	B	180/188 (95%)	0.83	20 (11%) 6 8	38, 42, 48, 53	4 (2%)
2	D	180/188 (95%)	0.85	22 (12%) 5 7	38, 42, 48, 51	4 (2%)
2	F	180/188 (95%)	0.96	28 (15%) 2 3	38, 43, 47, 49	4 (2%)
2	H	180/188 (95%)	0.85	22 (12%) 5 7	38, 43, 47, 50	4 (2%)
2	J	180/188 (95%)	0.57	13 (7%) 16 21	37, 42, 46, 48	4 (2%)
2	L	180/188 (95%)	0.82	24 (13%) 4 5	37, 41, 45, 47	4 (2%)
All	All	3678/3882 (94%)	1.20	800 (21%) 1 1	36, 42, 48, 58	132 (3%)

All (800) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	258	ILE	9.3
1	C	258	ILE	9.3
1	G	305	ALA	7.6
1	K	278	VAL	6.9
1	K	455	ALA	6.8
1	G	258	ILE	6.5
1	G	307	GLN	6.4
1	K	258	ILE	6.4
1	K	361	ASP	6.3
1	G	310	GLY	6.2
1	I	282	GLY	6.2

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Mol	Chain	Res	Type	RSRZ
1	G	278	VAL	6.1
1	K	204	GLY	5.9
2	F	160	ASP	5.8
1	K	282	GLY	5.7
1	A	224	ALA	5.7
1	G	253	LEU	5.7
1	C	339	ILE	5.7
1	G	294	GLN	5.7
1	A	227	PHE	5.6
1	G	204	GLY	5.6
1	K	22	GLU	5.6
1	I	416	GLY	5.6
1	K	433	TYR	5.5
1	C	331	SER	5.5
1	G	309	LEU	5.5
1	G	261	LYS	5.5
1	G	199	ASP	5.4
1	I	199	ASP	5.4
1	I	253	LEU	5.4
1	G	285	LEU	5.4
1	G	416	GLY	5.3
1	K	370	TYR	5.2
1	G	312	THR	5.2
1	K	311	HIS	5.2
1	E	105	MET	5.2
1	G	301	ALA	5.2
1	K	281	PRO	5.2
1	K	153	PHE	5.2
1	G	366	ILE	5.1
1	C	227	PHE	5.1
1	G	143	PHE	5.1
2	F	123	ALA	5.1
1	I	278	VAL	5.1
1	K	276	TRP	5.1
2	F	113	LEU	5.1
2	H	44	GLU	5.0
1	I	143	PHE	5.0
1	K	422	HIS	5.0
1	K	416	GLY	5.0
1	K	314	MET	4.9
1	A	341	VAL	4.9
1	A	228	CYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	K	18	ASN	4.9
1	G	153	PHE	4.9
1	C	333	LEU	4.8
1	A	258	ILE	4.8
2	B	113	LEU	4.8
1	A	260	THR	4.8
1	A	223	ALA	4.8
1	G	308	ARG	4.7
1	I	19	TRP	4.7
1	K	431	TYR	4.7
1	I	117	ALA	4.7
1	K	312	THR	4.7
1	E	257	GLN	4.7
1	A	325	THR	4.7
1	I	305	ALA	4.7
1	A	105	MET	4.7
1	G	203	ALA	4.6
1	G	251	MET	4.6
1	G	453	SER	4.6
2	L	160	ASP	4.6
2	D	113	LEU	4.6
1	C	341	VAL	4.5
1	I	261	LYS	4.5
1	K	424	ASP	4.5
1	K	143	PHE	4.5
2	J	113	LEU	4.5
1	A	331	SER	4.5
1	C	261	LYS	4.5
1	K	168	TYR	4.5
1	K	313	GLY	4.4
1	I	195	ASP	4.4
1	G	19	TRP	4.4
1	G	243	ILE	4.4
1	I	307	GLN	4.4
1	I	425	PHE	4.4
1	I	297	THR	4.4
1	A	342	TRP	4.4
1	G	277	TYR	4.4
1	K	277	TYR	4.4
1	G	420	THR	4.4
1	I	153	PHE	4.4
1	C	224	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	K	318	ARG	4.3
1	I	293	THR	4.3
1	E	253	LEU	4.3
1	I	202	PRO	4.3
1	A	226	GLN	4.3
1	G	138	PHE	4.3
1	K	290	PRO	4.3
1	I	268	ALA	4.3
1	A	259	PRO	4.3
1	E	260	THR	4.2
1	G	201	THR	4.2
1	C	325	THR	4.2
1	I	361	ASP	4.2
1	G	18	ASN	4.2
1	A	257	GLN	4.2
1	G	320	VAL	4.2
1	K	257	GLN	4.2
1	K	341	VAL	4.2
1	I	252	ASP	4.2
1	K	279	ASP	4.2
1	K	260	THR	4.2
1	K	459	PRO	4.2
1	G	415	LEU	4.2
1	K	19	TRP	4.2
1	A	326	ILE	4.2
1	A	256	ALA	4.1
1	K	253	LEU	4.1
1	I	418	SER	4.1
1	K	307	GLN	4.1
1	A	222	PHE	4.1
1	C	105	MET	4.1
1	K	292	VAL	4.1
1	K	31	GLU	4.1
1	A	251	MET	4.1
1	K	310	GLY	4.1
1	A	229	SER	4.0
1	A	327	PHE	4.0
1	C	273	GLY	4.0
1	E	250	GLU	4.0
1	C	342	TRP	4.0
1	E	258	ILE	4.0
1	K	420	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	283	SER	4.0
1	I	320	VAL	4.0
1	K	331	SER	4.0
1	C	228	CYS	4.0
1	C	259	PRO	4.0
1	E	252	ASP	4.0
1	G	303	GLU	4.0
1	G	454	TRP	4.0
1	K	303	GLU	3.9
1	K	309	LEU	3.9
2	H	113	LEU	3.9
1	G	268	ALA	3.9
1	A	395	ILE	3.9
2	B	160	ASP	3.9
1	G	304	LEU	3.9
1	G	333	LEU	3.9
1	K	295	TYR	3.9
1	K	304	LEU	3.9
1	I	178	VAL	3.9
1	G	431	TYR	3.9
1	K	261	LYS	3.9
1	G	281	PRO	3.8
2	L	125	PRO	3.8
1	K	283	SER	3.8
2	F	114	VAL	3.8
1	K	423	PRO	3.8
2	L	67	ARG	3.8
1	I	192	PRO	3.8
1	I	300	PRO	3.8
1	I	138	PHE	3.8
1	G	254	SER	3.8
1	I	254	SER	3.8
1	K	265	PHE	3.8
1	G	195	ASP	3.8
1	G	255	GLN	3.8
1	K	294	GLN	3.8
1	G	311	HIS	3.8
1	C	340	ARG	3.7
1	K	300	PRO	3.7
1	I	457	LEU	3.7
2	H	160	ASP	3.7
1	A	384	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	134	PHE	3.7
1	K	450	SER	3.7
1	I	303	GLU	3.7
1	K	236	THR	3.7
2	D	123	ALA	3.7
1	E	261	LYS	3.7
1	C	378	PHE	3.7
1	C	223	ALA	3.7
1	K	203	ALA	3.7
2	F	58	MET	3.7
2	H	75	GLY	3.7
2	L	90	TYR	3.6
1	G	142	ALA	3.6
1	A	59	LEU	3.6
1	I	363	PRO	3.6
1	G	260	THR	3.6
1	I	201	THR	3.6
1	I	48	LEU	3.6
2	H	71	LEU	3.6
1	G	155	LYS	3.6
1	K	248	PRO	3.6
1	G	157	GLU	3.6
1	K	364	ALA	3.6
1	I	31	GLU	3.6
1	K	70	THR	3.6
1	I	453	SER	3.6
1	C	332	PHE	3.6
1	G	339	ILE	3.6
1	K	456	THR	3.6
1	K	235	GLY	3.6
2	H	126	ASP	3.6
1	G	455	ALA	3.5
2	H	123	ALA	3.5
1	G	252	ASP	3.5
1	E	122	TYR	3.5
1	K	363	PRO	3.5
1	I	190	ALA	3.5
1	K	305	ALA	3.5
2	F	135	ILE	3.5
1	G	421	GLY	3.5
1	G	423	PRO	3.5
1	I	311	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	326	ILE	3.5
1	K	91	LYS	3.5
1	I	130	ALA	3.5
1	A	54	PHE	3.5
1	K	332	PHE	3.5
1	A	392	TRP	3.5
1	K	178	VAL	3.5
1	C	257	GLN	3.5
1	I	255	GLN	3.5
1	G	256	ALA	3.5
1	I	157	GLU	3.4
1	K	251	MET	3.4
1	I	455	ALA	3.4
1	K	268	ALA	3.4
1	G	300	PRO	3.4
1	A	60	LEU	3.4
1	E	341	VAL	3.4
1	E	259	PRO	3.4
1	I	32	LYS	3.4
2	D	58	MET	3.4
1	C	327	PHE	3.4
1	G	248	PRO	3.4
1	I	459	PRO	3.4
1	I	18	ASN	3.4
1	A	109	ARG	3.4
1	K	372	ARG	3.4
1	A	220	TRP	3.4
1	E	342	TRP	3.4
1	G	158	TRP	3.4
1	I	116	LYS	3.4
1	I	312	THR	3.4
1	K	223	ALA	3.3
1	I	315	PRO	3.3
1	G	34	LEU	3.3
1	G	198	LEU	3.3
1	I	183	LEU	3.3
1	G	156	ALA	3.3
1	G	245	ALA	3.3
1	G	93	ILE	3.3
1	K	229	SER	3.3
1	K	134	VAL	3.3
1	C	438	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	202	PRO	3.3
1	C	222	PHE	3.3
1	K	192	PRO	3.3
1	C	421	GLY	3.3
1	C	329	THR	3.3
1	A	35	LEU	3.3
1	C	395	ILE	3.3
1	I	279	ASP	3.3
1	I	456	THR	3.3
1	K	259	PRO	3.3
1	G	361	ASP	3.2
2	J	160	ASP	3.2
1	I	243	ILE	3.2
1	K	415	LEU	3.2
1	A	437	ALA	3.2
1	I	429	VAL	3.2
1	G	450	SER	3.2
1	E	251	MET	3.2
1	G	456	THR	3.2
1	C	255	GLN	3.2
1	K	199	ASP	3.2
1	C	392	TRP	3.2
1	E	332	PHE	3.2
1	I	161	LEU	3.2
1	G	179	GLN	3.2
1	E	278	VAL	3.2
1	G	317	ARG	3.2
1	K	297	THR	3.2
1	I	251	MET	3.2
1	K	317	ARG	3.2
1	K	269	TRP	3.2
1	K	458	LYS	3.2
1	A	330	CYS	3.1
1	I	290	PRO	3.1
1	G	140	LYS	3.1
1	G	20	THR	3.1
1	I	20	THR	3.1
1	C	328	PRO	3.1
1	G	134	VAL	3.1
1	K	315	PRO	3.1
1	K	454	TRP	3.1
1	K	319	MET	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	160	ASP	3.1
1	C	330	CYS	3.1
1	E	331	SER	3.1
1	I	330	CYS	3.1
1	G	282	GLY	3.1
1	K	26	GLY	3.1
1	E	214	TRP	3.1
1	I	142	ALA	3.1
1	E	294	GLN	3.1
1	K	25	ARG	3.1
1	K	93	ILE	3.1
2	D	115	SER	3.1
2	D	114	VAL	3.1
1	A	438	ALA	3.1
1	G	130	ALA	3.1
2	F	136	LEU	3.1
1	A	40	TYR	3.1
1	K	320	VAL	3.1
1	K	362	ALA	3.1
1	C	353	TRP	3.1
1	C	109	ARG	3.1
1	I	95	VAL	3.1
1	A	275	GLY	3.0
1	K	256	ALA	3.0
2	D	149	ALA	3.0
1	K	298	GLU	3.0
2	H	16	SER	3.0
1	G	279	ASP	3.0
1	C	60	LEU	3.0
2	D	134	PHE	3.0
2	F	137	TYR	3.0
1	E	254	SER	3.0
1	G	318	ARG	3.0
1	I	310	GLY	3.0
2	L	75	GLY	3.0
2	L	113	LEU	3.0
1	A	323	HIS	3.0
1	G	269	TRP	3.0
1	A	328	PRO	3.0
1	K	202	PRO	3.0
2	H	125	PRO	3.0
1	E	326	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	123	ALA	3.0
1	G	378	PHE	3.0
1	K	138	PHE	3.0
1	K	262	GLY	3.0
1	A	388	ASP	3.0
1	G	457	LEU	3.0
1	I	285	LEU	3.0
2	D	135	ILE	3.0
1	K	193	TYR	3.0
1	A	261	LYS	3.0
2	H	114	VAL	2.9
1	C	253	LEU	2.9
1	I	298	GLU	2.9
2	L	44	GLU	2.9
1	A	53	VAL	2.9
1	K	339	ILE	2.9
1	G	314	MET	2.9
2	H	67	ARG	2.9
2	H	70	GLU	2.9
2	D	103	ALA	2.9
1	K	90	ASP	2.9
1	G	67	VAL	2.9
1	I	366	ILE	2.9
1	K	425	PHE	2.9
1	E	392	TRP	2.9
1	K	130	ALA	2.9
1	A	333	LEU	2.9
1	K	140	LYS	2.9
1	K	365	GLU	2.9
1	I	23	ALA	2.9
1	A	225	GLU	2.9
2	B	136	LEU	2.9
1	A	233	HIS	2.9
1	E	305	ALA	2.9
1	I	115	ALA	2.9
1	C	214	TRP	2.9
1	C	220	TRP	2.9
1	E	361	ASP	2.9
2	J	114	VAL	2.8
1	A	339	ILE	2.8
1	C	226	GLN	2.8
1	G	70	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	254	SER	2.8
1	E	334	PRO	2.8
1	I	133	LEU	2.8
1	G	71	GLY	2.8
1	I	129	ILE	2.8
2	F	162	ASN	2.8
1	G	298	GLU	2.8
1	A	442	TYR	2.8
1	K	92	SER	2.8
1	K	418	SER	2.8
2	B	58	MET	2.8
1	I	191	ARG	2.8
1	C	59	LEU	2.8
1	G	382	GLY	2.8
1	I	196	VAL	2.8
1	A	39	ILE	2.8
1	A	216	ILE	2.8
1	K	243	ILE	2.8
1	G	132	LYS	2.8
1	G	306	GLU	2.8
1	K	414	GLY	2.8
1	I	134	VAL	2.8
1	E	220	TRP	2.8
1	G	418	SER	2.8
1	K	421	GLY	2.8
1	I	417	ARG	2.8
1	A	83	VAL	2.8
1	A	250	GLU	2.8
1	G	129	ILE	2.8
1	C	355	PHE	2.8
1	C	409	PHE	2.8
1	G	263	ASN	2.8
1	K	299	GLY	2.8
1	A	122	TYR	2.8
1	E	298	GLU	2.8
1	I	431	TYR	2.8
2	B	123	ALA	2.7
1	K	287	VAL	2.7
2	B	114	VAL	2.7
1	K	27	LEU	2.7
1	K	48	LEU	2.7
2	J	71	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	341	VAL	2.7
1	K	249	PRO	2.7
1	A	273	GLY	2.7
1	I	317	ARG	2.7
2	J	97	THR	2.7
2	J	52	LYS	2.7
1	C	238	THR	2.7
1	C	383	VAL	2.7
1	G	297	THR	2.7
2	B	135	ILE	2.7
1	A	332	PHE	2.7
2	F	17	LYS	2.7
1	I	179	GLN	2.7
1	C	260	THR	2.7
2	H	121	GLU	2.7
2	L	100	VAL	2.7
2	L	114	VAL	2.7
1	I	189	ASP	2.7
2	L	76	ASP	2.7
1	E	307	GLN	2.7
1	I	339	ILE	2.7
1	I	422	HIS	2.7
1	C	82	PRO	2.7
2	B	133	ALA	2.7
1	G	276	TRP	2.7
2	L	122	THR	2.7
1	K	419	GLN	2.7
1	G	257	GLN	2.7
1	K	201	THR	2.7
1	K	34	LEU	2.7
2	H	58	MET	2.7
1	K	186	TYR	2.6
1	G	326	ILE	2.6
1	A	354	ALA	2.6
1	K	286	ALA	2.6
1	I	184	GLU	2.6
2	H	122	THR	2.6
1	I	169	LYS	2.6
2	L	115	SER	2.6
1	C	122	TYR	2.6
1	A	104	GLY	2.6
1	A	350	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	149	ALA	2.6
1	I	420	THR	2.6
1	C	254	SER	2.6
1	K	457	LEU	2.6
1	E	325	THR	2.6
1	K	105	MET	2.6
1	I	365	GLU	2.6
1	E	383	VAL	2.6
1	G	358	VAL	2.6
1	C	441	MET	2.6
1	C	218	CYS	2.6
1	K	327	PHE	2.6
1	K	135	ASN	2.6
1	G	191	ARG	2.6
1	K	250	GLU	2.6
2	F	115	SER	2.6
2	F	133	ALA	2.6
1	E	246	GLY	2.6
1	A	253	LEU	2.6
1	A	393	VAL	2.5
1	K	360	ALA	2.5
2	J	115	SER	2.5
1	I	306	GLU	2.5
1	A	255	GLN	2.5
1	A	307	GLN	2.5
1	C	338	GLN	2.5
2	D	67	ARG	2.5
2	L	52	LYS	2.5
1	K	124	GLY	2.5
1	A	221	LYS	2.5
2	B	32	TYR	2.5
1	G	247	ILE	2.5
1	G	424	ASP	2.5
1	E	327	PHE	2.5
1	G	65	SER	2.5
1	G	313	GLY	2.5
1	G	414	GLY	2.5
2	H	149	ALA	2.5
2	H	162	ASN	2.5
2	L	169	LYS	2.5
1	I	447	ARG	2.5
1	K	316	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	154	ASP	2.5
1	K	137	PRO	2.5
2	B	125	PRO	2.5
2	F	125	PRO	2.5
1	E	311	HIS	2.5
1	I	94	LYS	2.5
2	D	162	ASN	2.5
1	A	214	TRP	2.5
1	K	342	TRP	2.5
2	L	163	LEU	2.5
1	I	324	MET	2.5
1	A	218	CYS	2.5
1	K	429	VAL	2.5
1	E	216	ILE	2.5
1	I	52	ARG	2.5
1	K	179	GLN	2.5
2	J	67	ARG	2.5
1	G	189	ASP	2.5
1	A	22	GLU	2.5
2	D	136	LEU	2.5
1	A	324	MET	2.5
1	C	324	MET	2.5
1	E	312	THR	2.5
1	C	323	HIS	2.5
2	D	32	TYR	2.5
1	E	339	ILE	2.5
1	K	246	GLY	2.5
1	I	156	ALA	2.5
1	A	231	MET	2.4
1	A	448	MET	2.4
1	I	314	MET	2.4
1	G	392	TRP	2.4
1	E	22	GLU	2.4
1	G	154	ASP	2.4
1	E	313	GLY	2.4
1	K	142	ALA	2.4
1	K	354	ALA	2.4
1	K	255	GLN	2.4
1	K	205	THR	2.4
1	E	61	LEU	2.4
1	I	22	GLU	2.4
1	C	53	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	100	CYS	2.4
1	A	366	ILE	2.4
1	E	365	GLU	2.4
1	I	302	ALA	2.4
1	E	116	LYS	2.4
1	I	248	PRO	2.4
1	I	281	PRO	2.4
1	E	227	PHE	2.4
1	G	118	PHE	2.4
1	G	425	PHE	2.4
1	I	198	LEU	2.4
1	A	352	VAL	2.4
1	A	383	VAL	2.4
1	C	393	VAL	2.4
1	G	165	VAL	2.4
1	G	250	GLU	2.4
1	I	139	GLU	2.4
1	I	419	GLN	2.4
1	I	392	TRP	2.4
2	F	149	ALA	2.4
1	K	185	THR	2.4
1	K	324	MET	2.4
2	H	32	TYR	2.4
1	A	329	THR	2.4
1	K	325	THR	2.4
1	K	330	CYS	2.4
2	D	21	LEU	2.4
2	F	13	GLU	2.4
2	L	121	GLU	2.4
1	E	109	ARG	2.4
1	G	178	VAL	2.4
2	L	78	ASP	2.4
1	I	335	ALA	2.4
1	C	76	THR	2.4
1	G	205	THR	2.4
1	I	185	THR	2.4
1	I	250	GLU	2.4
2	B	134	PHE	2.4
2	D	184	LEU	2.4
2	D	133	ALA	2.4
1	G	116	LYS	2.4
1	I	70	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	115	SER	2.4
1	G	186	TYR	2.4
1	I	402	TYR	2.4
1	G	265	PHE	2.3
2	F	148	PHE	2.3
1	A	334	PRO	2.3
1	I	301	ALA	2.3
1	K	224	ALA	2.3
2	D	150	GLY	2.3
1	C	40	TYR	2.3
1	K	402	TYR	2.3
1	K	392	TRP	2.3
1	I	88	GLN	2.3
1	E	352	VAL	2.3
1	I	67	VAL	2.3
1	E	104	GLY	2.3
1	E	283	SER	2.3
2	D	16	SER	2.3
1	E	297	THR	2.3
1	I	451	GLU	2.3
1	E	89	LYS	2.3
1	E	395	ILE	2.3
1	G	417	ARG	2.3
1	I	433	TYR	2.3
2	B	112	HIS	2.3
1	K	451	GLU	2.3
1	A	79	GLY	2.3
1	G	427	GLY	2.3
1	I	358	VAL	2.3
1	E	434	ALA	2.3
1	G	413	MET	2.3
2	F	186	MET	2.3
1	A	391	ASN	2.3
1	I	260	THR	2.3
1	K	417	ARG	2.3
1	A	298	GLU	2.3
1	C	229	SER	2.3
1	I	89	LYS	2.3
1	I	277	TYR	2.3
1	I	442	TYR	2.3
1	K	169	LYS	2.3
1	K	430	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	223	ALA	2.3
1	I	224	ALA	2.3
1	A	179	GLN	2.3
1	E	76	THR	2.3
1	G	325	THR	2.3
1	G	141	GLU	2.3
1	G	246	GLY	2.3
1	I	313	GLY	2.3
1	K	263	ASN	2.3
1	K	232	TYR	2.3
2	F	179	LEU	2.3
1	A	364	ALA	2.3
1	G	449	MET	2.3
1	I	203	ALA	2.3
2	B	44	GLU	2.3
2	B	188	PHE	2.3
2	L	58	MET	2.3
1	G	32	LYS	2.3
1	K	353	TRP	2.3
1	A	254	SER	2.3
1	G	334	PRO	2.3
1	G	64	GLU	2.3
2	B	13	GLU	2.3
1	K	302	ALA	2.2
1	C	384	PHE	2.2
1	G	332	PHE	2.2
1	E	316	VAL	2.2
1	G	280	GLU	2.2
1	K	321	GLY	2.2
1	K	39	ILE	2.2
1	I	424	ASP	2.2
1	A	163	ALA	2.2
1	E	333	LEU	2.2
2	F	180	LEU	2.2
1	G	22	GLU	2.2
1	I	186	TYR	2.2
2	J	70	GLU	2.2
1	C	352	VAL	2.2
1	G	352	VAL	2.2
1	I	372	ARG	2.2
1	E	218	CYS	2.2
1	E	329	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	67	ARG	2.2
1	I	410	ASN	2.2
2	L	126	ASP	2.2
1	G	365	GLU	2.2
1	A	294	GLN	2.2
1	K	88	GLN	2.2
1	K	340	ARG	2.2
1	C	380	ALA	2.2
1	G	360	ALA	2.2
2	D	102	TRP	2.2
2	L	161	ASN	2.2
1	A	389	GLY	2.2
2	L	179	LEU	2.2
1	C	143	PHE	2.2
1	A	340	ARG	2.2
1	E	91	LYS	2.2
2	F	52	LYS	2.2
1	G	428	ASN	2.2
1	I	256	ALA	2.2
1	C	388	ASP	2.2
1	K	198	LEU	2.2
1	K	452	PRO	2.2
1	C	89	LYS	2.2
1	E	215	VAL	2.2
1	G	295	TYR	2.2
2	F	117	VAL	2.2
1	G	23	ALA	2.2
1	G	169	LYS	2.2
1	I	257	GLN	2.1
1	K	308	ARG	2.2
1	C	216	ILE	2.1
1	C	97	LEU	2.1
2	L	180	LEU	2.1
2	H	87	GLU	2.1
1	G	228	CYS	2.1
1	G	422	HIS	2.1
1	I	193	TYR	2.1
1	I	228	CYS	2.1
1	A	416	GLY	2.1
1	C	354	ALA	2.1
2	B	150	GLY	2.1
1	I	407	GLN	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	16	SER	2.1
2	F	132	SER	2.1
2	J	133	ALA	2.1
1	G	137	PRO	2.1
1	E	59	LEU	2.1
1	I	276	TRP	2.1
1	K	128	ASP	2.1
1	K	195	ASP	2.1
1	G	384	PHE	2.1
1	I	332	PHE	2.1
1	A	271	GLY	2.1
1	I	168	TYR	2.1
1	A	441	MET	2.1
1	C	440	GLY	2.1
1	G	234	ALA	2.1
2	B	132	SER	2.1
2	D	80	ALA	2.1
1	E	281	PRO	2.1
1	K	21	PRO	2.1
1	C	233	HIS	2.1
1	I	90	ASP	2.1
1	I	443	HIS	2.1
1	I	171	LEU	2.1
1	K	284	LEU	2.1
1	G	235	GLY	2.1
1	G	321	GLY	2.1
1	K	159	GLY	2.1
1	K	306	GLU	2.1
1	I	220	TRP	2.1
2	F	128	PHE	2.1
1	K	20	THR	2.1
1	C	350	ILE	2.1
1	I	244	LEU	2.1
1	K	187	LEU	2.1
1	I	229	SER	2.1
1	K	446	MET	2.1
1	I	452	PRO	2.1
2	J	168	ALA	2.1
2	F	32	TYR	2.1
1	I	294	GLN	2.1
1	A	421	GLY	2.1
1	I	367	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	283	SER	2.1
1	G	194	MET	2.1
1	G	231	MET	2.1
1	G	459	PRO	2.1
1	K	447	ARG	2.1
1	I	167	THR	2.1
2	B	124	THR	2.1
1	A	378	PHE	2.1
1	E	222	PHE	2.1
1	G	227	PHE	2.1
2	F	188	PHE	2.1
2	J	128	PHE	2.1
1	I	200	ARG	2.0
1	K	177	ASP	2.0
2	H	66	ILE	2.0
1	G	324	MET	2.0
1	A	420	THR	2.0
1	C	221	LYS	2.0
2	H	52	LYS	2.0
2	J	90	TYR	2.0
1	C	391	ASN	2.0
1	I	158	TRP	2.0
1	K	160	PRO	2.0
1	G	133	LEU	2.0
2	F	184	LEU	2.0
1	E	380	ALA	2.0
1	G	207	ALA	2.0
1	K	180	ALA	2.0
1	K	132	LYS	2.0
1	C	437	ALA	2.0
1	G	316	VAL	2.0
2	D	126	ASP	2.0
2	L	77	GLN	2.0

## 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 [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	1IT	E	1451	13/13	0.82	0.90	21.63	29,29,29,29	13
3	FES	G	900	4/4	0.93	0.18	0.38	54,54,55,55	0
5	1IT	C	1451	13/13	0.83	0.27	0.25	61,61,61,61	0
3	FES	K	900	4/4	0.96	0.17	0.22	57,57,57,58	0
4	FE2	I	901	1/1	0.93	0.18	-0.11	55,55,55,55	0
5	1IT	A	1460	13/13	0.87	0.25	-0.13	61,61,61,61	0
3	FES	I	900	4/4	0.96	0.16	-0.22	58,58,58,58	0
3	FES	E	900	4/4	0.98	0.14	-0.81	31,32,32,32	0
3	FES	C	900	4/4	0.98	0.13	-0.95	31,32,33,33	0
3	FES	A	900	4/4	0.95	0.14	-1.14	29,30,31,31	0
4	FE2	C	901	1/1	0.99	0.14	-3.55	33,33,33,33	0
4	FE2	E	901	1/1	0.98	0.13	-	41,41,41,41	0
4	FE2	G	901	1/1	0.98	0.18	-	57,57,57,57	0
4	FE2	K	901	1/1	0.95	0.15	-	57,57,57,57	0
4	FE2	A	901	1/1	0.99	0.16	-	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.