



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:50 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

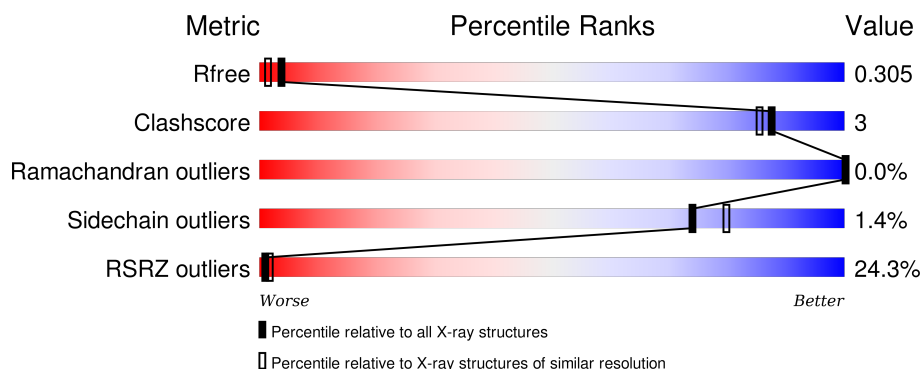
# 1 Overall quality at a glance i

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))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (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>20%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
1	C	459	<div> <div>19%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	E	459	<div> <div>15%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
1	G	459	<div> <div>36%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
1	I	459	<div> <div>34%</div> <div>87%</div> <div>8%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	459	
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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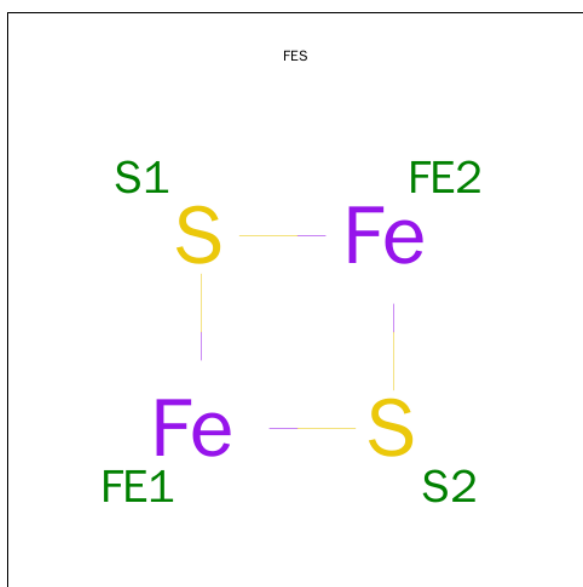
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Chain	Residue	Modelled	Actual	Comment	Reference
G	338	GLN	ASN	ENGINEERED MUTATION	UNP P37333
G	341	VAL	ILE	ENGINEERED MUTATION	UNP P37333
G	409	PHE	LEU	ENGINEERED MUTATION	UNP P37333
I	335	ALA	THR	ENGINEERED MUTATION	UNP P37333
I	336	MET	PHE	ENGINEERED 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>).

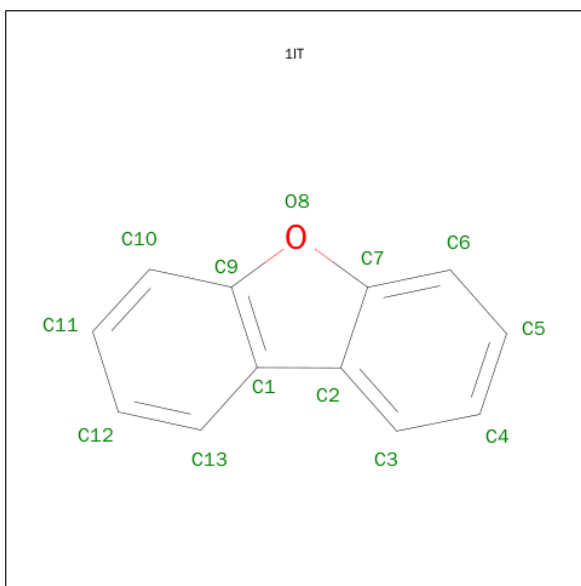


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		

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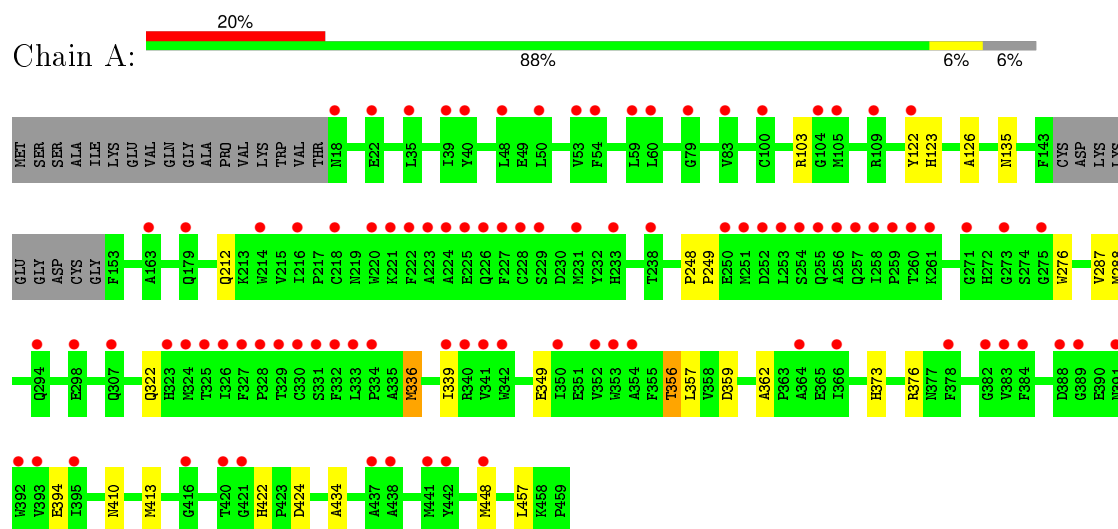
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	29	Total 29	O 29	0	0
6	J	31	Total 31	O 31	0	0
6	K	23	Total 23	O 23	0	0
6	L	17	Total 17	O 17	0	0

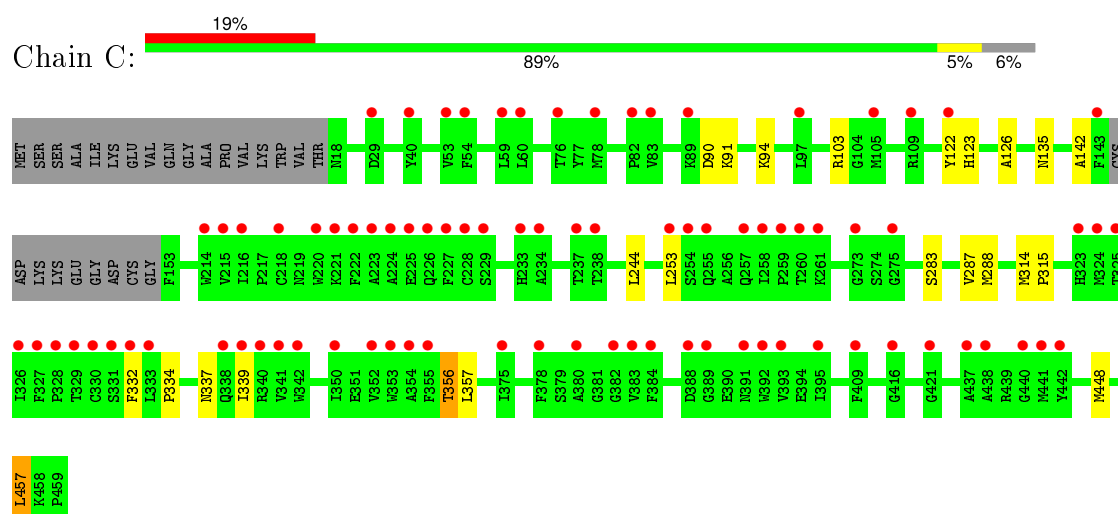
### 3 Residue-property plots

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

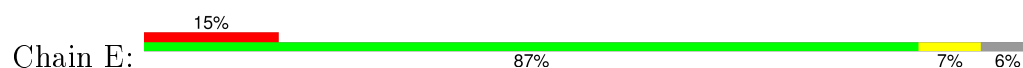
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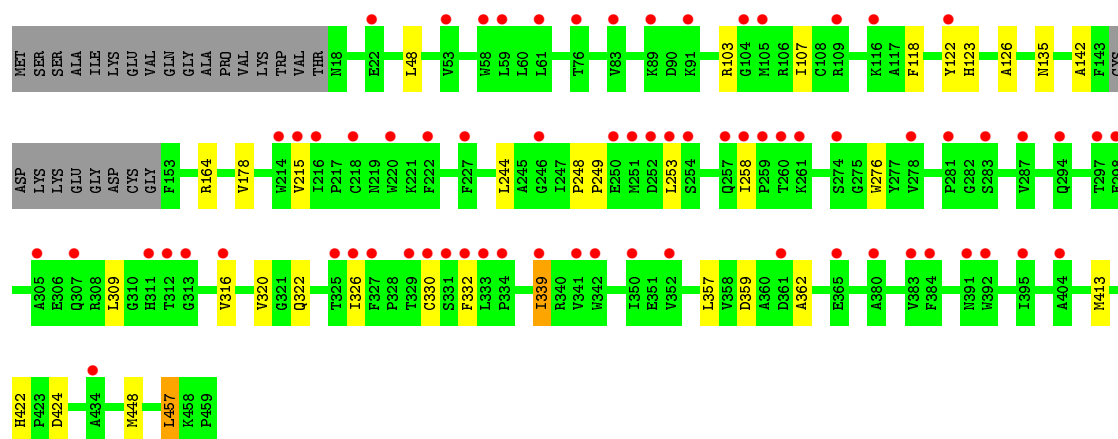


#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

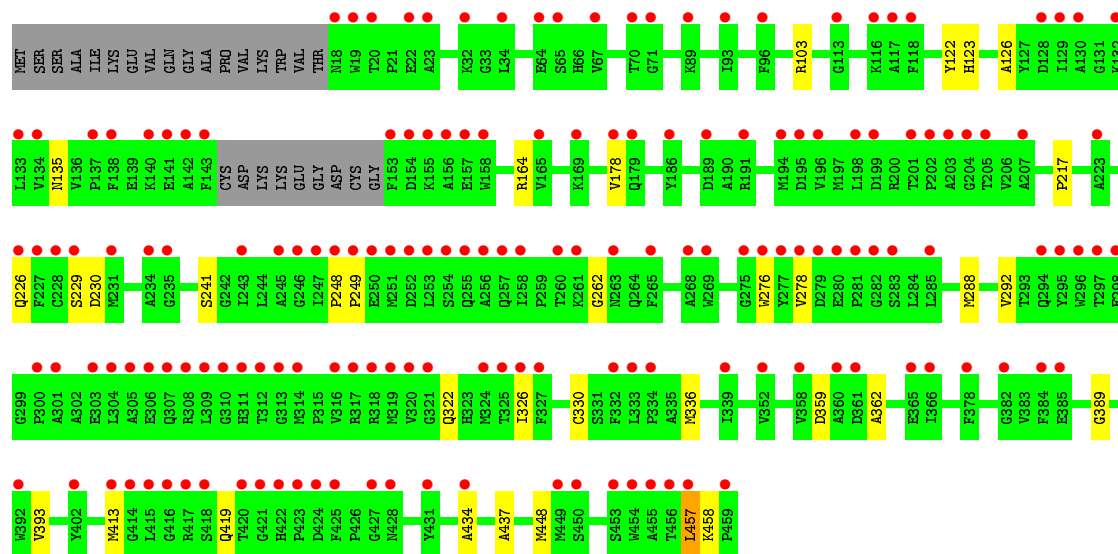
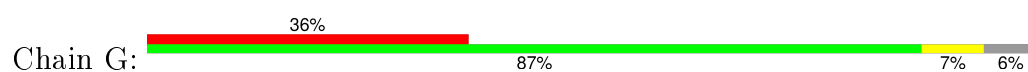


#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

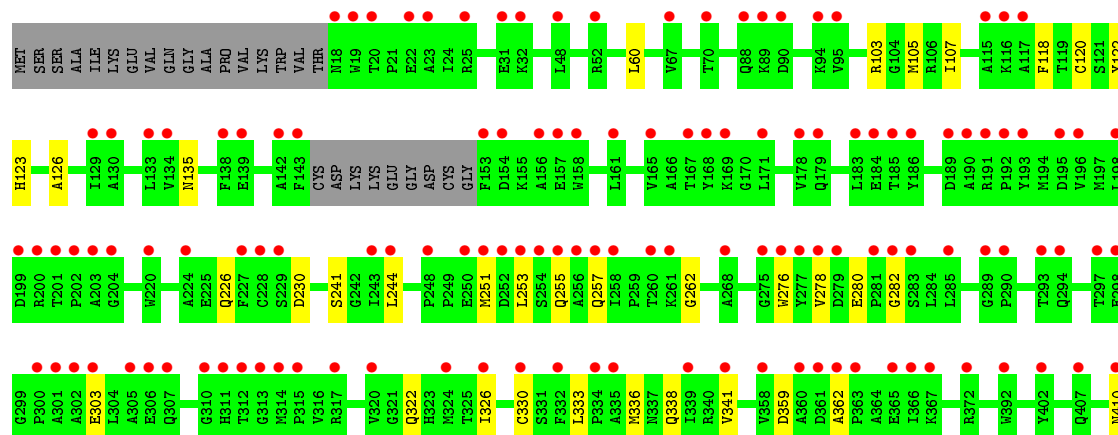
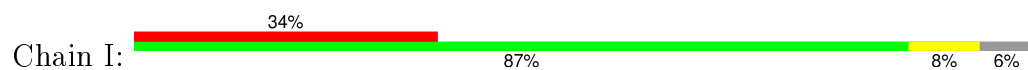


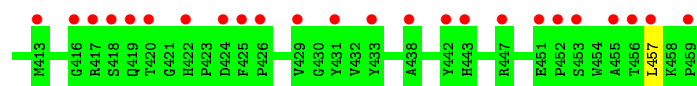


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

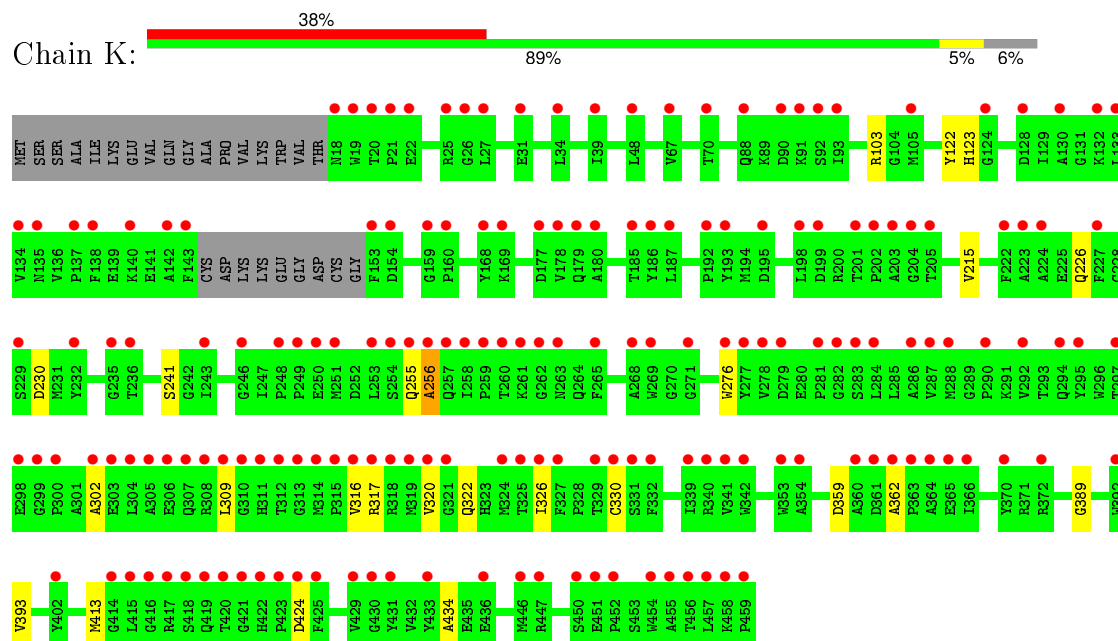


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

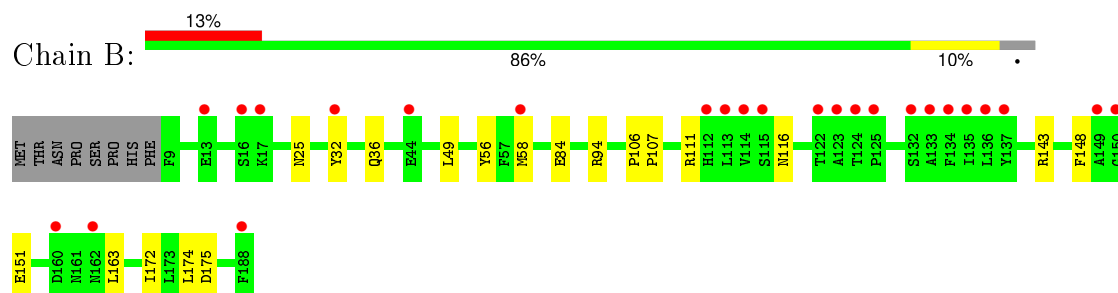




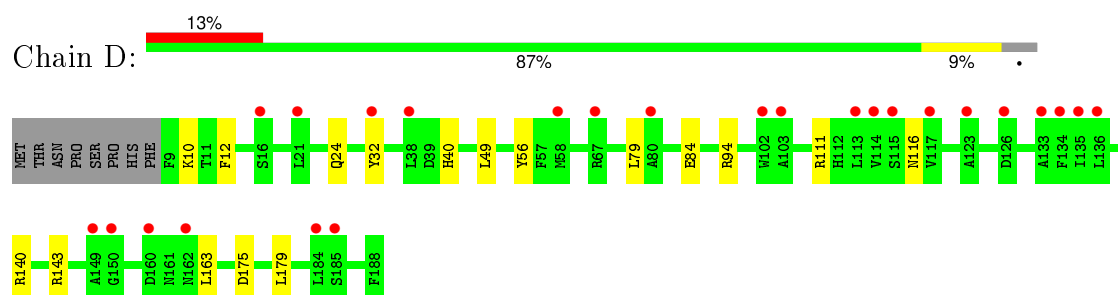
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



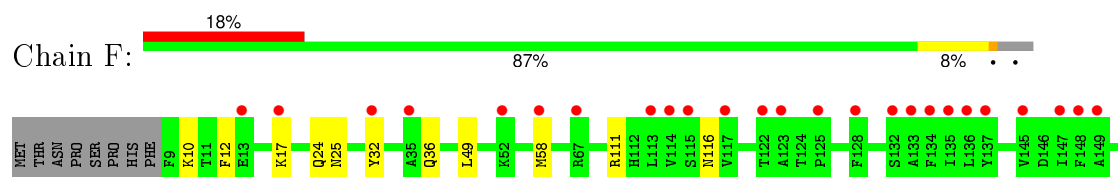
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

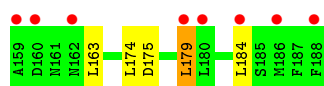


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

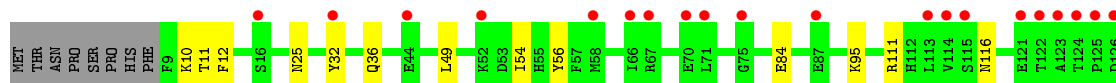
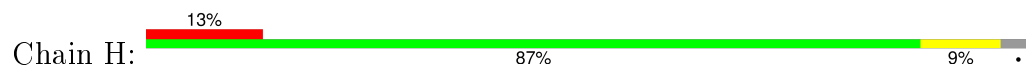


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

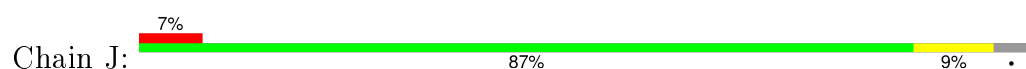




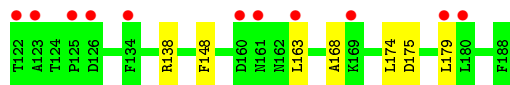
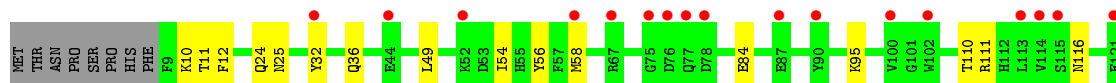
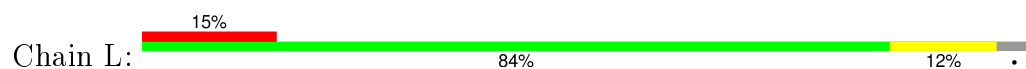
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• 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 0.285 , 0.305	Depositor DCC
$R_{free}$ test set	9870 reflections (5.28%)	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 , 36.3	EDS
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 196760 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:G:123:HIS:HB2	3:G:900:FES:S2	2.40	0.61
1:C:123:HIS:HB2	3:C:900:FES:S2	2.41	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
1:K:359:ASP:HB2	1:K:362:ALA:HB2	1.95	0.49
1:K:309:LEU:HD13	1:K:316:VAL:HG11	1.94	0.49
2:B:32:TYR:CD1	2:F:116:ASN:HA	2.47	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
2:D:24:GLN:HG2	2:F:25:ASN:HD21	1.78	0.48
1:A:349:GLU:OE2	2:D:143:ARG:NH2	2.42	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
1:I:126:ALA:HB3	1:I:135:ASN:HB3	1.96	0.47
2:D:175:ASP:OD2	2:F:111:ARG:HB2	2.14	0.47
1:I:257:GLN:HB3	1:I:282:GLY:HA3	1.97	0.47
1:C:287:VAL:HG12	1:C:288:MET:HE3	1.96	0.47
2:H:49:LEU:HD21	2:H:163:LEU:HD13	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:J:12:PHE:H	2:L:36:GLN:HE21	1.64	0.46
2:H:32:TYR:CD1	2:L:116:ASN:HA	2.50	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
2:L:54:ILE:HA	2:L:168:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:MET:HA	1:A:457:LEU:HD11	1.99	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:226:GLN:HA	1:G:230:ASP:HB3	2.00	0.44
1:G:126:ALA:HB3	1:G:135:ASN:HB3	1.99	0.44
1:I:107:ILE:HG22	1:I:118:PHE:HB3	1.99	0.44
2:D:116:ASN:HA	2:F:32:TYR:CD1	2.53	0.44
2:H:25:ASN:HD21	2:L:24:GLN:HG2	1.82	0.44
2:L:10:LYS:HG3	2:L:11:THR:N	2.32	0.44
2:J:116:ASN:HA	2:L:32:TYR:CD1	2.52	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:C:448:MET:HA	1:C:457:LEU:HD11	1.98	0.43
1:A:248:PRO:HA	1:A:249:PRO:HD3	1.93	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
2:H:111:ARG:HB2	2:L:175:ASP:OD2	2.18	0.43
1:G:262:GLY:HA2	1:G:278:VAL:HG23	2.00	0.43
1:C:283:SER:O	1:C:287:VAL:HG23	2.17	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:G:248:PRO:HA	1:G:249:PRO:HD3	1.91	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:A:126:ALA:HB3	1:A:135:ASN:HB3	2.00	0.43
2:L:10:LYS:HG3	2:L:11:THR:H	1.83	0.42
1:C:142:ALA:HB1	1:E:413:MET:HG3	2.01	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:326:ILE:HB	1:I:330:CYS:HB3	2.02	0.42
1:I:241:SER:HB2	2:J:95:LYS:HG3	2.00	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
2:H:12:PHE:H	2:J:36:GLN:NE2	2.19	0.41
1:G:326:ILE:HB	1:G:330:CYS:HB3	2.01	0.41
1:G:389:GLY:O	1:G:393:VAL:HG23	2.19	0.41
1:E:422:HIS:CD2	1:E:424:ASP:H	2.39	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:339:ILE:HD13	1:C:357:LEU:HG	2.02	0.40
1:C:314:MET:HA	1:C:315:PRO:HD3	1.89	0.40
1:C:90:ASP:O	1:C:91:LYS:HB2	2.20	0.40
1:I:105:MET:HB3	1:I:120:CYS:SG	2.62	0.40
1:G:164:ARG:HD2	1:G:178:VAL:HA	2.02	0.40
1:I:333:LEU:HD12	1:I:338:GLN:HB3	2.04	0.40
1:C:244:LEU:HD13	1:C:253:LEU:HG	2.02	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%)	52	51
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%)	68	74
1	C	350/372 (94%)	345 (99%)	5 (1%)	74	80
1	E	350/372 (94%)	343 (98%)	7 (2%)	63	67
1	G	350/372 (94%)	344 (98%)	6 (2%)	68	74
1	I	350/372 (94%)	343 (98%)	7 (2%)	63	67
1	K	350/372 (94%)	346 (99%)	4 (1%)	80	85
2	B	159/167 (95%)	158 (99%)	1 (1%)	90	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	159/167 (95%)	155 (98%)	4 (2%)	55	58
2	F	159/167 (95%)	156 (98%)	3 (2%)	65	69
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%)	90	94
All	All	3054/3234 (94%)	3010 (99%)	44 (1%)	74	80

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	-	11,15,15	1.23	0	12,21,21	1.99	4 (33%)
3	FES	A	900	1	0,4,4	0.00	-	0,4,4	0.00	-
5	1IT	C	1451	-	11,15,15	1.21	0	12,21,21	2.04	4 (33%)
3	FES	C	900	1	0,4,4	0.00	-	0,4,4	0.00	-
5	1IT	E	1451	-	11,15,15	1.20	0	12,21,21	1.99	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	IIT	C12-C13-C1	-2.50	116.48	120.79
5	E	1451	IIT	C4-C3-C2	-2.46	116.54	120.79
5	A	1460	IIT	C4-C3-C2	-2.44	116.58	120.79
5	E	1451	IIT	C12-C13-C1	-2.37	116.70	120.79
5	A	1460	IIT	C12-C13-C1	-2.35	116.74	120.79
5	C	1451	IIT	C4-C3-C2	-2.34	116.76	120.79
5	E	1451	IIT	C3-C2-C7	3.90	122.53	120.33
5	A	1460	IIT	C13-C1-C9	3.95	122.56	120.33
5	A	1460	IIT	C3-C2-C7	3.96	122.56	120.33
5	E	1451	IIT	C13-C1-C9	3.96	122.56	120.33
5	C	1451	IIT	C13-C1-C9	4.01	122.59	120.33
5	C	1451	IIT	C3-C2-C7	4.13	122.66	120.33

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%)	1.18	94 (21%) 1 2	37, 42, 48, 56	18 (4%)
1	C	433/459 (94%)	1.14	85 (19%) 1 2	37, 42, 48, 55	18 (4%)
1	E	433/459 (94%)	1.02	70 (16%) 3 4	36, 42, 50, 58	18 (4%)
1	G	433/459 (94%)	1.80	163 (37%) 0 1	37, 42, 48, 54	18 (4%)
1	I	433/459 (94%)	1.71	154 (35%) 0 1	38, 43, 47, 53	18 (4%)
1	K	433/459 (94%)	1.92	176 (40%) 0 1	38, 42, 48, 53	18 (4%)
2	B	180/188 (95%)	0.91	25 (13%) 4 6	38, 42, 48, 53	4 (2%)
2	D	180/188 (95%)	0.93	25 (13%) 4 6	38, 42, 48, 51	4 (2%)
2	F	180/188 (95%)	1.05	33 (18%) 2 3	38, 43, 47, 49	4 (2%)
2	H	180/188 (95%)	0.93	25 (13%) 4 6	38, 43, 47, 50	4 (2%)
2	J	180/188 (95%)	0.64	14 (7%) 16 22	37, 42, 46, 48	4 (2%)
2	L	180/188 (95%)	0.90	28 (15%) 3 4	37, 41, 45, 47	4 (2%)
All	All	3678/3882 (94%)	1.29	892 (24%) 1 2	36, 42, 48, 58	132 (3%)

All (892) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	258	ILE	9.8
1	C	258	ILE	9.7
1	G	305	ALA	8.0
1	K	278	VAL	7.3
1	K	455	ALA	7.1
1	G	258	ILE	6.8
1	K	258	ILE	6.7
1	G	307	GLN	6.5
1	K	361	ASP	6.5
1	G	278	VAL	6.5
1	G	310	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
1	I	282	GLY	6.4
1	K	204	GLY	6.1
2	F	160	ASP	6.1
1	C	339	ILE	6.0
1	A	224	ALA	6.0
1	G	253	LEU	6.0
1	K	282	GLY	6.0
1	A	227	PHE	5.9
1	G	204	GLY	5.9
1	I	416	GLY	5.8
1	G	294	GLN	5.8
1	K	22	GLU	5.8
1	G	309	LEU	5.7
1	C	331	SER	5.7
1	K	433	TYR	5.7
1	I	253	LEU	5.6
1	G	199	ASP	5.6
1	I	199	ASP	5.6
1	G	285	LEU	5.6
1	G	261	LYS	5.6
1	G	416	GLY	5.5
1	G	366	ILE	5.5
1	G	301	ALA	5.4
1	G	312	THR	5.4
1	K	153	PHE	5.4
1	I	278	VAL	5.4
2	F	123	ALA	5.4
1	K	370	TYR	5.4
1	K	281	PRO	5.4
1	C	227	PHE	5.4
1	K	311	HIS	5.3
1	G	143	PHE	5.3
1	E	105	MET	5.3
2	F	113	LEU	5.3
1	K	276	TRP	5.3
1	I	143	PHE	5.3
1	A	341	VAL	5.2
1	K	416	GLY	5.2
2	H	44	GLU	5.2
1	G	153	PHE	5.2
1	K	422	HIS	5.1
1	A	258	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	228	CYS	5.1
1	K	314	MET	5.1
1	C	333	LEU	5.1
2	B	113	LEU	5.0
1	A	223	ALA	5.0
1	K	18	ASN	5.0
1	I	117	ALA	5.0
1	A	260	THR	5.0
1	I	19	TRP	5.0
1	I	305	ALA	5.0
1	G	203	ALA	4.9
1	K	312	THR	4.9
1	K	431	TYR	4.9
1	A	325	THR	4.9
1	G	308	ARG	4.9
1	C	341	VAL	4.8
1	E	257	GLN	4.8
1	A	105	MET	4.8
2	D	113	LEU	4.8
1	G	453	SER	4.8
2	L	160	ASP	4.8
1	K	143	PHE	4.7
1	G	251	MET	4.7
1	G	243	ILE	4.7
2	J	113	LEU	4.7
1	K	424	ASP	4.7
1	A	331	SER	4.7
1	G	19	TRP	4.7
1	I	261	LYS	4.7
1	K	168	TYR	4.6
1	K	313	GLY	4.6
1	I	425	PHE	4.6
1	I	195	ASP	4.6
1	C	261	LYS	4.6
1	A	342	TRP	4.6
1	C	224	ALA	4.6
1	I	153	PHE	4.6
1	G	420	THR	4.5
1	I	297	THR	4.5
1	I	268	ALA	4.5
1	I	307	GLN	4.5
1	G	277	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	253	LEU	4.5
1	G	138	PHE	4.5
1	K	277	TYR	4.5
1	I	293	THR	4.5
1	G	320	VAL	4.5
1	I	202	PRO	4.5
1	K	318	ARG	4.5
1	K	341	VAL	4.4
1	E	260	THR	4.4
1	A	256	ALA	4.4
1	A	326	ILE	4.4
1	A	259	PRO	4.4
1	K	290	PRO	4.4
1	C	325	THR	4.4
1	A	226	GLN	4.4
1	G	415	LEU	4.4
1	K	253	LEU	4.4
1	G	201	THR	4.4
1	I	361	ASP	4.4
1	K	19	TRP	4.4
1	K	260	THR	4.4
1	G	18	ASN	4.3
1	K	279	ASP	4.3
1	K	292	VAL	4.3
1	A	222	PHE	4.3
1	A	257	GLN	4.3
1	K	257	GLN	4.3
1	K	459	PRO	4.3
1	I	252	ASP	4.3
1	I	418	SER	4.3
1	E	258	ILE	4.3
1	I	320	VAL	4.3
1	A	327	PHE	4.3
1	K	310	GLY	4.3
1	C	273	GLY	4.2
1	C	342	TRP	4.2
1	K	307	GLN	4.2
1	A	229	SER	4.2
1	K	31	GLU	4.2
1	C	105	MET	4.2
1	K	420	THR	4.2
1	A	251	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	395	ILE	4.2
1	C	228	CYS	4.2
1	K	331	SER	4.2
1	G	454	TRP	4.2
1	E	252	ASP	4.2
1	C	259	PRO	4.2
1	E	250	GLU	4.1
1	G	268	ALA	4.1
1	I	283	SER	4.1
1	K	309	LEU	4.1
1	I	178	VAL	4.1
2	H	113	LEU	4.1
1	G	333	LEU	4.1
2	F	114	VAL	4.1
1	G	303	GLU	4.1
1	G	304	LEU	4.1
2	B	160	ASP	4.1
1	K	304	LEU	4.1
1	K	303	GLU	4.0
1	I	138	PHE	4.0
1	K	295	TYR	4.0
1	G	431	TYR	4.0
1	K	283	SER	4.0
1	G	281	PRO	4.0
2	L	125	PRO	4.0
1	I	192	PRO	4.0
1	K	423	PRO	4.0
1	K	265	PHE	4.0
1	K	261	LYS	4.0
1	I	254	SER	4.0
1	I	300	PRO	4.0
1	I	457	LEU	3.9
2	L	67	ARG	3.9
1	A	384	PHE	3.9
2	F	134	PHE	3.9
1	G	254	SER	3.9
1	K	450	SER	3.9
1	G	195	ASP	3.9
2	H	160	ASP	3.9
1	K	300	PRO	3.9
2	D	123	ALA	3.9
1	C	378	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	311	HIS	3.9
1	C	340	ARG	3.9
1	C	223	ALA	3.9
1	G	142	ALA	3.9
1	G	255	GLN	3.9
1	K	203	ALA	3.9
1	K	236	THR	3.9
1	K	294	GLN	3.9
1	A	59	LEU	3.8
1	G	260	THR	3.8
1	I	303	GLU	3.8
1	I	201	THR	3.8
2	H	75	GLY	3.8
1	G	339	ILE	3.8
2	L	90	TYR	3.8
1	I	48	LEU	3.8
2	H	71	LEU	3.8
1	E	261	LYS	3.8
1	I	363	PRO	3.8
1	G	455	ALA	3.8
1	K	364	ALA	3.8
2	H	123	ALA	3.8
2	F	58	MET	3.8
1	C	332	PHE	3.8
1	G	155	LYS	3.8
1	K	248	PRO	3.8
1	I	190	ALA	3.7
1	K	70	THR	3.7
1	C	326	ILE	3.7
2	F	135	ILE	3.7
1	K	235	GLY	3.7
1	K	305	ALA	3.7
1	K	456	THR	3.7
1	G	157	GLU	3.7
1	K	178	VAL	3.7
2	H	126	ASP	3.7
1	I	453	SER	3.7
1	I	130	ALA	3.7
1	I	31	GLU	3.7
1	A	54	PHE	3.7
1	G	252	ASP	3.7
1	G	421	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	423	PRO	3.7
1	K	363	PRO	3.7
1	G	256	ALA	3.7
1	K	332	PHE	3.7
1	E	341	VAL	3.7
1	A	392	TRP	3.7
1	E	122	TYR	3.7
1	K	268	ALA	3.7
1	I	311	HIS	3.6
1	A	60	LEU	3.6
1	I	455	ALA	3.6
1	C	257	GLN	3.6
1	K	91	LYS	3.6
1	C	327	PHE	3.6
1	K	134	VAL	3.6
1	I	255	GLN	3.6
1	E	259	PRO	3.6
1	G	300	PRO	3.6
1	I	312	THR	3.6
1	K	223	ALA	3.6
1	K	251	MET	3.6
1	G	34	LEU	3.5
1	G	93	ILE	3.5
1	I	183	LEU	3.5
1	I	157	GLU	3.5
1	A	220	TRP	3.5
1	G	156	ALA	3.5
1	G	245	ALA	3.5
1	G	198	LEU	3.5
1	G	248	PRO	3.5
1	E	342	TRP	3.5
1	G	158	TRP	3.5
1	C	438	ALA	3.5
1	I	32	LYS	3.5
1	I	459	PRO	3.5
1	C	222	PHE	3.5
2	D	58	MET	3.5
1	I	429	VAL	3.5
1	I	315	PRO	3.5
1	C	395	ILE	3.5
1	K	372	ARG	3.5
1	I	116	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	18	ASN	3.5
1	A	109	ARG	3.5
1	I	243	ILE	3.5
1	C	421	GLY	3.5
1	K	229	SER	3.4
1	A	35	LEU	3.4
1	C	329	THR	3.4
1	K	415	LEU	3.4
1	A	437	ALA	3.4
1	G	202	PRO	3.4
1	G	361	ASP	3.4
1	I	279	ASP	3.4
2	J	160	ASP	3.4
1	K	192	PRO	3.4
1	K	259	PRO	3.4
1	E	332	PHE	3.4
1	G	456	THR	3.4
1	I	456	THR	3.4
1	G	450	SER	3.4
1	E	278	VAL	3.4
1	G	134	VAL	3.4
1	I	161	LEU	3.4
1	C	392	TRP	3.4
1	K	297	THR	3.3
1	K	199	ASP	3.3
2	D	114	VAL	3.3
1	C	255	GLN	3.3
1	K	93	ILE	3.3
1	E	251	MET	3.3
1	I	290	PRO	3.3
1	K	269	TRP	3.3
1	G	179	GLN	3.3
1	I	142	ALA	3.3
1	A	330	CYS	3.3
1	K	26	GLY	3.3
1	I	20	THR	3.3
2	D	160	ASP	3.3
1	E	214	TRP	3.3
1	G	317	ARG	3.3
1	K	320	VAL	3.3
1	K	454	TRP	3.3
1	K	458	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	330	CYS	3.3
1	I	330	CYS	3.3
2	F	136	LEU	3.3
1	E	331	SER	3.3
1	G	20	THR	3.3
1	I	251	MET	3.3
1	C	328	PRO	3.3
1	K	317	ARG	3.3
1	G	140	LYS	3.3
1	G	282	GLY	3.3
1	A	438	ALA	3.3
1	G	130	ALA	3.3
1	K	362	ALA	3.3
1	I	95	VAL	3.3
1	C	353	TRP	3.3
1	K	315	PRO	3.3
1	K	256	ALA	3.2
2	D	115	SER	3.2
1	K	319	MET	3.2
2	D	149	ALA	3.2
2	D	134	PHE	3.2
1	C	60	LEU	3.2
1	K	25	ARG	3.2
1	E	326	ILE	3.2
1	A	40	TYR	3.2
1	E	294	GLN	3.2
1	A	275	GLY	3.2
1	K	138	PHE	3.2
2	L	113	LEU	3.2
2	D	135	ILE	3.2
2	H	16	SER	3.2
1	I	310	GLY	3.2
1	C	109	ARG	3.2
1	G	378	PHE	3.2
1	G	279	ASP	3.2
2	L	123	ALA	3.2
1	G	269	TRP	3.2
1	K	262	GLY	3.2
2	L	75	GLY	3.2
1	K	298	GLU	3.2
2	F	137	TYR	3.2
1	A	53	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	114	VAL	3.2
1	I	285	LEU	3.2
1	E	254	SER	3.1
1	G	318	ARG	3.1
1	G	67	VAL	3.1
1	G	457	LEU	3.1
1	A	328	PRO	3.1
2	H	125	PRO	3.1
1	A	388	ASP	3.1
1	K	339	ILE	3.1
1	K	193	TYR	3.1
1	A	323	HIS	3.1
1	K	202	PRO	3.1
2	D	103	ALA	3.1
1	I	366	ILE	3.1
1	C	253	LEU	3.1
1	K	130	ALA	3.1
1	K	425	PHE	3.1
1	A	261	LYS	3.1
1	A	333	LEU	3.1
2	J	114	VAL	3.1
1	E	392	TRP	3.1
1	A	339	ILE	3.1
1	E	305	ALA	3.0
1	I	23	ALA	3.0
1	I	115	ALA	3.0
1	K	90	ASP	3.0
1	I	129	ILE	3.0
1	G	314	MET	3.0
1	I	196	VAL	3.0
2	B	136	LEU	3.0
1	C	214	TRP	3.0
1	C	220	TRP	3.0
1	I	298	GLU	3.0
2	L	44	GLU	3.0
1	A	39	ILE	3.0
1	A	216	ILE	3.0
2	H	67	ARG	3.0
1	C	59	LEU	3.0
1	I	133	LEU	3.0
1	I	134	VAL	3.0
1	G	71	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	361	ASP	3.0
2	H	70	GLU	3.0
1	K	243	ILE	3.0
1	G	70	THR	3.0
1	A	83	VAL	3.0
1	K	365	GLU	3.0
1	K	254	SER	3.0
1	K	418	SER	3.0
1	A	233	HIS	3.0
1	K	140	LYS	3.0
1	A	225	GLU	3.0
1	E	334	PRO	3.0
1	I	341	VAL	3.0
1	K	287	VAL	3.0
2	B	114	VAL	3.0
1	C	409	PHE	3.0
1	K	92	SER	3.0
2	F	162	ASN	3.0
1	G	382	GLY	2.9
1	E	220	TRP	2.9
1	G	129	ILE	2.9
1	A	442	TYR	2.9
1	C	226	GLN	2.9
1	K	414	GLY	2.9
2	B	123	ALA	2.9
1	K	48	LEU	2.9
1	C	383	VAL	2.9
1	I	191	ARG	2.9
2	B	58	MET	2.9
1	C	355	PHE	2.9
1	K	299	GLY	2.9
1	K	421	GLY	2.9
1	G	132	LYS	2.9
1	G	298	GLU	2.9
1	G	418	SER	2.9
2	J	71	LEU	2.9
2	L	100	VAL	2.9
1	G	263	ASN	2.9
1	I	339	ILE	2.9
2	B	135	ILE	2.9
1	K	27	LEU	2.9
2	L	114	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	122	TYR	2.9
1	I	431	TYR	2.9
1	A	332	PHE	2.9
1	A	250	GLU	2.9
1	G	306	GLU	2.9
1	A	273	GLY	2.9
1	I	417	ARG	2.9
1	K	249	PRO	2.9
2	B	133	ALA	2.9
1	C	238	THR	2.9
1	G	297	THR	2.9
2	J	97	THR	2.9
1	G	326	ILE	2.8
1	E	298	GLU	2.8
1	A	354	ALA	2.8
1	I	189	ASP	2.8
1	C	260	THR	2.8
1	G	276	TRP	2.8
1	I	317	ARG	2.8
2	J	52	LYS	2.8
2	L	76	ASP	2.8
1	A	350	ILE	2.8
1	C	82	PRO	2.8
1	K	34	LEU	2.8
1	K	286	ALA	2.8
2	L	122	THR	2.8
1	I	179	GLN	2.8
1	E	383	VAL	2.8
2	F	17	LYS	2.8
2	H	121	GLU	2.8
1	I	422	HIS	2.8
2	B	149	ALA	2.8
1	A	104	GLY	2.8
1	K	201	THR	2.8
2	H	122	THR	2.8
1	E	307	GLN	2.8
1	G	358	VAL	2.8
1	K	419	GLN	2.8
1	C	122	TYR	2.8
1	K	186	TYR	2.8
1	K	327	PHE	2.8
2	L	115	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	257	GLN	2.8
1	I	420	THR	2.8
1	K	457	LEU	2.8
1	A	393	VAL	2.8
2	H	58	MET	2.7
1	K	360	ALA	2.7
1	E	325	THR	2.7
1	I	169	LYS	2.7
1	I	184	GLU	2.7
1	C	254	SER	2.7
2	F	133	ALA	2.7
1	C	218	CYS	2.7
1	G	247	ILE	2.7
1	K	316	VAL	2.7
1	E	246	GLY	2.7
1	K	105	MET	2.7
1	A	253	LEU	2.7
2	F	115	SER	2.7
2	J	115	SER	2.7
2	H	149	ALA	2.7
1	E	327	PHE	2.7
1	K	135	ASN	2.7
1	C	441	MET	2.7
1	I	365	GLU	2.7
1	K	124	GLY	2.7
1	E	216	ILE	2.7
1	K	429	VAL	2.7
1	K	250	GLU	2.7
1	G	313	GLY	2.7
1	G	191	ARG	2.6
1	E	339	ILE	2.6
1	G	424	ASP	2.6
1	A	214	TRP	2.6
1	K	342	TRP	2.6
1	G	65	SER	2.6
1	K	137	PRO	2.6
2	F	125	PRO	2.6
2	B	32	TYR	2.6
1	A	307	GLN	2.6
1	C	338	GLN	2.6
1	G	414	GLY	2.6
2	D	67	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	52	LYS	2.6
2	L	163	LEU	2.6
1	C	53	VAL	2.6
1	I	156	ALA	2.6
1	A	221	LYS	2.6
1	A	218	CYS	2.6
1	K	246	GLY	2.6
1	I	154	ASP	2.6
2	D	162	ASN	2.6
2	D	136	LEU	2.6
1	A	255	GLN	2.6
2	L	169	LYS	2.6
1	A	366	ILE	2.6
1	E	312	THR	2.6
1	A	352	VAL	2.6
1	A	383	VAL	2.6
1	C	393	VAL	2.6
1	G	178	VAL	2.6
1	I	306	GLU	2.6
1	I	447	ARG	2.6
1	K	354	ALA	2.6
2	B	125	PRO	2.6
1	E	313	GLY	2.6
1	G	189	ASP	2.6
2	H	162	ASN	2.6
1	E	311	HIS	2.6
1	G	392	TRP	2.6
1	I	94	LYS	2.6
1	K	142	ALA	2.6
1	G	165	VAL	2.6
1	I	324	MET	2.6
1	I	52	ARG	2.6
2	D	32	TYR	2.6
2	J	67	ARG	2.6
1	G	425	PHE	2.6
1	E	61	LEU	2.6
1	K	205	THR	2.6
1	I	302	ALA	2.6
1	C	324	MET	2.6
1	K	179	GLN	2.6
1	G	154	ASP	2.6
1	E	227	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	118	PHE	2.5
1	A	22	GLU	2.5
1	A	100	CYS	2.5
1	I	392	TRP	2.5
1	K	185	THR	2.5
1	I	198	LEU	2.5
2	D	21	LEU	2.5
2	F	149	ALA	2.5
1	A	324	MET	2.5
1	A	448	MET	2.5
1	C	323	HIS	2.5
1	I	314	MET	2.5
1	E	22	GLU	2.5
1	I	248	PRO	2.5
1	I	281	PRO	2.5
1	K	255	GLN	2.5
1	A	329	THR	2.5
1	G	265	PHE	2.5
1	K	325	THR	2.5
2	B	134	PHE	2.5
1	A	231	MET	2.5
1	I	335	ALA	2.5
1	K	330	CYS	2.5
2	D	184	LEU	2.5
1	I	22	GLU	2.5
1	E	352	VAL	2.5
1	I	67	VAL	2.5
1	I	419	GLN	2.5
1	C	76	THR	2.5
1	G	205	THR	2.5
1	I	185	THR	2.5
1	E	116	LYS	2.5
2	H	32	TYR	2.5
1	E	365	GLU	2.5
2	D	133	ALA	2.5
2	F	148	PHE	2.5
2	L	78	ASP	2.5
1	E	395	ILE	2.5
1	I	358	VAL	2.5
1	I	139	GLU	2.5
2	L	121	GLU	2.5
1	E	434	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	301	ALA	2.5
1	K	224	ALA	2.5
1	K	324	MET	2.5
1	E	109	ARG	2.5
2	H	115	SER	2.5
1	G	250	GLU	2.5
1	I	250	GLU	2.5
2	F	13	GLU	2.5
1	K	392	TRP	2.5
1	I	70	THR	2.5
1	G	116	LYS	2.5
1	C	40	TYR	2.5
1	G	186	TYR	2.5
1	I	402	TYR	2.5
1	E	283	SER	2.5
1	E	104	GLY	2.5
2	D	150	GLY	2.5
1	A	334	PRO	2.5
1	E	297	THR	2.5
1	I	224	ALA	2.4
1	A	79	GLY	2.4
1	G	427	GLY	2.4
1	K	402	TYR	2.4
1	G	325	THR	2.4
1	K	39	ILE	2.4
1	A	364	ALA	2.4
1	G	223	ALA	2.4
1	I	203	ALA	2.4
2	D	16	SER	2.4
1	I	433	TYR	2.4
2	F	179	LEU	2.4
1	E	76	THR	2.4
1	C	352	VAL	2.4
1	E	316	VAL	2.4
1	G	352	VAL	2.4
1	G	413	MET	2.4
1	I	260	THR	2.4
1	E	89	LYS	2.4
1	G	246	GLY	2.4
1	I	88	GLN	2.4
1	I	313	GLY	2.4
1	K	430	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	353	TRP	2.4
1	C	384	PHE	2.4
1	I	442	TYR	2.4
2	B	188	PHE	2.4
1	K	169	LYS	2.4
1	C	229	SER	2.4
1	G	417	ARG	2.4
1	K	417	ARG	2.4
1	A	163	ALA	2.4
1	K	302	ALA	2.4
2	B	112	HIS	2.4
1	A	391	ASN	2.4
1	K	263	ASN	2.4
1	A	298	GLU	2.4
1	I	451	GLU	2.4
1	K	451	GLU	2.4
2	B	44	GLU	2.4
1	A	179	GLN	2.4
1	E	333	LEU	2.4
1	G	332	PHE	2.4
1	I	277	TYR	2.4
1	K	232	TYR	2.4
1	G	449	MET	2.4
2	F	186	MET	2.4
1	G	141	GLU	2.4
1	I	89	LYS	2.4
1	I	424	ASP	2.4
1	E	218	CYS	2.4
1	A	254	SER	2.4
1	C	143	PHE	2.4
1	K	321	GLY	2.4
2	F	180	LEU	2.4
2	B	13	GLU	2.4
1	C	380	ALA	2.3
1	G	23	ALA	2.3
1	G	334	PRO	2.3
1	E	215	VAL	2.3
1	G	32	LYS	2.3
1	G	64	GLU	2.3
2	L	58	MET	2.3
2	L	179	LEU	2.3
1	I	186	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	102	TRP	2.3
1	G	360	ALA	2.3
2	F	117	VAL	2.3
1	C	216	ILE	2.3
1	A	389	GLY	2.3
1	E	329	THR	2.3
2	L	126	ASP	2.3
1	I	372	ARG	2.3
1	K	198	LEU	2.3
1	G	22	GLU	2.3
1	G	280	GLU	2.3
1	I	256	ALA	2.3
2	J	70	GLU	2.3
2	F	67	ARG	2.3
1	C	97	LEU	2.3
2	L	180	LEU	2.3
1	G	234	ALA	2.3
2	J	133	ALA	2.3
1	A	294	GLN	2.3
1	C	388	ASP	2.3
1	I	410	ASN	2.3
1	I	276	TRP	2.3
1	K	88	GLN	2.3
2	L	161	ASN	2.3
1	G	365	GLU	2.3
1	C	354	ALA	2.3
1	E	59	LEU	2.3
1	I	171	LEU	2.3
2	D	80	ALA	2.3
1	A	340	ARG	2.3
1	K	340	ARG	2.3
1	G	384	PHE	2.3
1	I	332	PHE	2.3
1	C	440	GLY	2.3
1	G	228	CYS	2.3
1	I	228	CYS	2.3
1	C	350	ILE	2.3
1	G	137	PRO	2.3
1	K	452	PRO	2.3
1	E	91	LYS	2.3
1	K	195	ASP	2.3
1	G	428	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	52	LYS	2.3
1	I	244	LEU	2.3
1	K	284	LEU	2.3
1	A	416	GLY	2.2
2	B	16	SER	2.2
2	B	150	GLY	2.2
2	F	132	SER	2.2
1	G	295	TYR	2.2
1	I	168	TYR	2.2
1	I	193	TYR	2.2
2	F	128	PHE	2.2
2	H	87	GLU	2.2
1	C	89	LYS	2.2
1	G	169	LYS	2.2
1	I	257	GLN	2.2
1	K	308	ARG	2.2
1	K	128	ASP	2.2
1	I	220	TRP	2.2
1	A	271	GLY	2.2
1	G	235	GLY	2.2
1	G	321	GLY	2.2
1	G	422	HIS	2.2
2	B	132	SER	2.2
2	J	168	ALA	2.2
1	K	187	LEU	2.2
1	I	407	GLN	2.2
1	I	90	ASP	2.2
1	K	21	PRO	2.2
2	H	66	ILE	2.2
1	K	159	GLY	2.2
1	A	441	MET	2.2
1	E	281	PRO	2.2
1	E	222	PHE	2.2
1	G	227	PHE	2.2
2	F	32	TYR	2.2
2	F	188	PHE	2.2
2	J	128	PHE	2.2
1	K	20	THR	2.2
1	C	233	HIS	2.2
1	I	443	HIS	2.2
1	A	421	GLY	2.2
1	I	229	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	446	MET	2.2
1	K	306	GLU	2.2
1	A	378	PHE	2.2
1	I	167	THR	2.2
2	B	124	THR	2.2
1	G	283	SER	2.2
1	G	316	VAL	2.2
1	G	207	ALA	2.2
1	K	180	ALA	2.2
1	G	459	PRO	2.2
1	I	452	PRO	2.2
1	G	133	LEU	2.2
1	G	231	MET	2.2
2	F	184	LEU	2.2
1	I	158	TRP	2.2
1	K	177	ASP	2.2
1	E	380	ALA	2.2
1	E	350	ILE	2.2
1	K	366	ILE	2.2
1	G	194	MET	2.1
1	I	294	GLN	2.1
1	A	420	THR	2.1
1	A	353	TRP	2.1
1	C	221	LYS	2.1
1	I	367	LYS	2.1
2	J	90	TYR	2.1
1	C	437	ALA	2.1
1	K	160	PRO	2.1
1	K	447	ARG	2.1
1	G	324	MET	2.1
2	H	52	LYS	2.1
1	A	50	LEU	2.1
1	C	391	ASN	2.1
1	G	327	PHE	2.1
1	I	200	ARG	2.1
1	K	222	PHE	2.1
2	F	35	ALA	2.1
1	E	287	VAL	2.1
2	D	117	VAL	2.1
2	D	126	ASP	2.1
1	A	382	GLY	2.1
1	C	382	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	113	GLY	2.1
1	G	229	SER	2.1
2	J	184	LEU	2.1
1	K	132	LYS	2.1
1	G	117	ALA	2.1
1	I	362	ALA	2.1
1	C	442	TYR	2.1
2	L	32	TYR	2.1
2	L	102	TRP	2.1
1	C	78	MET	2.1
1	G	275	GLY	2.1
1	I	204	GLY	2.1
1	I	275	GLY	2.1
2	F	145	VAL	2.1
1	E	391	ASN	2.1
1	A	238	THR	2.1
1	C	375	ILE	2.1
1	K	436	GLU	2.1
2	L	77	GLN	2.1
1	K	133	LEU	2.1
1	G	249	PRO	2.1
1	C	234	ALA	2.1
1	A	18	ASN	2.1
1	C	389	GLY	2.1
1	E	330	CYS	2.1
1	K	227	PHE	2.1
1	K	271	GLY	2.1
2	L	87	GLU	2.1
1	C	215	VAL	2.1
1	E	53	VAL	2.1
1	G	226	GLN	2.1
1	G	296	TRP	2.1
1	I	165	VAL	2.1
1	K	329	THR	2.1
2	B	122	THR	2.1
2	F	122	THR	2.1
2	H	124	THR	2.1
2	H	184	LEU	2.1
1	G	434	ALA	2.1
2	B	115	SER	2.1
2	D	185	SER	2.1
1	E	384	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	96	PHE	2.1
1	I	227	PHE	2.1
2	L	134	PHE	2.1
1	G	402	TYR	2.1
1	C	83	VAL	2.1
1	C	237	THR	2.0
1	E	58	TRP	2.0
1	I	326	ILE	2.0
1	G	89	LYS	2.0
1	I	25	ARG	2.0
1	I	334	PRO	2.0
1	C	416	GLY	2.0
1	I	289	GLY	2.0
1	I	438	ALA	2.0
1	K	288	MET	2.0
1	A	252	ASP	2.0
1	C	29	ASP	2.0
1	C	225	GLU	2.0
1	G	385	GLU	2.0
1	C	54	PHE	2.0
1	G	196	VAL	2.0
2	B	17	LYS	2.0
2	B	137	TYR	2.0
2	B	162	ASN	2.0
1	K	326	ILE	2.0
1	A	48	LEU	2.0
2	D	38	LEU	2.0
1	E	404	ALA	2.0
1	G	128	ASP	2.0
1	G	319	MET	2.0
1	I	360	ALA	2.0
1	I	413	MET	2.0
1	K	154	ASP	2.0
2	F	159	ALA	2.0
2	H	133	ALA	2.0
1	E	83	VAL	2.0
1	K	67	VAL	2.0
1	I	426	PRO	2.0
1	C	275	GLY	2.0
1	E	274	SER	2.0
2	F	147	ILE	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	1IT	E	1451	13/13	0.82	0.90	21.60	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	-0.14	61,61,61,61	0
3	FES	I	900	4/4	0.96	0.16	-0.21	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	-3.58	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.