



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 5, 2016 – 03:38 PM EDT

PDB ID : 5AEW  
Title : Crystal structure of II9 variant of Biphenyl dioxygenase from Burkholderia xenovorans LB400 in complex with biphenyl  
Authors : Dhindwal, S.; Gomez-Gil, L.; Sylvestre, M.; Eltis, L.D.; Bolin, J.T.; Kumar, P.  
Deposited on : 2015-01-10  
Resolution : 1.88 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

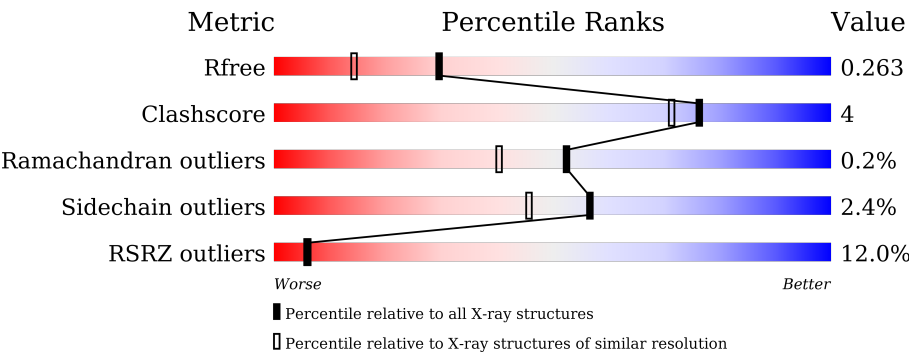
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027457  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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></div><div><div></div><div></div><div></div><div></div></div><div>87%7%6%</div></div>
1	C	459	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>89%5%6%</div></div>
1	E	459	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>88%6%6%</div></div>
1	G	459	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>88%5%6%</div></div>
1	I	459	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>83%10%6%</div></div>
1	K	459	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>87%7%6%</div></div>

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Mol	Chain	Length	Quality of chain
1	M	459	
1	O	459	
1	Q	459	
1	S	459	
1	U	459	
1	W	459	
2	B	188	
2	D	188	
2	F	188	
2	H	188	
2	J	188	
2	L	188	
2	N	188	
2	P	188	
2	R	188	
2	T	188	
2	V	188	
2	X	188	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	Q	460	-	-	X	-
3	FES	W	460	-	-	X	-
5	BNL	E	462	-	-	-	X
5	BNL	Q	462	-	-	-	X
5	BNL	S	462	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 63519 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	2	0
			3442	2189	604	625	24			
1	C	433	Total	C	N	O	S	0	2	0
			3444	2190	606	624	24			
1	E	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	G	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	I	433	Total	C	N	O	S	0	1	0
			3433	2184	602	623	24			
1	K	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	M	433	Total	C	N	O	S	0	1	0
			3434	2184	603	624	23			
1	O	433	Total	C	N	O	S	0	1	0
			3433	2184	602	623	24			
1	Q	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	S	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	U	430	Total	C	N	O	S	0	0	0
			3405	2163	599	620	23			
1	W	432	Total	C	N	O	S	0	0	0
			3417	2171	601	622	23			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
A	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
A	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
A	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
C	335	GLY	THR	ENGINEERED MUTATION	UNP P37333

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Chain	Residue	Modelled	Actual	Comment	Reference
C	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
C	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
C	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
E	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
E	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
E	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
E	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
G	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
G	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
G	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
G	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
I	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
I	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
I	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
I	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
K	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
K	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
K	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
K	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
M	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
M	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
M	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
M	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
O	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
O	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
O	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
O	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
Q	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
Q	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
Q	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
Q	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
S	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
S	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
S	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
S	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
U	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
U	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
U	338	THR	ASN	ENGINEERED MUTATION	UNP P37333
U	341	THR	ILE	ENGINEERED MUTATION	UNP P37333
W	335	GLY	THR	ENGINEERED MUTATION	UNP P37333
W	336	ILE	PHE	ENGINEERED MUTATION	UNP P37333
W	338	THR	ASN	ENGINEERED MUTATION	UNP P37333

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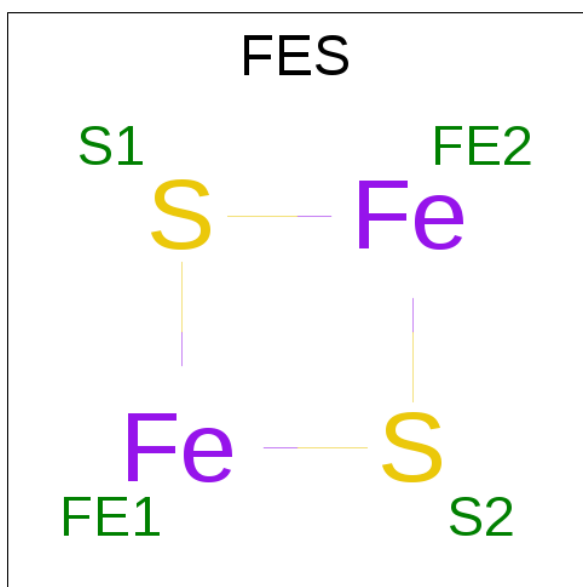
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Chain	Residue	Modelled	Actual	Comment	Reference
W	341	THR	ILE	ENGINEERED MUTATION	UNP P37333

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	1	0
			1532	972	271	285	4			
2	D	183	Total	C	N	O	S	0	2	0
			1541	977	272	288	4			
2	F	184	Total	C	N	O	S	0	2	0
			1544	979	272	289	4			
2	H	181	Total	C	N	O	S	0	1	0
			1515	961	267	283	4			
2	J	175	Total	C	N	O	S	0	1	0
			1454	918	259	273	4			
2	L	182	Total	C	N	O	S	0	1	0
			1522	966	269	283	4			
2	N	183	Total	C	N	O	S	0	0	0
			1524	968	270	282	4			
2	P	181	Total	C	N	O	S	0	3	0
			1522	967	266	284	5			
2	R	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	T	182	Total	C	N	O	S	0	0	0
			1517	963	269	281	4			
2	V	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	X	180	Total	C	N	O	S	0	1	0
			1501	951	265	281	4			

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

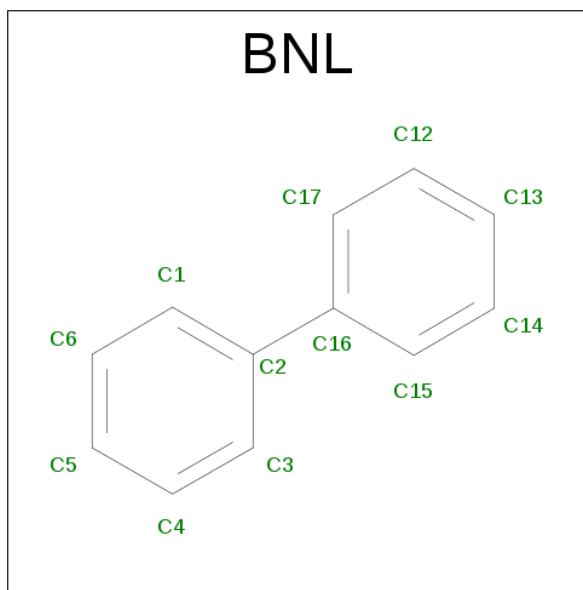


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		
3	M	1	Total	Fe	S	0	0
			4	2	2		
3	O	1	Total	Fe	S	0	0
			4	2	2		
3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

- Molecule 5 is BIPHENYL (three-letter code: BNL) (formula:  $C_{12}H_{10}$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C 12 12	0	0
5	E	1	Total C 12 12	0	0
5	I	1	Total C 12 12	0	0
5	K	1	Total C 12 12	0	0
5	M	1	Total C 12 12	0	0
5	O	1	Total C 12 12	0	0
5	Q	1	Total C 12 12	0	0
5	S	1	Total C 12 12	0	0
5	W	1	Total C 12 12	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	381	Total O 381 381	0	0
6	B	194	Total O 194 194	0	0
6	C	376	Total O 376 376	0	0
6	D	169	Total O 169 169	0	0
6	E	266	Total O 266 266	0	0
6	F	177	Total O 177 177	0	0
6	G	239	Total O 239 239	0	0
6	H	138	Total O 138 138	0	0
6	I	241	Total O 241 241	0	0
6	J	136	Total O 136 136	0	0
6	K	241	Total O 241 241	0	0

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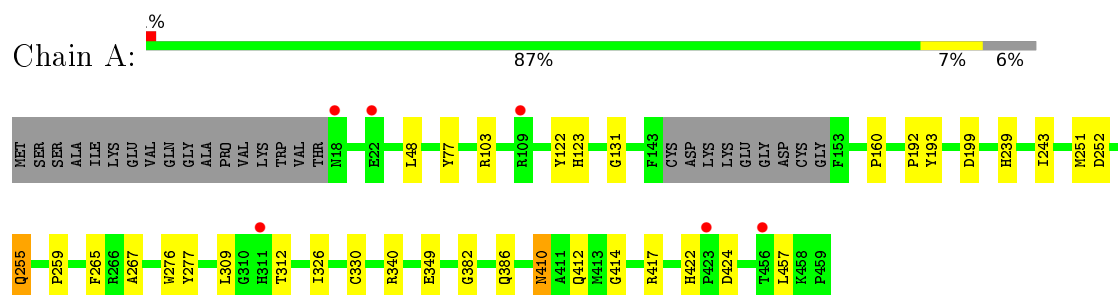
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	130	Total 130	O 130	0	0
6	M	204	Total 204	O 204	0	0
6	N	101	Total 101	O 101	0	0
6	O	205	Total 205	O 205	0	0
6	P	108	Total 108	O 108	0	0
6	Q	150	Total 150	O 150	0	0
6	R	124	Total 124	O 124	0	0
6	S	95	Total 95	O 95	0	0
6	T	73	Total 73	O 73	0	0
6	U	107	Total 107	O 107	0	0
6	V	54	Total 54	O 54	0	0
6	W	73	Total 73	O 73	0	0
6	X	35	Total 35	O 35	0	0

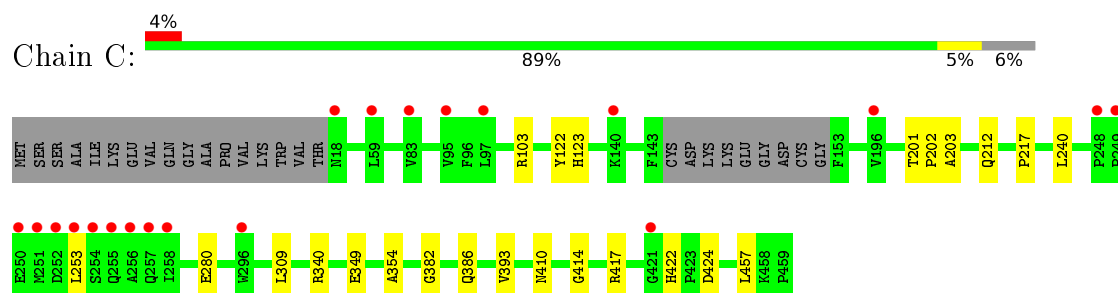
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

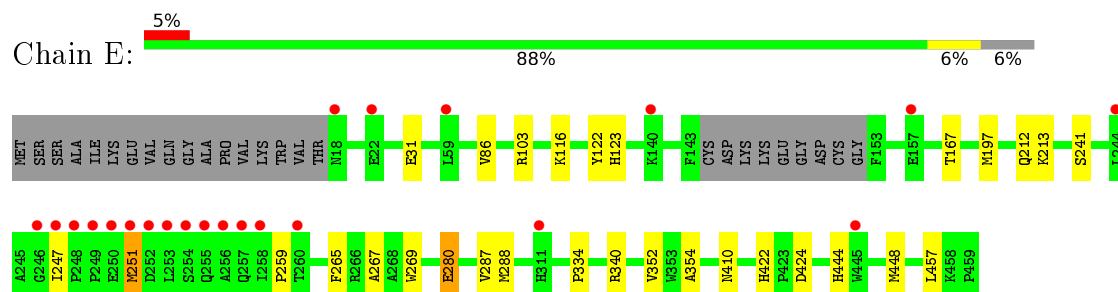
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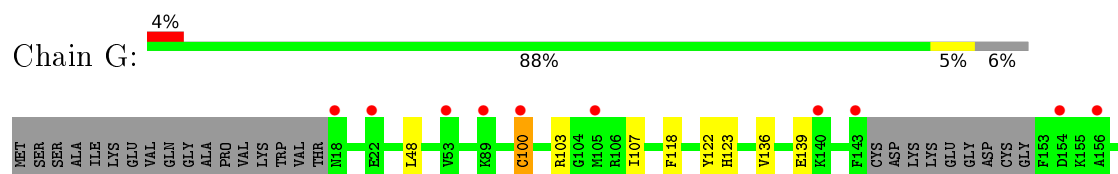
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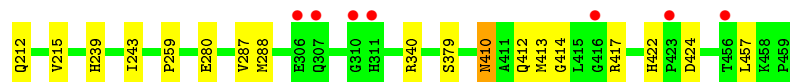


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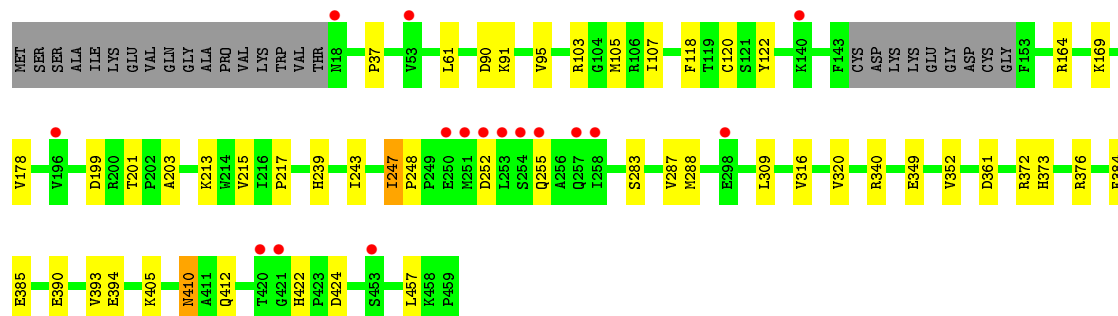
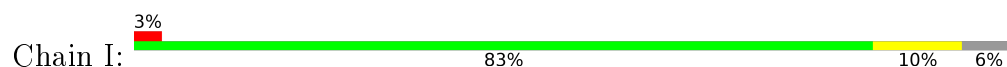


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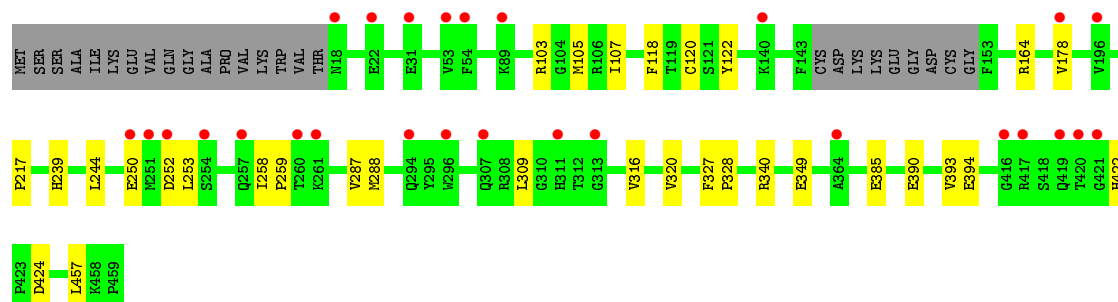
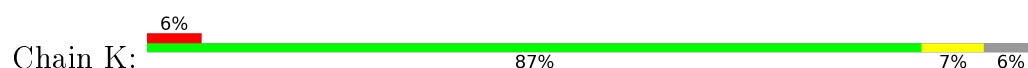




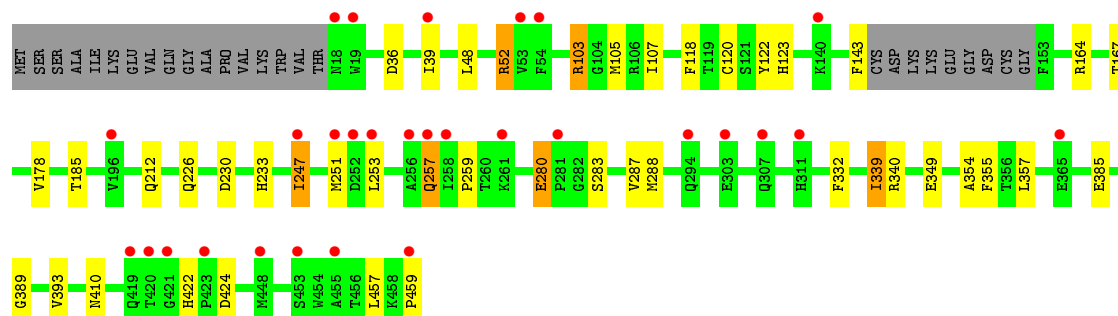
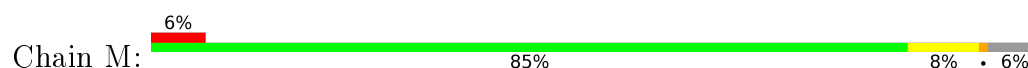
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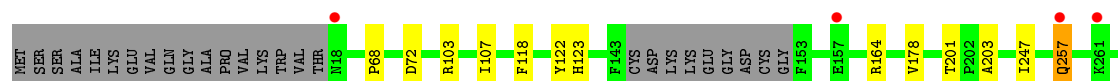
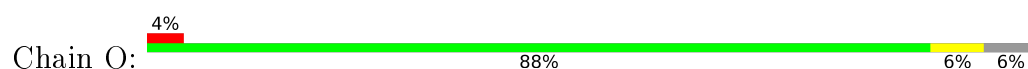
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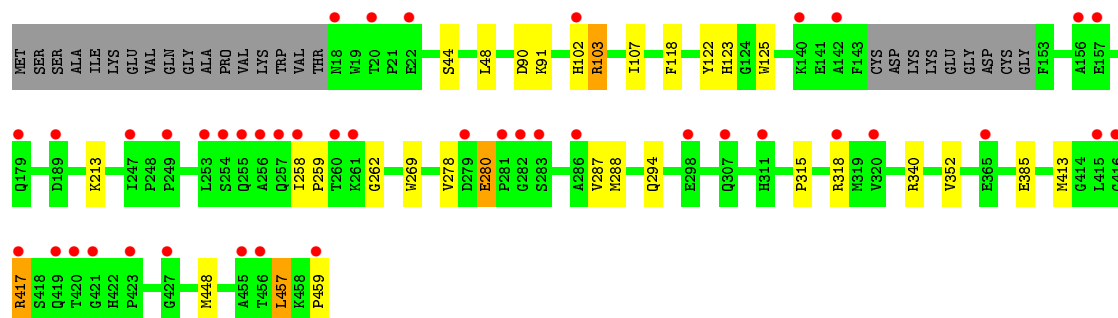
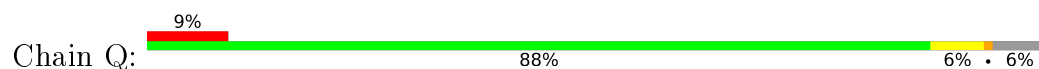


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

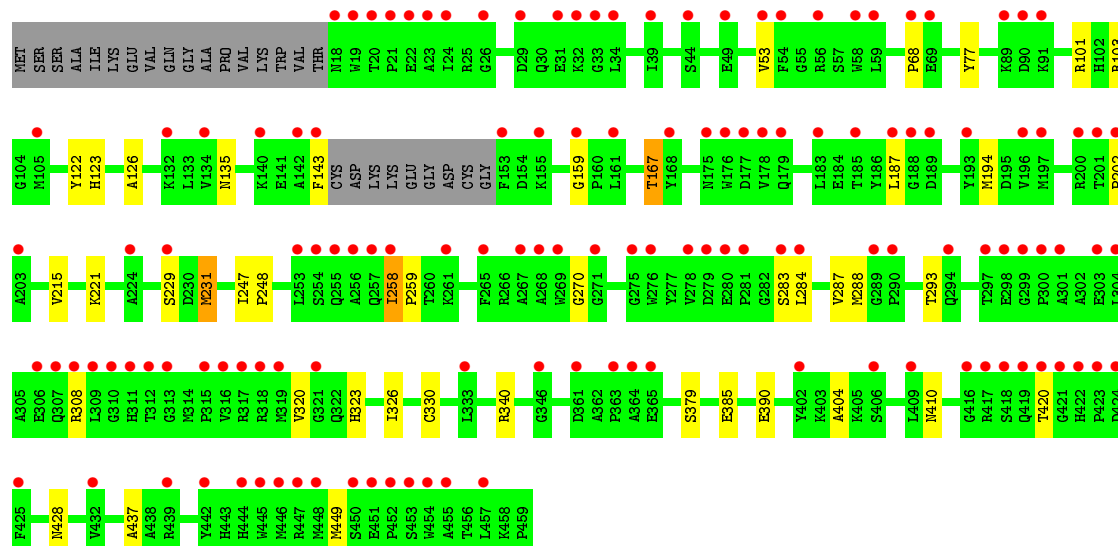
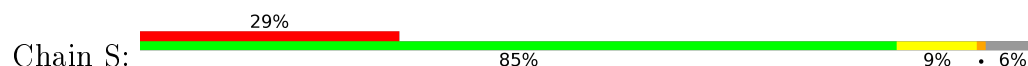




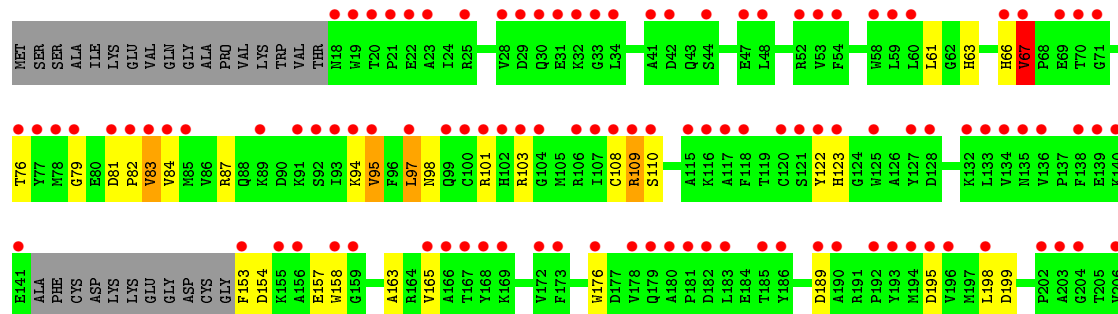
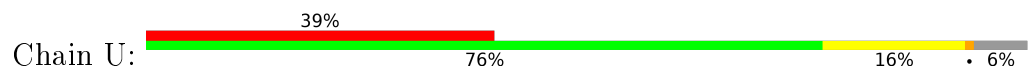
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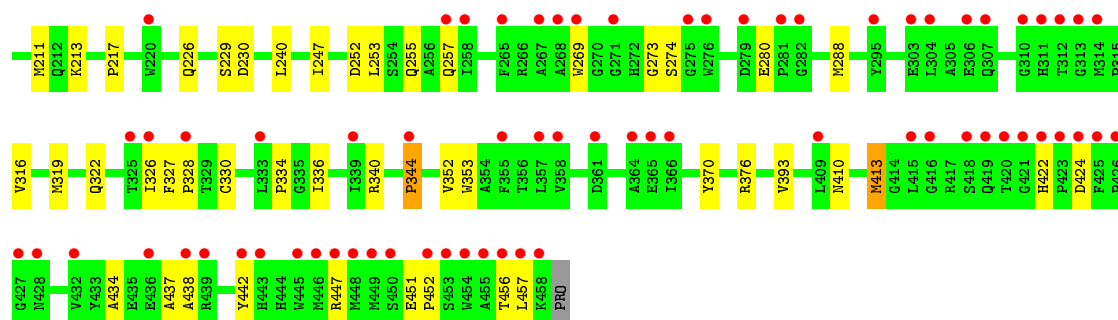


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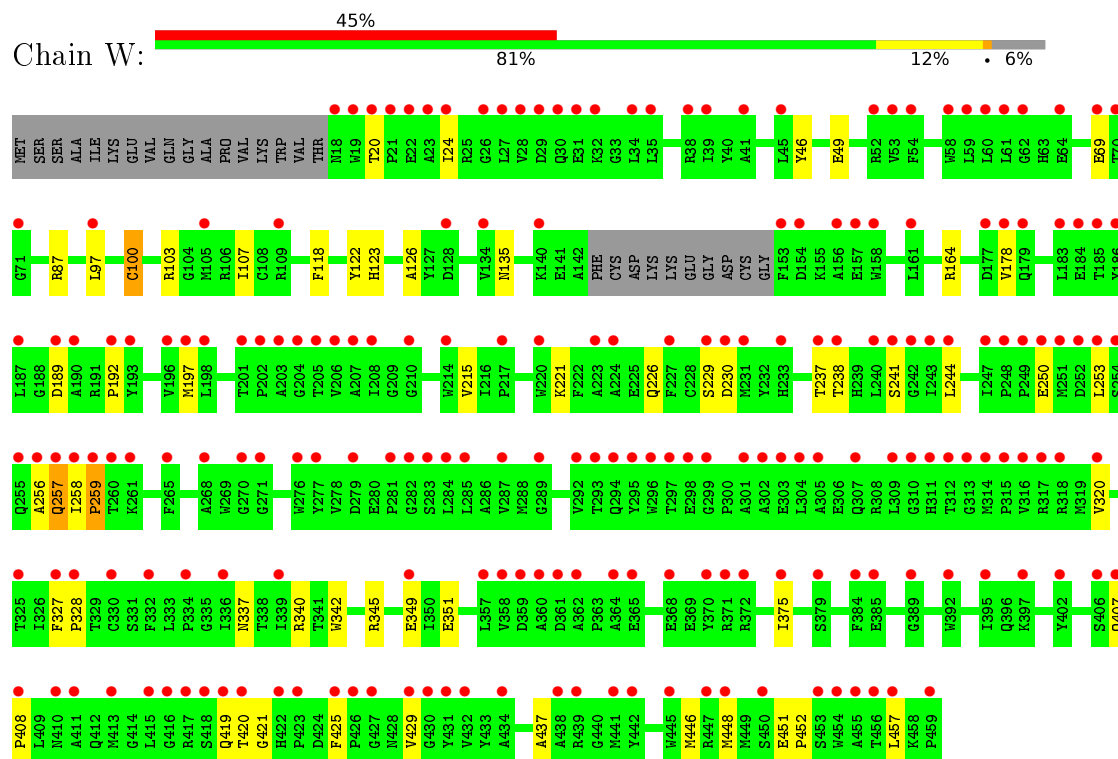


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

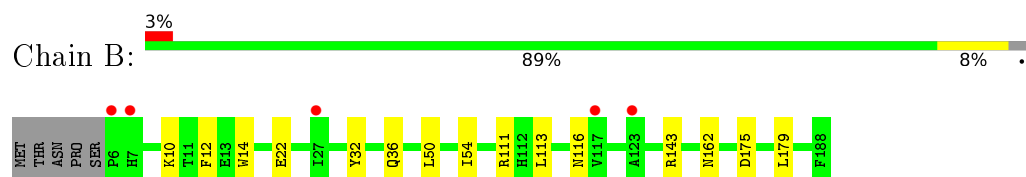




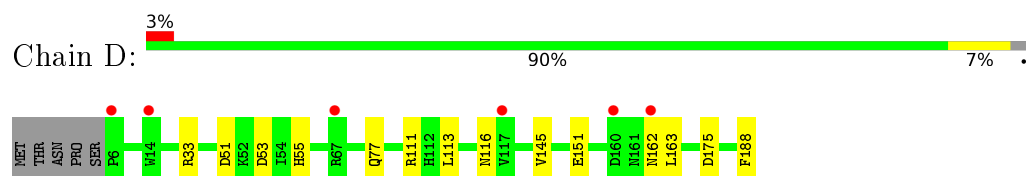
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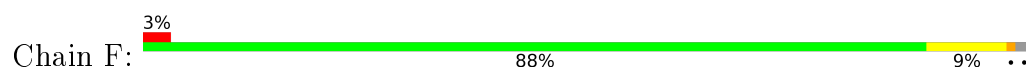
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

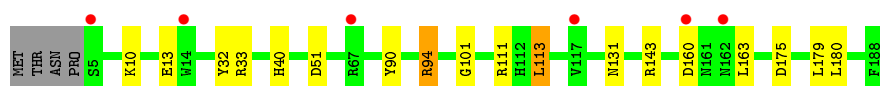


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

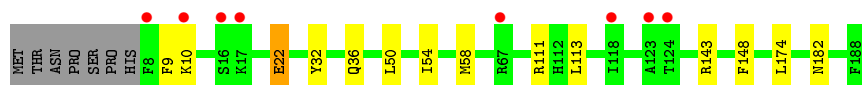
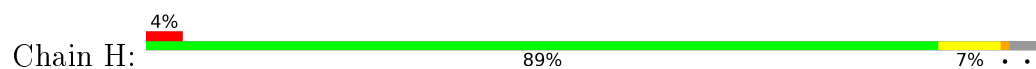


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

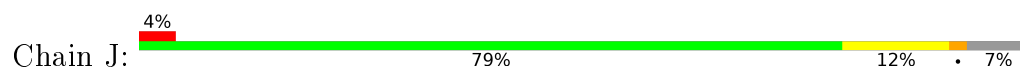




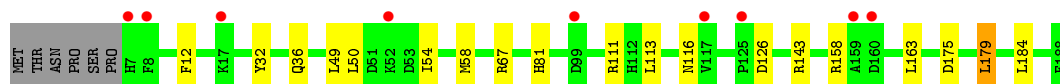
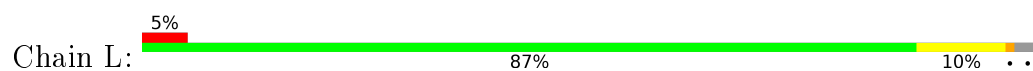
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



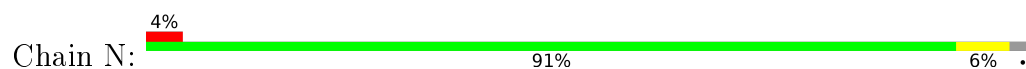
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



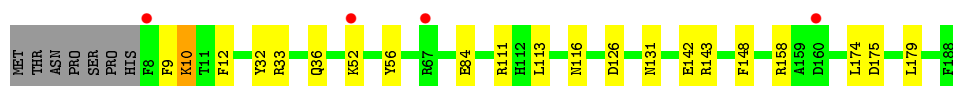
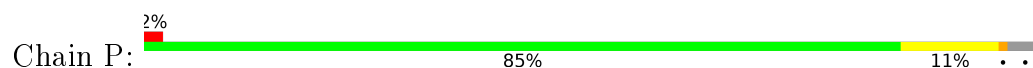
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



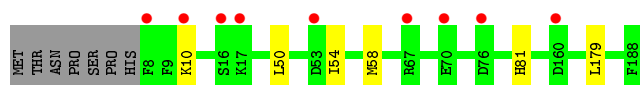
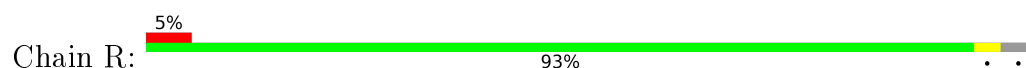
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



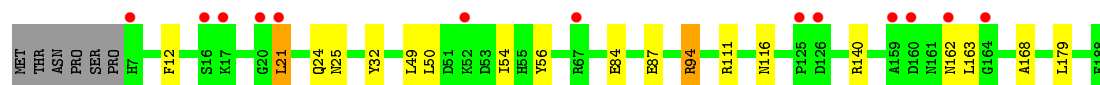
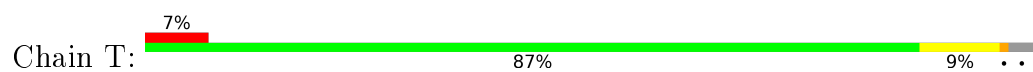
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



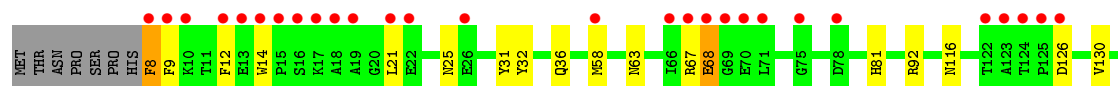
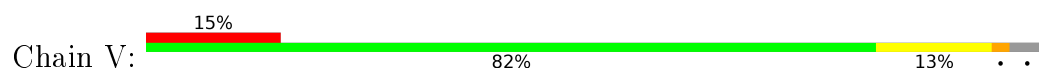
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



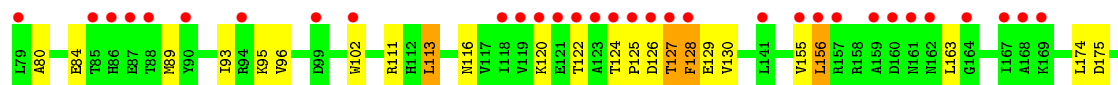
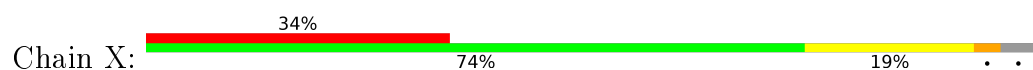
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.77Å 133.19Å 133.97Å 102.31° 102.54° 104.54°	Depositor
Resolution (Å)	23.34 – 1.88 23.33 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.1 (23.34-1.88) 87.2 (23.33-1.88)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.225 , 0.263 0.225 , 0.263	Depositor DCC
$R_{free}$ test set	32697 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for k,l,h 0.027 for l,h,k 0.013 for -k,-h,-l 0.018 for -l,-k,-h 0.016 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	63519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: FE2, FES, BNL

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	0.37	0/3547	0.55	0/4814
1	C	0.38	0/3549	0.56	0/4816
1	E	0.37	0/3530	0.56	0/4792
1	G	0.36	0/3530	0.56	1/4792 (0.0%)
1	I	0.36	0/3538	0.55	0/4802
1	K	0.35	0/3530	0.53	0/4792
1	M	0.35	0/3539	0.53	0/4804
1	O	0.33	0/3538	0.52	0/4802
1	Q	0.34	0/3530	0.53	0/4792
1	S	0.31	0/3530	0.49	0/4792
1	U	0.31	0/3505	0.50	0/4757
1	W	0.30	0/3518	0.48	0/4776
2	B	0.39	0/1569	0.59	0/2121
2	D	0.40	0/1578	0.62	0/2133
2	F	0.40	0/1584	0.63	0/2142
2	H	0.38	0/1550	0.58	0/2095
2	J	0.40	0/1489	0.60	1/2014 (0.0%)
2	L	0.38	0/1561	0.56	0/2110
2	N	0.38	0/1561	0.57	0/2110
2	P	0.39	0/1566	0.58	0/2117
2	R	0.37	0/1542	0.55	0/2084
2	T	0.35	0/1553	0.53	0/2099
2	V	0.34	0/1542	0.53	0/2084
2	X	0.31	0/1538	0.51	0/2079
All	All	0.35	0/61017	0.54	2/82719 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	143	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	G	100	CYS	CA-CB-SG	5.08	123.14	114.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	0	3300	20	0
1	C	3444	0	3305	12	0
1	E	3428	0	3284	17	0
1	G	3428	0	3284	16	0
1	I	3433	0	3293	26	0
1	K	3428	0	3284	15	0
1	M	3434	0	3292	29	0
1	O	3433	0	3293	15	0
1	Q	3428	0	3284	17	0
1	S	3428	0	3284	26	0
1	U	3405	0	3263	61	0
1	W	3417	0	3275	39	0
2	B	1532	0	1474	15	0
2	D	1541	0	1479	12	0
2	F	1544	0	1484	16	0
2	H	1515	0	1459	15	0
2	J	1454	0	1407	23	0
2	L	1522	0	1467	17	0
2	N	1524	0	1471	16	0
2	P	1522	0	1473	15	0
2	R	1507	0	1456	3	0
2	T	1517	0	1463	20	0
2	V	1507	0	1456	32	0
2	X	1501	0	1451	35	0
3	A	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
3	K	4	0	0	0	0
3	M	4	0	0	1	0
3	O	4	0	0	1	0
3	Q	4	0	0	2	0
3	S	4	0	0	1	0
3	U	4	0	0	1	0
3	W	4	0	0	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
4	S	1	0	0	0	0
4	U	1	0	0	0	0
4	W	1	0	0	0	0
5	C	12	0	10	3	0
5	E	12	0	10	1	0
5	I	12	0	10	0	0
5	K	12	0	10	0	0
5	M	12	0	10	1	0
5	O	12	0	10	0	0
5	Q	12	0	10	0	0
5	S	12	0	10	0	0
5	W	12	0	10	0	0
6	A	381	0	0	1	0
6	B	194	0	0	1	0
6	C	376	0	0	5	0
6	D	169	0	0	1	0
6	E	266	0	0	2	0
6	F	177	0	0	1	0
6	G	239	0	0	0	0
6	H	138	0	0	0	0
6	I	241	0	0	3	0
6	J	136	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	241	0	0	1	0
6	L	130	0	0	1	0
6	M	204	0	0	1	0
6	N	101	0	0	1	0
6	O	205	0	0	0	0
6	P	108	0	0	1	0
6	Q	150	0	0	0	0
6	R	124	0	0	0	0
6	S	95	0	0	4	0
6	T	73	0	0	0	0
6	U	107	0	0	5	0
6	V	54	0	0	0	0
6	W	73	0	0	0	0
6	X	35	0	0	1	0
All	All	63519	0	57071	443	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 4.

The worst 5 of 443 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)
2:V:67:ARG:O	2:V:68:GLU:HG3	1.21	1.28
1:E:167:THR:HB	6:E:2123:HOH:O	1.39	1.19
2:H:58:MET:HE3	2:H:174:LEU:HD22	1.28	1.14
1:U:109:ARG:HG3	1:U:109:ARG:HH11	1.01	1.12
2:V:67:ARG:O	2:V:68:GLU:CG	2.01	1.08

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	431/459 (94%)	419 (97%)	12 (3%)	0	100	100
1	C	431/459 (94%)	418 (97%)	13 (3%)	0	100	100
1	E	429/459 (94%)	419 (98%)	10 (2%)	0	100	100
1	G	429/459 (94%)	416 (97%)	13 (3%)	0	100	100
1	I	430/459 (94%)	415 (96%)	15 (4%)	0	100	100
1	K	429/459 (94%)	413 (96%)	16 (4%)	0	100	100
1	M	430/459 (94%)	413 (96%)	17 (4%)	0	100	100
1	O	430/459 (94%)	413 (96%)	17 (4%)	0	100	100
1	Q	429/459 (94%)	415 (97%)	13 (3%)	1 (0%)	52	40
1	S	429/459 (94%)	411 (96%)	17 (4%)	1 (0%)	52	40
1	U	426/459 (93%)	400 (94%)	22 (5%)	4 (1%)	21	8
1	W	428/459 (93%)	406 (95%)	19 (4%)	3 (1%)	26	13
2	B	182/188 (97%)	177 (97%)	5 (3%)	0	100	100
2	D	183/188 (97%)	176 (96%)	7 (4%)	0	100	100
2	F	184/188 (98%)	179 (97%)	5 (3%)	0	100	100
2	H	180/188 (96%)	174 (97%)	6 (3%)	0	100	100
2	J	174/188 (93%)	167 (96%)	6 (3%)	1 (1%)	30	16
2	L	181/188 (96%)	176 (97%)	5 (3%)	0	100	100
2	N	181/188 (96%)	177 (98%)	4 (2%)	0	100	100
2	P	182/188 (97%)	172 (94%)	9 (5%)	1 (0%)	34	20
2	R	179/188 (95%)	173 (97%)	5 (3%)	1 (1%)	30	16
2	T	180/188 (96%)	175 (97%)	5 (3%)	0	100	100
2	V	179/188 (95%)	170 (95%)	8 (4%)	1 (1%)	30	16
2	X	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	30	16
All	All	7315/7764 (94%)	7043 (96%)	258 (4%)	14 (0%)	52	40

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	67	VAL
1	U	83	VAL
2	V	68	GLU
1	W	257	GLN
1	W	259	PRO

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/372 (95%)	346 (98%)	7 (2%)	63	54
1	C	353/372 (95%)	346 (98%)	7 (2%)	63	54
1	E	351/372 (94%)	343 (98%)	8 (2%)	58	48
1	G	351/372 (94%)	344 (98%)	7 (2%)	63	54
1	I	352/372 (95%)	343 (97%)	9 (3%)	54	42
1	K	351/372 (94%)	341 (97%)	10 (3%)	51	39
1	M	352/372 (95%)	338 (96%)	14 (4%)	38	24
1	O	352/372 (95%)	345 (98%)	7 (2%)	63	54
1	Q	351/372 (94%)	341 (97%)	10 (3%)	51	39
1	S	351/372 (94%)	342 (97%)	9 (3%)	54	42
1	U	349/372 (94%)	334 (96%)	15 (4%)	35	21
1	W	350/372 (94%)	345 (99%)	5 (1%)	74	69
2	B	163/167 (98%)	161 (99%)	2 (1%)	78	74
2	D	164/167 (98%)	163 (99%)	1 (1%)	90	89
2	F	165/167 (99%)	159 (96%)	6 (4%)	42	28
2	H	161/167 (96%)	160 (99%)	1 (1%)	90	89
2	J	155/167 (93%)	150 (97%)	5 (3%)	46	33
2	L	162/167 (97%)	161 (99%)	1 (1%)	90	89
2	N	162/167 (97%)	159 (98%)	3 (2%)	65	56
2	P	163/167 (98%)	160 (98%)	3 (2%)	66	59
2	R	160/167 (96%)	159 (99%)	1 (1%)	90	89
2	T	161/167 (96%)	156 (97%)	5 (3%)	47	34
2	V	160/167 (96%)	158 (99%)	2 (1%)	76	71
2	X	160/167 (96%)	153 (96%)	7 (4%)	35	20
All	All	6152/6468 (95%)	6007 (98%)	145 (2%)	57	46

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	52	ARG
1	O	103	ARG
1	W	103	ARG
1	M	122	TYR
1	M	339	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	444	HIS
2	N	162	ASN
1	W	257	GLN
2	L	36	GLN
1	M	391	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 12 are monoatomic - leaving 21 for Mogul analysis.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FES	A	460	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	C	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	C	462	-	13,13,13	1.07	1 (7%)	16,16,16	0.45	0
3	FES	E	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	E	462	-	13,13,13	1.10	1 (7%)	16,16,16	0.70	0
3	FES	G	460	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	I	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	I	462	-	13,13,13	1.13	1 (7%)	16,16,16	0.47	0
3	FES	K	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	K	462	-	13,13,13	1.12	1 (7%)	16,16,16	0.51	0
3	FES	M	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	M	462	-	13,13,13	1.10	1 (7%)	16,16,16	0.46	0
3	FES	O	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	O	462	-	13,13,13	1.15	1 (7%)	16,16,16	0.65	0
3	FES	Q	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	Q	462	-	13,13,13	1.14	1 (7%)	16,16,16	0.52	0
3	FES	S	460	1,6	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	S	462	-	13,13,13	1.07	1 (7%)	16,16,16	0.65	0
3	FES	U	460	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	W	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	W	462	-	13,13,13	1.11	1 (7%)	16,16,16	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	A	460	1	-	0/0/4/4	0/1/1/1
3	FES	C	460	1	-	0/0/4/4	0/1/1/1
5	BNL	C	462	-	-	0/4/4/4	0/2/2/2
3	FES	E	460	1	-	0/0/4/4	0/1/1/1
5	BNL	E	462	-	-	0/4/4/4	0/2/2/2
3	FES	G	460	1	-	0/0/4/4	0/1/1/1
3	FES	I	460	1	-	0/0/4/4	0/1/1/1
5	BNL	I	462	-	-	0/4/4/4	0/2/2/2
3	FES	K	460	1	-	0/0/4/4	0/1/1/1
5	BNL	K	462	-	-	0/4/4/4	0/2/2/2
3	FES	M	460	1	-	0/0/4/4	0/1/1/1
5	BNL	M	462	-	-	0/4/4/4	0/2/2/2
3	FES	O	460	1	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BNL	O	462	-	-	0/4/4/4	0/2/2/2
3	FES	Q	460	1	-	0/0/4/4	0/1/1/1
5	BNL	Q	462	-	-	0/4/4/4	0/2/2/2
3	FES	S	460	1,6	-	0/0/4/4	0/1/1/1
5	BNL	S	462	-	-	0/4/4/4	0/2/2/2
3	FES	U	460	1	-	0/0/4/4	0/1/1/1
3	FES	W	460	1	-	0/0/4/4	0/1/1/1
5	BNL	W	462	-	-	0/4/4/4	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	462	BNL	C16-C2	-3.63	1.39	1.49
5	O	462	BNL	C16-C2	-3.46	1.40	1.49
5	W	462	BNL	C16-C2	-3.42	1.40	1.49
5	Q	462	BNL	C16-C2	-3.42	1.40	1.49
5	K	462	BNL	C16-C2	-3.39	1.40	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	460	FES	1	0
3	C	460	FES	1	0
5	C	462	BNL	3	0
3	E	460	FES	1	0
5	E	462	BNL	1	0
3	G	460	FES	1	0
3	M	460	FES	1	0
5	M	462	BNL	1	0
3	O	460	FES	1	0
3	Q	460	FES	2	0
3	S	460	FES	1	0
3	U	460	FES	1	0
3	W	460	FES	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	433/459 (94%)	0.08	6 (1%) 78 80	23, 26, 40, 53	11 (2%)
1	C	433/459 (94%)	0.24	20 (4%) 36 38	23, 26, 41, 87	15 (3%)
1	E	433/459 (94%)	0.14	22 (5%) 32 33	22, 29, 47, 96	12 (2%)
1	G	433/459 (94%)	0.08	17 (3%) 43 45	23, 29, 46, 63	16 (3%)
1	I	433/459 (94%)	0.05	16 (3%) 45 47	22, 30, 45, 61	16 (3%)
1	K	433/459 (94%)	0.19	27 (6%) 24 26	22, 33, 51, 64	15 (3%)
1	M	433/459 (94%)	0.22	29 (6%) 21 22	22, 33, 54, 65	16 (3%)
1	O	433/459 (94%)	0.12	20 (4%) 36 38	22, 36, 54, 68	20 (4%)
1	Q	433/459 (94%)	0.43	42 (9%) 10 10	25, 39, 65, 85	12 (2%)
1	S	433/459 (94%)	1.67	134 (30%) 1 0	43, 77, 113, 129	48 (11%)
1	U	430/459 (93%)	2.10	179 (41%) 0 0	42, 81, 106, 122	53 (12%)
1	W	432/459 (94%)	2.29	205 (47%) 0 0	46, 72, 97, 112	71 (16%)
2	B	183/188 (97%)	0.22	5 (2%) 58 60	24, 25, 31, 50	3 (1%)
2	D	183/188 (97%)	0.26	6 (3%) 50 52	24, 25, 33, 43	7 (3%)
2	F	184/188 (97%)	0.14	6 (3%) 50 52	24, 26, 33, 40	4 (2%)
2	H	181/188 (96%)	-0.00	8 (4%) 38 40	24, 26, 37, 47	3 (1%)
2	J	175/188 (93%)	0.19	8 (4%) 36 38	24, 26, 33, 67	8 (4%)
2	L	182/188 (96%)	0.03	9 (4%) 33 35	23, 27, 35, 58	4 (2%)
2	N	183/188 (97%)	0.04	8 (4%) 38 40	24, 27, 37, 58	6 (3%)
2	P	181/188 (96%)	-0.00	4 (2%) 65 67	23, 27, 38, 53	3 (1%)
2	R	181/188 (96%)	-0.02	9 (4%) 32 34	23, 30, 40, 48	3 (1%)
2	T	182/188 (96%)	0.40	13 (7%) 19 20	28, 41, 61, 68	3 (1%)
2	V	181/188 (96%)	0.68	28 (15%) 3 3	25, 44, 87, 107	11 (6%)
2	X	180/188 (95%)	1.77	64 (35%) 0 0	45, 72, 101, 111	21 (11%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	7368/7764 (94%)	0.54	885 (12%) <b>6</b> <b>6</b>	22, 32, 89, 129	381 (5%)

The worst 5 of 885 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	418	SER	22.0
1	U	409	LEU	13.5
1	W	284	LEU	12.0
1	W	230	ASP	11.6
1	U	100	CYS	11.6

## 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	BNL	E	462	12/12	0.70	0.24	<b>6.06</b>	47,50,52,52	0
5	BNL	S	462	12/12	0.66	0.63	<b>3.79</b>	56,57,58,58	12
5	BNL	Q	462	12/12	0.74	0.19	<b>2.80</b>	56,58,60,60	0
5	BNL	C	462	12/12	0.80	0.17	1.32	33,34,35,35	0
5	BNL	K	462	12/12	0.90	0.11	0.74	42,43,44,44	0
3	FES	S	460	4/4	0.85	0.17	0.44	82,83,84,86	0
5	BNL	M	462	12/12	0.90	0.12	0.39	49,50,52,52	0
5	BNL	I	462	12/12	0.91	0.11	0.32	32,32,33,33	0
5	BNL	O	462	12/12	0.90	0.10	-0.06	38,38,40,40	0
5	BNL	W	462	12/12	0.79	0.15	-0.64	80,81,83,83	0
3	FES	K	460	4/4	0.99	0.10	-0.91	23,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FES	E	460	4/4	0.99	0.08	-1.24	24,24,24,25	0
4	FE2	E	461	1/1	0.94	0.06	-1.27	31,31,31,31	0
3	FES	U	460	4/4	0.92	0.12	-1.41	65,66,67,67	4
3	FES	M	460	4/4	0.99	0.07	-1.46	24,24,24,24	0
3	FES	G	460	4/4	0.97	0.06	-1.64	33,34,35,35	0
3	FES	Q	460	4/4	0.99	0.05	-1.77	29,30,30,31	0
4	FE2	C	461	1/1	0.96	0.06	-1.99	25,25,25,25	0
3	FES	C	460	4/4	0.98	0.07	-2.20	26,26,26,26	0
3	FES	O	460	4/4	0.98	0.05	-2.32	33,34,34,34	0
3	FES	I	460	4/4	0.98	0.05	-2.47	28,28,28,28	0
3	FES	A	460	4/4	0.98	0.05	-2.77	26,26,26,26	0
3	FES	W	460	4/4	0.97	0.04	-2.95	55,56,57,57	0
4	FE2	S	461	1/1	0.97	0.06	-4.07	68,68,68,68	0
4	FE2	M	461	1/1	0.99	0.02	-5.08	29,29,29,29	0
4	FE2	W	461	1/1	0.88	0.06	-	75,75,75,75	0
4	FE2	A	461	1/1	1.00	0.08	-	24,24,24,24	0
4	FE2	U	461	1/1	0.95	0.12	-	62,62,62,62	0
4	FE2	G	461	1/1	1.00	0.05	-	23,23,23,23	0
4	FE2	O	461	1/1	0.99	0.07	-	26,26,26,26	0
4	FE2	I	461	1/1	0.99	0.04	-	25,25,25,25	0
4	FE2	Q	461	1/1	0.95	0.05	-	50,50,50,50	0
4	FE2	K	461	1/1	0.99	0.04	-	30,30,30,30	0

## 6.5 Other polymers

There are no such residues in this entry.