



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:04 PM GMT

PDB ID : 2XRX  
Title : CRYSTAL STRUCTURE OF BIPHENYL DIOXYGENASE IN COMPLEX  
WITH BIPHENYL FROM BURKHOLDERIA XENOVORANS LB400  
Authors : Kumar, P.; Bolin, J.T.  
Deposited on : 2010-09-23  
Resolution : 2.42 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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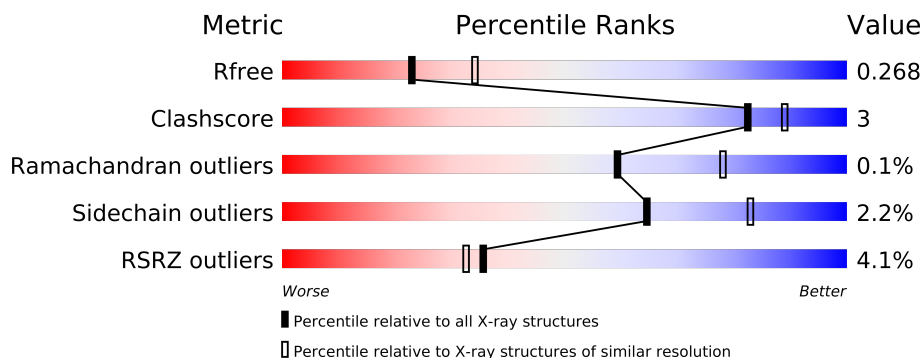
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.42 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.












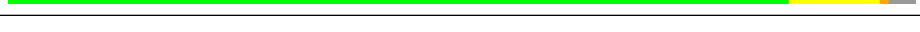
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2496 (2.44-2.40)
Clashscore	79885	3124 (2.44-2.40)
Ramachandran outliers	78287	3067 (2.44-2.40)
Sidechain outliers	78261	3068 (2.44-2.40)
RSRZ outliers	66119	2499 (2.44-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	459	
1	C	459	
1	E	459	
1	G	459	
1	I	459	
1	K	459	
1	M	459	
1	O	459	
1	Q	459	
1	S	459	
1	U	459	
1	W	459	
2	B	188	
2	D	188	

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Mol	Chain	Length	Quality of chain
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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	BNL	A	1462	-	X
5	BNL	C	1462	-	X
5	BNL	E	1462	-	X
5	BNL	G	1462	-	X
5	BNL	I	1462	-	X
5	BNL	K	1462	-	X
5	BNL	O	1462	-	X
5	BNL	Q	1462	-	X
5	BNL	S	1462	-	X
5	BNL	U	1462	-	X
5	BNL	W	1462	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59977 atoms, of which 0 are hydrogen and 0 are deuterium.

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	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	C	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	E	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	G	432	Total	C	N	O	S	0	0	0
			3416	2172	600	621	23			
1	I	432	Total	C	N	O	S	0	0	0
			3416	2172	600	621	23			
1	K	432	Total	C	N	O	S	0	0	0
			3416	2172	600	621	23			
1	M	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	O	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	Q	432	Total	C	N	O	S	0	0	0
			3421	2175	601	622	23			
1	S	432	Total	C	N	O	S	0	0	0
			3417	2172	600	622	23			
1	U	432	Total	C	N	O	S	0	0	0
			3417	2172	600	622	23			
1	W	432	Total	C	N	O	S	0	0	0
			3417	2172	600	622	23			

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

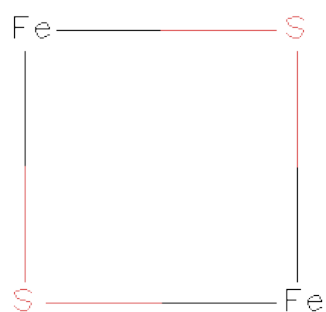
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			
2	D	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			
2	H	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	J	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	L	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	N	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	P	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	R	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	T	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	V	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	X	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	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		

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

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

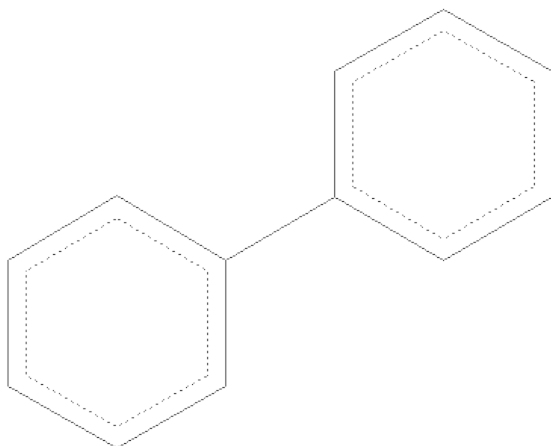
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Fe 1	0	0
4	Q	1	Total 1	Fe 1	0	0
4	K	1	Total 1	Fe 1	0	0
4	E	1	Total 1	Fe 1	0	0
4	I	1	Total 1	Fe 1	0	0
4	C	1	Total 1	Fe 1	0	0
4	W	1	Total 1	Fe 1	0	0
4	A	1	Total 1	Fe 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	U	1	Total 1	Fe 1	0	0
4	O	1	Total 1	Fe 1	0	0
4	S	1	Total 1	Fe 1	0	0
4	M	1	Total 1	Fe 1	0	0

- Molecule 5 is BIPHENYL (three-letter code: BNL) (formula: C<sub>12</sub>H<sub>10</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 12	C 12	0	0
5	C	1	Total 12	C 12	0	0
5	E	1	Total 12	C 12	0	0
5	G	1	Total 12	C 12	0	0
5	I	1	Total 12	C 12	0	0
5	K	1	Total 12	C 12	0	0
5	M	1	Total 12	C 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	U	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	44	Total O 44 44	0	0
6	B	19	Total O 19 19	0	0
6	C	31	Total O 31 31	0	0
6	D	21	Total O 21 21	0	0
6	E	50	Total O 50 50	0	0
6	F	35	Total O 35 35	0	0
6	G	24	Total O 24 24	0	0
6	H	12	Total O 12 12	0	0
6	I	25	Total O 25 25	0	0
6	J	7	Total O 7 7	0	0
6	K	16	Total O 16 16	0	0
6	L	12	Total O 12 12	0	0
6	M	38	Total O 38 38	0	0
6	N	25	Total O 25 25	0	0

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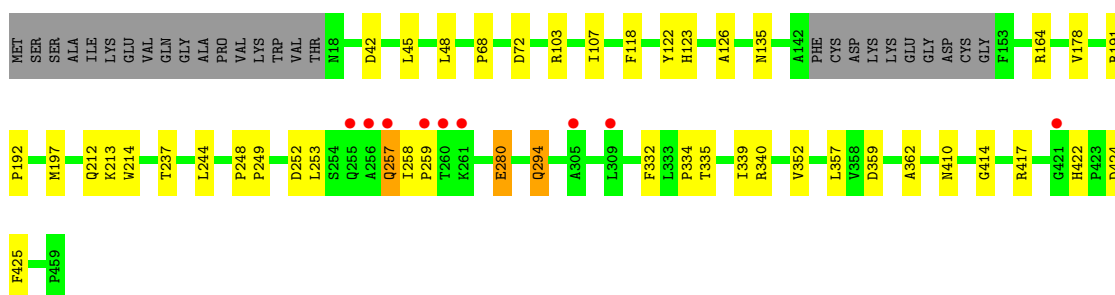
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	O	65	Total 65	O 65	0	0
6	P	26	Total 26	O 26	0	0
6	Q	83	Total 83	O 83	0	0
6	R	30	Total 30	O 30	0	0
6	S	33	Total 33	O 33	0	0
6	T	18	Total 18	O 18	0	0
6	U	25	Total 25	O 25	0	0
6	V	11	Total 11	O 11	0	0
6	W	30	Total 30	O 30	0	0
6	X	14	Total 14	O 14	0	0

### 3 Residue-property plots

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

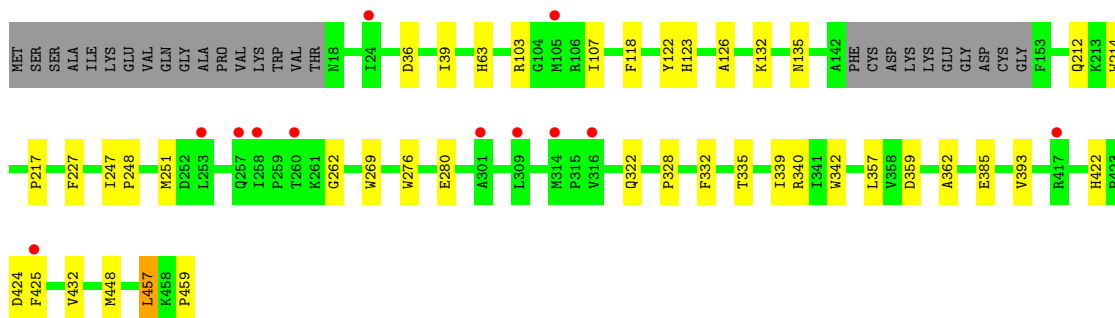
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain A: 



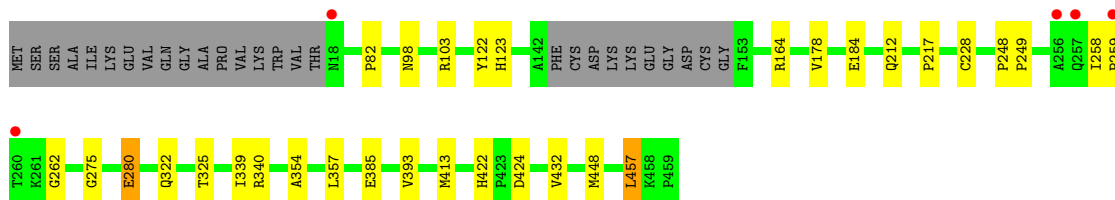
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain C: 



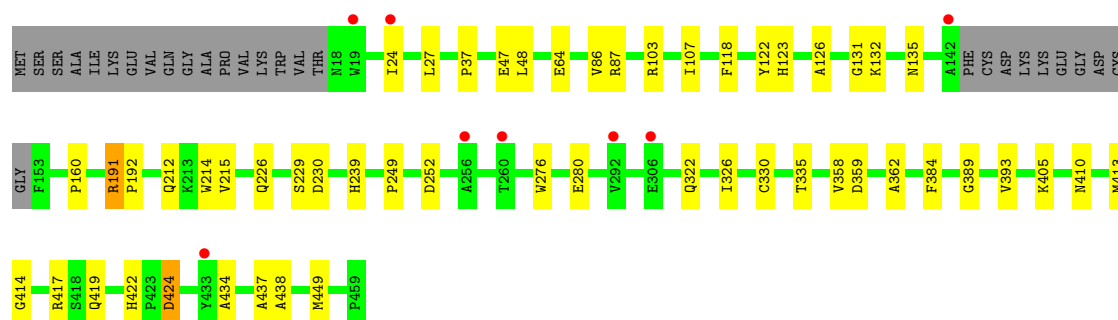
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain E: 



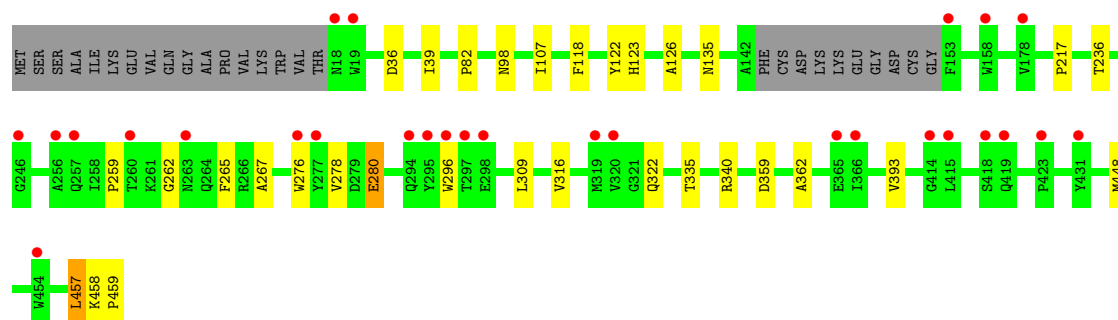
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain G: 



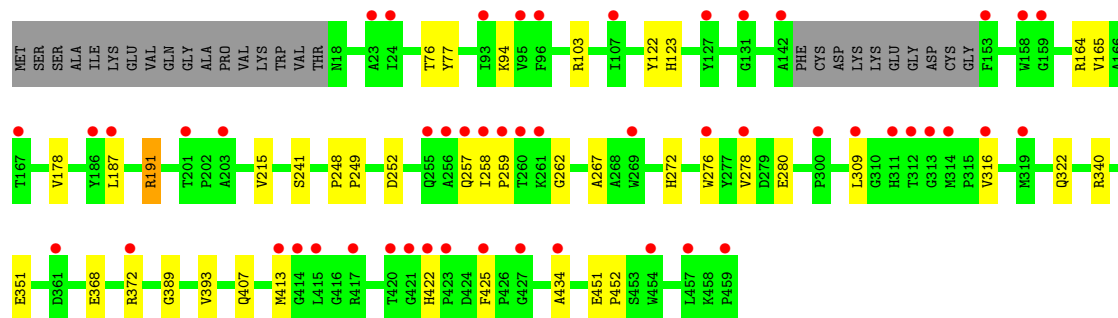
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain I:



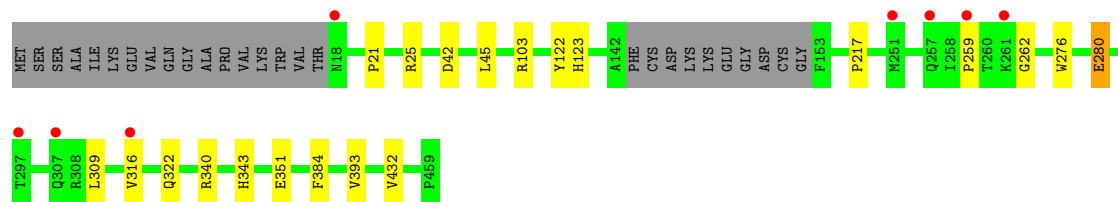
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain K:



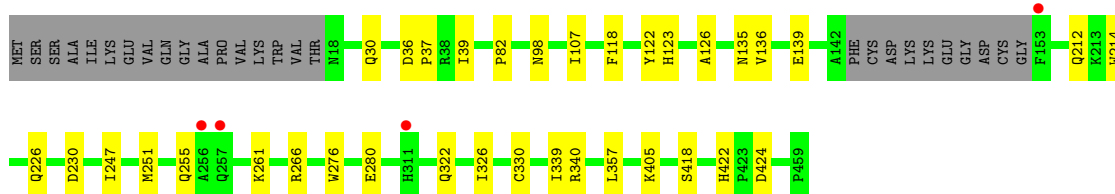
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain M:



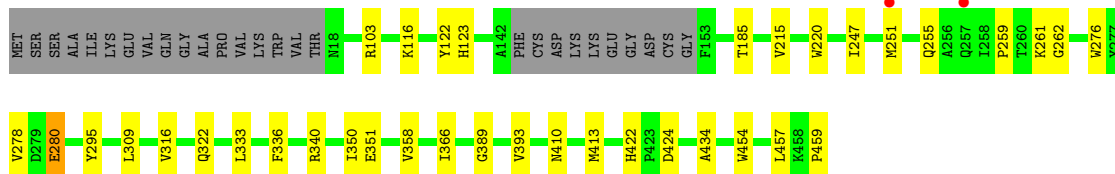
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain O:



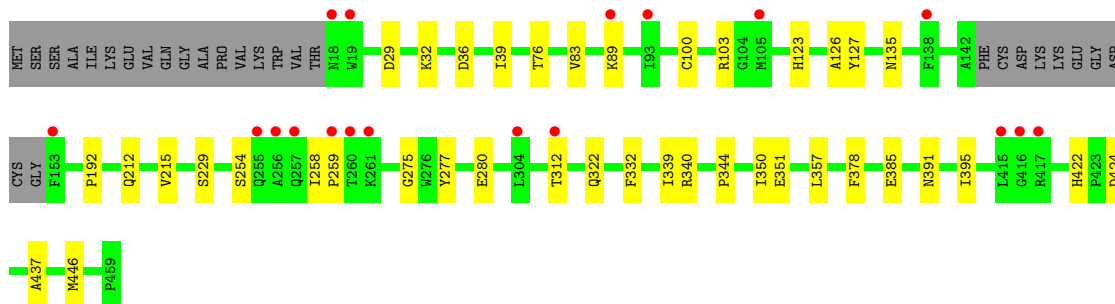
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain Q:



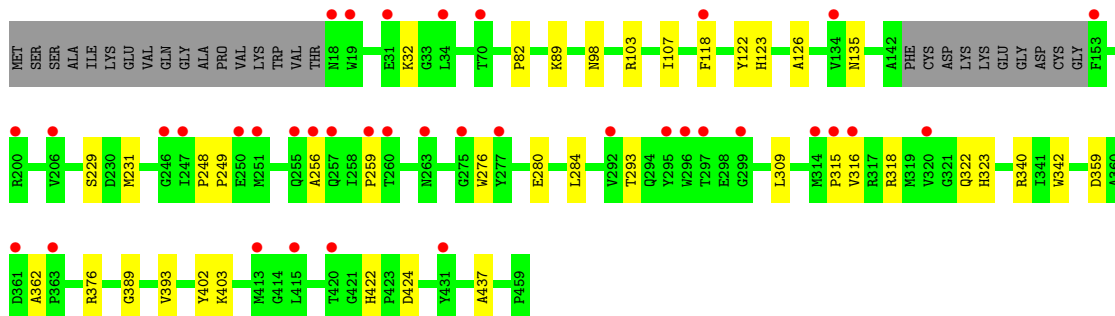
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain S:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

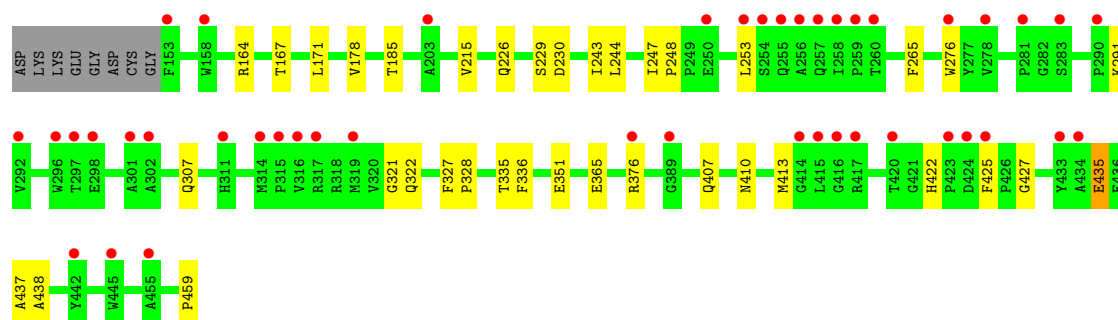
Chain U:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain W:





• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain B:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain D:



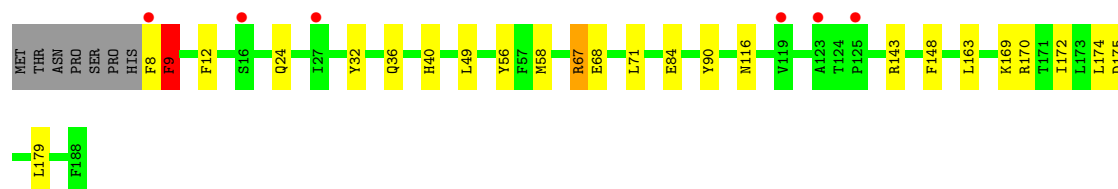
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain F:



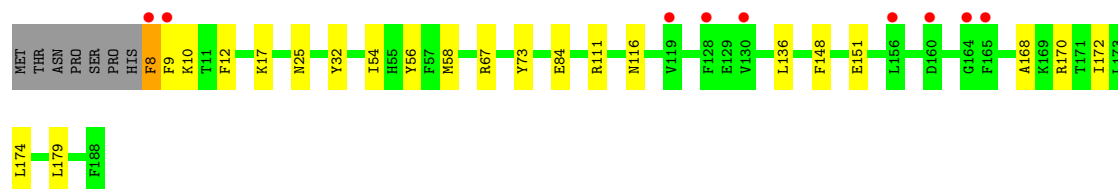
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain H:



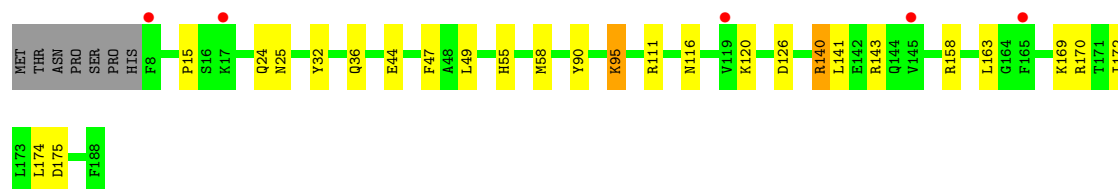
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain J:



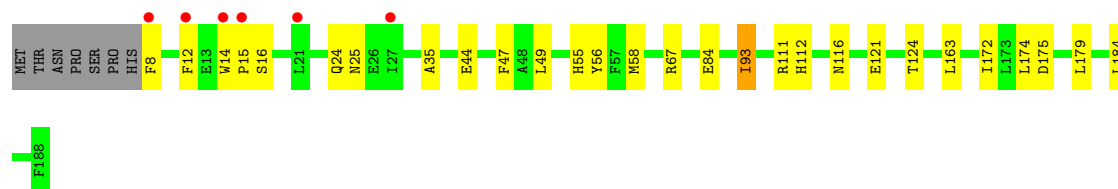
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain L:



- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain N:



- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain P:



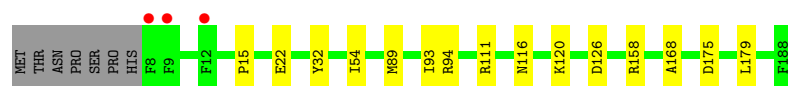
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain R:



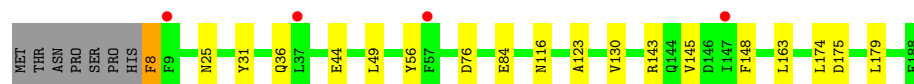
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain T:



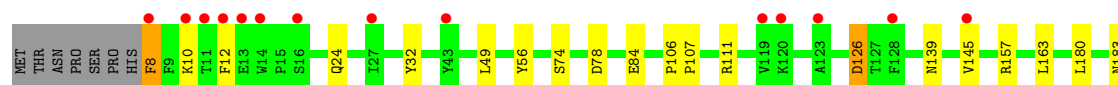
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain V:



- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain X:



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F186

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.82Å 132.65Å 130.42Å 102.65° 101.11° 105.31°	Depositor
Resolution (Å)	119.52 – 2.42 49.50 – 2.42	Depositor EDS
% Data completeness (in resolution range)	95.0 (119.52-2.42) 82.5 (49.50-2.42)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.233 , 0.270 0.236 , 0.268	Depositor DCC
$R_{free}$ test set	2612 reflections (1.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 21.7	EDS
Estimated twinning fraction	0.007 for l,h,k 0.007 for k,l,h 0.010 for -h,-l,-k 0.008 for -l,-k,-h 0.010 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 255377 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	59977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, FES, 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	0.32	0/3523	0.48	0/4784
1	C	0.32	0/3523	0.47	0/4784
1	E	0.32	0/3523	0.49	0/4784
1	G	0.33	0/3518	0.47	0/4777
1	I	0.33	0/3518	0.47	0/4777
1	K	0.33	0/3518	0.47	0/4777
1	M	0.33	0/3523	0.48	0/4784
1	O	0.32	0/3523	0.48	0/4784
1	Q	0.33	0/3523	0.49	0/4784
1	S	0.32	0/3519	0.47	0/4780
1	U	0.34	0/3519	0.46	0/4780
1	W	0.34	0/3519	0.47	0/4780
2	B	0.34	0/1532	0.51	0/2072
2	D	0.34	0/1532	0.50	0/2072
2	F	0.35	0/1532	0.50	0/2072
2	H	0.34	0/1542	0.51	0/2084
2	J	0.35	0/1542	0.49	0/2084
2	L	0.34	0/1542	0.49	0/2084
2	N	0.35	0/1542	0.52	0/2084
2	P	0.34	0/1542	0.52	0/2084
2	R	0.34	0/1542	0.53	0/2084
2	T	0.34	0/1542	0.49	0/2084
2	V	0.35	0/1542	0.49	0/2084
2	X	0.36	0/1542	0.49	0/2084
All	All	0.33	0/60723	0.48	0/82347

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3421	0	3269	25	0
1	C	3421	0	3269	21	0
1	E	3421	0	3269	17	0
1	G	3416	0	3262	26	0
1	I	3416	0	3262	16	0
1	K	3416	0	3262	21	0
1	M	3421	0	3269	10	0
1	O	3421	0	3269	15	0
1	Q	3421	0	3269	16	0
1	S	3417	0	3258	22	0
1	U	3417	0	3258	19	0
1	W	3417	0	3258	22	0
2	B	1497	0	1441	13	0
2	D	1497	0	1441	16	0
2	F	1497	0	1441	11	0
2	H	1507	0	1456	20	0
2	J	1507	0	1456	18	0
2	L	1507	0	1456	21	0
2	N	1507	0	1456	17	0
2	P	1507	0	1456	17	0
2	R	1507	0	1456	19	0
2	T	1507	0	1456	11	0
2	V	1507	0	1456	15	0
2	X	1507	0	1456	15	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
3	M	4	0	0	1	0
3	O	4	0	0	1	0
3	Q	4	0	0	1	0
3	S	4	0	0	1	0
3	U	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	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
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	A	12	0	10	0	0
5	C	12	0	10	0	0
5	E	12	0	10	0	0
5	G	12	0	10	0	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	U	12	0	10	0	0
5	W	12	0	10	0	0
6	A	44	0	0	1	0
6	B	19	0	0	0	0
6	C	31	0	0	0	0
6	D	21	0	0	0	0
6	E	50	0	0	1	0
6	F	35	0	0	0	0
6	G	24	0	0	0	0
6	H	12	0	0	0	0
6	I	25	0	0	0	0
6	J	7	0	0	0	0
6	K	16	0	0	0	0
6	L	12	0	0	0	0
6	M	38	0	0	0	0
6	N	25	0	0	1	0
6	O	65	0	0	0	0
6	P	26	0	0	0	0
6	Q	83	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	30	0	0	0	0
6	S	33	0	0	0	0
6	T	18	0	0	0	0
6	U	25	0	0	0	0
6	V	11	0	0	1	0
6	W	30	0	0	1	0
6	X	14	0	0	0	0
All	All	59977	0	56721	362	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (362) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:8:PHE:HA	2:H:9:PHE:HB2	1.28	1.16
2:X:8:PHE:HD1	2:X:8:PHE:O	1.54	0.90
2:P:94:ARG:HH11	2:P:94:ARG:HG2	1.36	0.89
2:J:8:PHE:HA	2:J:73:TYR:HD2	1.37	0.88
2:R:8:PHE:N	2:R:9:PHE:HB2	1.87	0.88
1:S:123:HIS:HB2	3:S:1460:FES:S2	2.14	0.88
1:M:123:HIS:HB2	3:M:1460:FES:S2	2.16	0.86
1:I:123:HIS:HB2	3:I:1460:FES:S2	2.21	0.80
2:H:8:PHE:HA	2:H:9:PHE:CB	2.10	0.78
1:W:123:HIS:HB2	3:W:1460:FES:S2	2.24	0.77
1:E:339:ILE:CD1	1:E:357:LEU:HG	2.15	0.76
1:A:259:PRO:HB3	1:A:280:GLU:HG2	1.67	0.75
1:K:259:PRO:HB3	1:K:280:GLU:HG2	1.69	0.75
1:Q:259:PRO:HB3	1:Q:280:GLU:HG2	1.68	0.74
1:C:123:HIS:HB2	3:C:1460:FES:S2	2.27	0.74
1:Q:123:HIS:HB2	3:Q:1460:FES:S2	2.27	0.74
2:R:58:MET:HE1	2:R:174:LEU:HD22	1.69	0.74
1:W:413:MET:HB2	1:W:435:GLU:HB2	1.69	0.73
1:E:339:ILE:HD11	1:E:357:LEU:HG	1.72	0.71
1:A:123:HIS:HB2	3:A:1460:FES:S2	2.31	0.70
1:Q:422:HIS:HD2	1:Q:424:ASP:H	1.41	0.69
2:R:8:PHE:N	2:R:9:PHE:CB	2.56	0.68
2:P:94:ARG:NH1	2:P:94:ARG:HG2	2.07	0.67
2:B:94:ARG:HG2	2:B:94:ARG:HH11	1.61	0.66
1:S:339:ILE:HD11	1:S:357:LEU:HG	1.77	0.66
2:J:56:TYR:HB3	2:J:84:GLU:HB2	1.78	0.65
1:M:309:LEU:HD13	1:M:316:VAL:HG11	1.78	0.65
1:G:123:HIS:HB2	3:G:1460:FES:S2	2.37	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:175:ASP:OD2	2:R:111:ARG:HB2	1.98	0.64
2:V:8:PHE:N	2:V:8:PHE:CD1	2.66	0.64
1:C:247:ILE:HG13	1:C:248:PRO:HD2	1.79	0.64
1:W:291:LYS:HE2	1:W:365:GLU:HG2	1.80	0.63
2:X:8:PHE:CD1	2:X:8:PHE:O	2.44	0.63
2:V:143:ARG:HD3	1:W:215:VAL:HG21	1.80	0.63
2:H:148:PHE:HB3	2:H:174:LEU:HD11	1.80	0.63
1:S:339:ILE:CD1	1:S:357:LEU:HG	2.29	0.61
2:T:111:ARG:HB2	2:V:175:ASP:OD2	1.99	0.61
2:J:8:PHE:HA	2:J:73:TYR:CD2	2.29	0.61
1:I:448:MET:HG2	1:I:457:LEU:HD21	1.82	0.60
1:I:217:PRO:HD2	1:I:393:VAL:HG22	1.83	0.60
2:D:58:MET:HE1	2:D:174:LEU:HD22	1.82	0.60
2:P:10:LYS:HG2	2:P:10:LYS:O	2.02	0.60
1:G:229:SER:OG	1:G:438:ALA:HB2	2.01	0.60
1:K:123:HIS:HB2	3:K:1460:FES:S2	2.42	0.59
2:V:56:TYR:HB3	2:V:84:GLU:HB2	1.84	0.59
1:E:339:ILE:HD13	1:E:357:LEU:HG	1.84	0.59
1:S:215:VAL:HG22	1:S:351:GLU:HG2	1.84	0.59
2:D:58:MET:CE	2:D:174:LEU:HD22	2.33	0.59
2:V:25:ASN:HD21	2:X:24:GLN:HG2	1.68	0.58
1:A:339:ILE:HD13	1:A:357:LEU:HG	1.85	0.58
1:E:259:PRO:HB3	1:E:280:GLU:HG2	1.85	0.57
2:V:8:PHE:N	2:V:8:PHE:HD1	2.01	0.57
1:K:257:GLN:NE2	2:P:8:PHE:HB3	2.18	0.57
1:E:123:HIS:HB2	3:E:1460:FES:S2	2.45	0.57
2:N:25:ASN:HD21	2:P:24:GLN:HG2	1.68	0.57
2:D:56:TYR:HB3	2:D:84:GLU:HB2	1.87	0.57
1:K:94:LYS:HA	1:K:165:VAL:HG21	1.86	0.57
1:S:229:SER:HB2	1:S:437:ALA:HB3	1.87	0.56
2:R:58:MET:CE	2:R:174:LEU:HD22	2.36	0.55
2:H:24:GLN:HG2	2:L:25:ASN:HD21	1.71	0.55
1:O:123:HIS:HB2	3:O:1460:FES:S2	2.46	0.55
1:I:448:MET:HA	1:I:457:LEU:HD11	1.87	0.55
1:Q:185:THR:HG22	1:Q:459:PRO:HG2	1.89	0.55
1:I:259:PRO:HB3	1:I:280:GLU:HG2	1.89	0.55
1:A:107:ILE:HG22	1:A:118:PHE:HB3	1.88	0.55
2:B:111:ARG:HB2	2:D:175:ASP:OD2	2.07	0.55
2:T:126:ASP:HB3	2:T:158:ARG:HB2	1.87	0.55
2:L:140:ARG:HG3	2:L:141:LEU:HG	1.89	0.55
1:K:413:MET:HG2	1:K:434:ALA:HA	1.88	0.55
1:W:226:GLN:HA	1:W:230:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:359:ASP:HB2	1:U:362:ALA:HB2	1.89	0.55
1:U:123:HIS:HB2	3:U:1460:FES:S2	2.47	0.55
2:N:56:TYR:HB3	2:N:84:GLU:HB2	1.88	0.55
1:W:229:SER:HB3	1:W:437:ALA:HB3	1.89	0.54
2:L:55:HIS:HB3	2:L:169:LYS:HG3	1.90	0.54
2:B:94:ARG:NH1	2:B:94:ARG:HG2	2.18	0.54
1:O:107:ILE:HG22	1:O:118:PHE:HB3	1.89	0.54
2:X:56:TYR:HB3	2:X:84:GLU:HB2	1.88	0.54
1:C:269:TRP:CD2	1:C:459:PRO:HG3	2.43	0.54
1:S:340:ARG:HH12	1:S:385:GLU:CD	2.10	0.54
2:D:111:ARG:HB2	2:F:175:ASP:OD2	2.08	0.54
1:W:226:GLN:HA	1:W:230:ASP:CB	2.39	0.53
1:I:359:ASP:HB2	1:I:362:ALA:HB2	1.90	0.53
1:I:262:GLY:HA2	1:I:278:VAL:HG23	1.88	0.53
1:Q:413:MET:HG2	1:Q:434:ALA:HA	1.91	0.53
1:U:309:LEU:HD13	1:U:316:VAL:HG11	1.89	0.53
1:G:24:ILE:HD11	1:G:449:MET:HB3	1.91	0.53
2:H:175:ASP:OD2	2:L:111:ARG:HB2	2.09	0.53
2:B:175:ASP:OD2	2:F:111:ARG:HB2	2.08	0.53
2:D:49:LEU:HD21	2:D:163:LEU:HD13	1.91	0.53
1:A:258:ILE:HD11	2:N:8:PHE:C	2.29	0.53
2:N:24:GLN:HG2	2:R:25:ASN:HD21	1.74	0.53
2:L:58:MET:HE1	2:L:174:LEU:HD22	1.90	0.53
1:W:215:VAL:HG22	1:W:351:GLU:HG2	1.89	0.53
1:W:422:HIS:HD2	1:W:425:PHE:H	1.56	0.52
2:P:25:ASN:HD21	2:R:24:GLN:HG2	1.74	0.52
1:E:448:MET:HA	1:E:457:LEU:HD11	1.90	0.52
1:G:249:PRO:HB3	2:H:90:TYR:CE2	2.45	0.52
1:K:164:ARG:HD2	1:K:178:VAL:HA	1.91	0.52
2:H:56:TYR:HB3	2:H:84:GLU:HB2	1.90	0.52
1:C:227:PHE:CZ	1:C:340:ARG:HD2	2.45	0.52
1:G:64:GLU:HG2	1:G:87:ARG:HH22	1.73	0.52
1:A:359:ASP:HB2	1:A:362:ALA:HB2	1.91	0.52
2:D:123:ALA:HA	1:G:132:LYS:HD3	1.92	0.52
2:V:148:PHE:HB3	2:V:174:LEU:HD11	1.92	0.52
2:H:32:TYR:CD1	2:J:116:ASN:HA	2.44	0.52
2:N:49:LEU:HD21	2:N:163:LEU:HD13	1.92	0.52
2:B:36:GLN:HE21	2:D:12:PHE:H	1.58	0.52
1:G:413:MET:HG2	1:G:434:ALA:HA	1.92	0.52
2:J:9:PHE:O	2:J:10:LYS:HG2	2.10	0.52
1:A:126:ALA:HB3	1:A:135:ASN:HB3	1.91	0.52
1:M:259:PRO:HB3	1:M:280:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:309:LEU:HD13	1:I:316:VAL:HG11	1.91	0.51
2:H:36:GLN:HE21	2:J:12:PHE:H	1.57	0.51
1:K:262:GLY:HA2	1:K:278:VAL:HG23	1.92	0.51
1:K:241:SER:HB2	2:L:95:LYS:HG2	1.92	0.51
2:J:25:ASN:HD21	2:L:24:GLN:HG2	1.75	0.51
1:A:237:THR:HG22	2:N:12:PHE:HB3	1.93	0.51
1:I:82:PRO:HB2	1:I:98:ASN:HB3	1.93	0.51
2:H:12:PHE:H	2:L:36:GLN:HE21	1.57	0.51
1:A:422:HIS:CD2	1:A:424:ASP:H	2.28	0.51
1:O:276:TRP:HB3	1:O:322:GLN:HG3	1.92	0.51
1:E:217:PRO:HD2	1:E:393:VAL:HG22	1.93	0.50
1:C:340:ARG:HH12	1:C:385:GLU:CD	2.15	0.50
2:B:25:ASN:HD21	2:D:24:GLN:HG2	1.76	0.50
1:Q:309:LEU:HD22	1:Q:316:VAL:HG11	1.94	0.50
1:G:131:GLY:O	1:G:160:PRO:HD2	2.12	0.50
2:J:32:TYR:CD1	2:L:116:ASN:HA	2.46	0.50
1:G:229:SER:HB3	1:G:437:ALA:HB3	1.92	0.50
1:A:414:GLY:HA2	1:A:417:ARG:HD2	1.94	0.50
1:C:422:HIS:HD2	1:C:425:PHE:H	1.60	0.49
1:G:215:VAL:HG21	2:L:143:ARG:HD3	1.93	0.49
2:N:58:MET:HE1	2:N:174:LEU:HD22	1.94	0.49
2:J:170:ARG:HD3	2:J:172:ILE:HD11	1.94	0.49
1:E:340:ARG:HH12	1:E:385:GLU:CD	2.16	0.49
1:G:126:ALA:HB3	1:G:135:ASN:HB3	1.93	0.49
1:Q:276:TRP:HB3	1:Q:322:GLN:HG3	1.94	0.49
2:X:49:LEU:HD21	2:X:163:LEU:HD13	1.95	0.49
2:N:111:ARG:HB2	2:P:175:ASP:OD2	2.12	0.49
2:B:116:ASN:HA	2:F:32:TYR:CD1	2.48	0.49
1:I:265:PHE:CZ	1:I:267:ALA:HA	2.48	0.48
1:S:422:HIS:HD2	1:S:424:ASP:H	1.60	0.48
2:F:49:LEU:HD21	2:F:163:LEU:HD13	1.94	0.48
2:N:116:ASN:HA	2:R:32:TYR:CD1	2.48	0.48
1:W:36:ASP:O	1:W:39:ILE:HG12	2.13	0.48
2:J:8:PHE:CD1	2:J:8:PHE:C	2.87	0.48
1:Q:422:HIS:CD2	1:Q:424:ASP:H	2.26	0.48
1:U:259:PRO:HB3	1:U:280:GLU:HG2	1.94	0.48
2:N:35:ALA:HB1	2:N:112:HIS:HB2	1.95	0.48
1:S:332:PHE:HB3	1:S:339:ILE:HG23	1.96	0.48
1:K:309:LEU:HD13	1:K:316:VAL:HG11	1.95	0.48
1:E:422:HIS:HD2	1:E:424:ASP:H	1.60	0.48
1:O:37:PRO:HG2	1:O:405:LYS:HA	1.94	0.48
2:J:54:ILE:HA	2:J:168:ALA:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:422:HIS:HD2	1:A:424:ASP:H	1.62	0.47
1:C:36:ASP:O	1:C:39:ILE:HG12	2.13	0.47
1:A:258:ILE:HD11	2:N:8:PHE:O	2.13	0.47
2:H:68:GLU:HB3	2:H:71:LEU:HD12	1.96	0.47
1:O:82:PRO:HB2	1:O:98:ASN:HB3	1.96	0.47
1:M:42:ASP:HB3	1:M:45:LEU:HB2	1.96	0.47
1:S:126:ALA:HB3	1:S:135:ASN:HB3	1.96	0.47
2:P:40:HIS:HE1	2:R:151:GLU:OE2	1.97	0.47
1:U:402:TYR:CE2	1:U:403:LYS:HE3	2.49	0.47
1:U:389:GLY:O	1:U:393:VAL:HG23	2.15	0.47
2:N:47:PHE:HB2	2:N:93:ILE:HD13	1.97	0.47
2:T:116:ASN:HA	2:X:32:TYR:CD1	2.49	0.47
1:C:359:ASP:HB2	1:C:362:ALA:HB2	1.95	0.47
1:G:359:ASP:HB2	1:G:362:ALA:HB2	1.97	0.47
1:W:126:ALA:HB3	1:W:135:ASN:HB3	1.96	0.47
1:M:217:PRO:HG2	1:M:393:VAL:HG22	1.96	0.47
2:R:56:TYR:HB3	2:R:84:GLU:HB2	1.96	0.47
2:N:55:HIS:HB3	6:N:2014:HOH:O	2.14	0.47
1:S:36:ASP:O	1:S:39:ILE:HG12	2.14	0.47
1:G:107:ILE:HG22	1:G:118:PHE:HB3	1.95	0.47
2:B:116:ASN:HA	2:F:32:TYR:CG	2.50	0.47
1:S:259:PRO:HB2	1:S:277:TYR:CE2	2.50	0.47
1:A:332:PHE:HB3	1:A:339:ILE:HG13	1.97	0.47
1:C:448:MET:HA	1:C:457:LEU:HD11	1.97	0.47
2:P:90:TYR:CE2	2:P:94:ARG:HD2	2.50	0.46
1:S:192:PRO:HB3	1:S:312:THR:HG21	1.97	0.46
1:U:82:PRO:HB2	1:U:98:ASN:HB3	1.98	0.46
2:X:106:PRO:HA	2:X:107:PRO:HD3	1.83	0.46
1:G:24:ILE:HG13	1:G:27:LEU:HD12	1.97	0.46
1:I:126:ALA:HB3	1:I:135:ASN:HB3	1.97	0.46
2:L:47:PHE:CZ	2:L:90:TYR:HB2	2.50	0.46
1:O:247:ILE:HD12	1:O:251:MET:HB3	1.96	0.46
1:U:284:LEU:HD23	1:U:293:THR:HG23	1.98	0.46
1:Q:215:VAL:HG22	1:Q:351:GLU:HG2	1.97	0.46
1:W:276:TRP:HB3	1:W:322:GLN:HG3	1.95	0.46
1:C:107:ILE:HG22	1:C:118:PHE:HB3	1.97	0.46
2:X:74:SER:HB2	2:X:78:ASP:HB2	1.98	0.45
1:A:191:ARG:N	1:A:192:PRO:HD2	2.31	0.45
1:O:36:ASP:O	1:O:39:ILE:HG12	2.16	0.45
2:T:175:ASP:OD2	2:X:111:ARG:HB2	2.16	0.45
1:E:164:ARG:HD2	1:E:178:VAL:HA	1.97	0.45
2:R:49:LEU:HD21	2:R:163:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:T:32:TYR:CD1	2:V:116:ASN:HA	2.51	0.45
1:O:136:VAL:O	1:O:139:GLU:HB2	2.17	0.45
1:E:82:PRO:HB2	1:E:98:ASN:HB3	1.98	0.45
1:G:24:ILE:CD1	1:G:449:MET:HB3	2.47	0.45
6:W:2026:HOH:O	2:X:183:ASN:HB3	2.16	0.45
1:U:276:TRP:HB3	1:U:322:GLN:HG3	1.98	0.45
2:L:58:MET:CE	2:L:174:LEU:HD22	2.46	0.45
2:X:126:ASP:O	2:X:157:ARG:HA	2.17	0.45
2:V:145:VAL:HG21	2:X:180:LEU:HD11	1.99	0.45
2:J:111:ARG:HB2	2:L:175:ASP:OD2	2.16	0.45
2:R:126:ASP:HB3	2:R:158:ARG:HB2	1.98	0.45
2:T:89:MET:O	2:T:93:ILE:HG12	2.16	0.45
1:W:244:LEU:HD13	1:W:253:LEU:HG	1.99	0.45
2:P:32:TYR:CD1	2:R:116:ASN:HA	2.52	0.45
2:T:15:PRO:HD3	2:T:120:LYS:HG3	1.99	0.45
2:N:116:ASN:HA	2:R:32:TYR:CG	2.52	0.44
1:K:187:LEU:HB2	1:K:191:ARG:HD3	1.99	0.44
2:B:24:GLN:HG2	2:F:25:ASN:HD21	1.82	0.44
1:W:164:ARG:HD2	1:W:178:VAL:HA	1.99	0.44
1:Q:454:TRP:HA	1:Q:457:LEU:HB2	1.99	0.44
2:N:58:MET:HG3	2:N:172:ILE:HB	1.99	0.44
2:H:170:ARG:HD3	2:H:172:ILE:HD11	1.99	0.44
1:A:213:LYS:HA	1:A:352:VAL:O	2.17	0.44
1:M:384:PHE:CE2	5:M:1462:BNL:H12	2.53	0.44
1:Q:262:GLY:HA2	1:Q:278:VAL:HG23	1.99	0.44
1:E:262:GLY:C	1:E:432:VAL:HB	2.38	0.44
2:T:22:GLU:CD	2:T:22:GLU:H	2.21	0.44
1:G:422:HIS:HD2	1:G:424:ASP:H	1.65	0.44
1:W:105:MET:CE	1:W:109:ARG:HD2	2.47	0.44
1:U:422:HIS:CD2	1:U:424:ASP:H	2.36	0.44
1:S:76:THR:HG23	1:S:83:VAL:HG23	1.99	0.44
1:G:37:PRO:HG2	1:G:405:LYS:HA	1.99	0.44
1:E:212:GLN:HG3	1:E:354:ALA:HB3	2.00	0.44
1:U:422:HIS:HD2	1:U:424:ASP:H	1.66	0.44
1:G:276:TRP:HB3	1:G:322:GLN:HG3	1.98	0.44
2:R:9:PHE:H	1:S:258:ILE:HD11	1.83	0.43
1:M:343:HIS:HB2	1:M:351:GLU:HB2	2.00	0.43
2:D:172:ILE:HD13	2:D:188:PHE:HB2	2.00	0.43
2:T:116:ASN:HA	2:X:32:TYR:CG	2.54	0.43
2:L:44:GLU:HG2	2:P:155:VAL:HG21	2.00	0.43
2:T:54:ILE:HA	2:T:168:ALA:O	2.18	0.43
1:E:248:PRO:HA	1:E:249:PRO:HD3	1.93	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:212:GLN:HG3	1:C:214:TRP:HZ3	1.82	0.43
1:C:251:MET:O	2:D:94:ARG:NH2	2.50	0.43
2:H:49:LEU:HD21	2:H:163:LEU:HD13	1.99	0.43
1:C:217:PRO:HG2	1:C:393:VAL:HG22	2.00	0.43
1:M:262:GLY:C	1:M:432:VAL:HB	2.38	0.43
1:K:389:GLY:O	1:K:393:VAL:HG23	2.19	0.43
2:L:49:LEU:HD21	2:L:163:LEU:HD13	2.01	0.43
1:K:422:HIS:HD2	1:K:425:PHE:H	1.64	0.43
1:U:107:ILE:HG22	1:U:118:PHE:HB3	2.00	0.43
2:V:36:GLN:NE2	2:X:12:PHE:H	2.16	0.43
2:R:10:LYS:HG3	1:S:254:SER:HB3	2.01	0.43
2:V:49:LEU:HD21	2:V:163:LEU:HD13	2.01	0.43
2:B:94:ARG:CG	2:B:94:ARG:HH11	2.29	0.43
2:H:58:MET:HE1	2:H:174:LEU:HD22	2.00	0.43
2:L:170:ARG:HD3	2:L:172:ILE:HD11	2.01	0.43
1:A:244:LEU:HD13	1:A:253:LEU:HG	1.99	0.43
1:S:344:PRO:HA	1:S:350:ILE:HG22	1.99	0.43
1:U:315:PRO:HB2	1:U:318:ARG:HD3	2.01	0.43
1:C:63:HIS:CD2	1:C:357:LEU:HD21	2.53	0.43
2:P:179:LEU:HD21	2:P:184:LEU:HD11	2.01	0.43
1:I:107:ILE:HG22	1:I:118:PHE:HB3	2.01	0.43
2:H:116:ASN:HA	2:L:32:TYR:CD1	2.54	0.43
1:U:229:SER:HB2	1:U:437:ALA:HB3	2.00	0.43
1:K:215:VAL:HG22	1:K:351:GLU:HG2	1.99	0.43
1:A:294:GLN:HA	1:A:294:GLN:HE21	1.84	0.43
1:W:185:THR:HG22	1:W:459:PRO:HG2	2.00	0.43
1:G:414:GLY:HA2	1:G:417:ARG:HD2	2.01	0.43
1:E:184:GLU:HB2	6:E:2022:HOH:O	2.19	0.43
1:C:132:LYS:HD2	2:V:123:ALA:HA	2.01	0.43
1:O:226:GLN:HA	1:O:230:ASP:HB3	2.01	0.43
1:I:276:TRP:HB3	1:I:322:GLN:HG3	2.01	0.43
2:L:126:ASP:HB3	2:L:158:ARG:HB2	2.00	0.43
1:W:229:SER:OG	1:W:438:ALA:HB2	2.18	0.42
1:U:126:ALA:HB3	1:U:135:ASN:HB3	2.00	0.42
2:B:126:ASP:HB3	2:B:158:ARG:HB2	2.00	0.42
1:E:228:CYS:HB2	1:E:325:THR:HB	2.01	0.42
2:P:111:ARG:HB2	2:R:175:ASP:OD2	2.20	0.42
1:C:276:TRP:HB3	1:C:322:GLN:HG3	2.01	0.42
2:D:32:TYR:CD1	2:F:116:ASN:HA	2.54	0.42
1:G:389:GLY:O	1:G:393:VAL:HG23	2.19	0.42
1:K:451:GLU:HA	1:K:452:PRO:HD3	1.79	0.42
1:C:262:GLY:C	1:C:432:VAL:HB	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:220:TRP:HA	1:Q:350:ILE:HG21	2.02	0.42
2:P:32:TYR:CG	2:R:116:ASN:HA	2.54	0.42
1:Q:247:ILE:HD12	1:Q:251:MET:HB3	2.02	0.42
1:A:164:ARG:HD2	1:A:178:VAL:HA	2.01	0.42
2:H:40:HIS:NE2	2:J:151:GLU:OE2	2.48	0.42
1:K:257:GLN:HE22	2:P:8:PHE:HB3	1.81	0.42
1:G:212:GLN:HG3	1:G:214:TRP:HZ3	1.85	0.42
1:C:126:ALA:HB3	1:C:135:ASN:HB3	2.01	0.42
1:W:247:ILE:HG13	1:W:248:PRO:HD2	2.00	0.42
1:K:368:GLU:O	1:K:372:ARG:HG3	2.20	0.42
2:V:143:ARG:NH2	6:V:2011:HOH:O	2.53	0.42
2:B:36:GLN:NE2	2:D:12:PHE:H	2.18	0.42
2:J:58:MET:HE1	2:J:174:LEU:HD22	2.01	0.42
1:G:191:ARG:N	1:G:192:PRO:HD2	2.35	0.42
1:A:42:ASP:HB3	1:A:45:LEU:HB2	2.01	0.42
1:Q:333:LEU:HD13	1:Q:336:PHE:HD1	1.84	0.42
1:Q:295:TYR:CD1	1:Q:366:ILE:HD13	2.54	0.42
1:A:257:GLN:HB2	6:A:2030:HOH:O	2.19	0.42
1:O:126:ALA:HB3	1:O:135:ASN:HB3	2.02	0.42
1:U:248:PRO:HA	1:U:249:PRO:HD3	1.90	0.42
1:S:100:CYS:SG	1:S:127:TYR:OH	2.78	0.42
2:L:15:PRO:HG3	2:L:120:LYS:HG3	2.01	0.42
2:P:58:MET:HE1	2:P:174:LEU:HD22	2.02	0.42
1:I:458:LYS:HB2	1:I:459:PRO:HD2	2.00	0.42
1:I:296:TRP:CE2	1:I:335:THR:HG23	2.55	0.42
1:M:276:TRP:HB3	1:M:322:GLN:HG3	2.02	0.42
2:H:36:GLN:NE2	2:J:12:PHE:H	2.17	0.41
2:T:32:TYR:CG	2:V:116:ASN:HA	2.55	0.41
1:G:422:HIS:CD2	1:G:424:ASP:H	2.37	0.41
1:C:340:ARG:HD3	1:C:342:TRP:CH2	2.55	0.41
1:A:422:HIS:HD2	1:A:425:PHE:H	1.67	0.41
2:J:32:TYR:CG	2:L:116:ASN:HA	2.55	0.41
1:U:340:ARG:HD3	1:U:342:TRP:CH2	2.55	0.41
1:W:265:PHE:HE1	1:W:427:GLY:HA3	1.84	0.41
1:K:267:ALA:HB2	1:K:272:HIS:HB2	2.02	0.41
2:P:58:MET:HE2	2:P:81:HIS:CB	2.50	0.41
1:M:21:PRO:O	1:M:25:ARG:HG3	2.20	0.41
1:O:30:GLN:OE1	1:O:266:ARG:NH2	2.44	0.41
1:I:36:ASP:O	1:I:39:ILE:HG12	2.20	0.41
1:S:212:GLN:HE21	1:S:212:GLN:HB2	1.67	0.41
2:R:54:ILE:HA	2:R:168:ALA:O	2.20	0.41
2:B:56:TYR:HB3	2:B:84:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:248:PRO:HA	1:A:249:PRO:HD3	1.94	0.41
1:O:339:ILE:HD11	1:O:357:LEU:HD11	2.03	0.41
1:K:276:TRP:HB3	1:K:322:GLN:HG3	2.01	0.41
1:U:231:MET:HB2	1:U:323:HIS:NE2	2.35	0.41
1:A:212:GLN:HG3	1:A:214:TRP:HZ3	1.85	0.41
1:K:76:THR:OG1	1:K:77:TYR:N	2.53	0.41
2:H:32:TYR:CG	2:J:116:ASN:HA	2.56	0.41
1:O:326:ILE:HB	1:O:330:CYS:HB3	2.03	0.41
2:D:36:GLN:HE21	2:F:12:PHE:H	1.68	0.41
1:E:275:GLY:O	1:E:322:GLN:HA	2.21	0.41
1:W:60:LEU:HD11	1:W:171:LEU:HD22	2.02	0.41
2:V:31:TYR:HE2	2:V:130:VAL:HG11	1.86	0.41
1:A:197:MET:HB2	1:A:334:PRO:HB3	2.03	0.41
1:W:321:GLY:HA2	1:W:336:PHE:CZ	2.56	0.41
1:G:226:GLN:HA	1:G:230:ASP:HB3	2.03	0.41
1:S:340:ARG:NH2	1:S:378:PHE:HB3	2.36	0.41
1:W:327:PHE:CG	1:W:328:PRO:HA	2.56	0.41
2:X:139:ASN:HD22	2:X:145:VAL:HG22	1.85	0.41
1:K:248:PRO:HA	1:K:249:PRO:HD3	1.93	0.41
2:H:24:GLN:HG2	2:L:25:ASN:ND2	2.35	0.40
1:C:422:HIS:CD2	1:C:424:ASP:H	2.38	0.40
1:O:422:HIS:CD2	1:O:424:ASP:H	2.40	0.40
1:S:275:GLY:O	1:S:322:GLN:HA	2.22	0.40
1:C:332:PHE:HB3	1:C:339:ILE:HG23	2.03	0.40
2:F:19:ALA:HB1	2:F:23:LEU:HD23	2.03	0.40
1:K:258:ILE:HA	1:K:259:PRO:HD2	1.93	0.40
1:Q:389:GLY:O	1:Q:393:VAL:HG23	2.22	0.40
2:N:179:LEU:HD21	2:N:184:LEU:HD11	2.03	0.40
2:J:136:LEU:HB3	2:J:148:PHE:HB2	2.03	0.40
2:D:179:LEU:HD21	2:D:184:LEU:HD11	2.03	0.40
1:A:68:PRO:HD2	1:A:72:ASP:OD2	2.21	0.40
2:H:67:ARG:HG2	2:H:68:GLU:HG3	2.03	0.40
1:S:391:ASN:O	1:S:395:ILE:HG13	2.22	0.40
1:G:326:ILE:HB	1:G:330:CYS:HB3	2.04	0.40
1:U:107:ILE:CG2	1:U:118:PHE:HB3	2.52	0.40
2:D:36:GLN:NE2	2:F:12:PHE:H	2.19	0.40
1:O:212:GLN:HG3	1:O:214:TRP:HZ3	1.87	0.40
1:S:29:ASP:OD1	1:S:32:LYS:HE3	2.21	0.40
1:G:239:HIS:CE1	1:G:384:PHE:O	2.74	0.40
2:F:9:PHE:O	2:F:10:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	428/459 (93%)	414 (97%)	14 (3%)	0	100	100
1	C	428/459 (93%)	411 (96%)	16 (4%)	1 (0%)	56	74
1	E	428/459 (93%)	413 (96%)	15 (4%)	0	100	100
1	G	428/459 (93%)	413 (96%)	15 (4%)	0	100	100
1	I	428/459 (93%)	412 (96%)	15 (4%)	1 (0%)	56	74
1	K	428/459 (93%)	411 (96%)	17 (4%)	0	100	100
1	M	428/459 (93%)	417 (97%)	11 (3%)	0	100	100
1	O	428/459 (93%)	411 (96%)	17 (4%)	0	100	100
1	Q	428/459 (93%)	415 (97%)	13 (3%)	0	100	100
1	S	428/459 (93%)	414 (97%)	14 (3%)	0	100	100
1	U	428/459 (93%)	407 (95%)	20 (5%)	1 (0%)	56	74
1	W	428/459 (93%)	404 (94%)	24 (6%)	0	100	100
2	B	179/188 (95%)	170 (95%)	9 (5%)	0	100	100
2	D	179/188 (95%)	168 (94%)	10 (6%)	1 (1%)	33	46
2	F	179/188 (95%)	171 (96%)	7 (4%)	1 (1%)	33	46
2	H	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	33	46
2	J	179/188 (95%)	168 (94%)	11 (6%)	0	100	100
2	L	179/188 (95%)	171 (96%)	8 (4%)	0	100	100
2	N	179/188 (95%)	170 (95%)	7 (4%)	2 (1%)	21	28
2	P	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	33	46
2	R	179/188 (95%)	170 (95%)	9 (5%)	0	100	100
2	T	179/188 (95%)	172 (96%)	7 (4%)	0	100	100
2	V	179/188 (95%)	171 (96%)	8 (4%)	0	100	100
2	X	179/188 (95%)	171 (96%)	7 (4%)	1 (1%)	33	46
All	All	7284/7764 (94%)	6982 (96%)	292 (4%)	10 (0%)	59	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	9	PHE
2	X	10	LYS
2	F	10	LYS
1	U	256	ALA
2	D	10	LYS
2	N	16	SER
1	I	236	THR
2	N	15	PRO
2	P	16	SER
1	C	328	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/373 (94%)	340 (97%)	10 (3%)	55	75
1	C	350/373 (94%)	345 (99%)	5 (1%)	78	91
1	E	350/373 (94%)	344 (98%)	6 (2%)	73	88
1	G	349/373 (94%)	336 (96%)	13 (4%)	45	66
1	I	349/373 (94%)	345 (99%)	4 (1%)	84	94
1	K	349/373 (94%)	343 (98%)	6 (2%)	73	88
1	M	350/373 (94%)	346 (99%)	4 (1%)	84	94
1	O	350/373 (94%)	344 (98%)	6 (2%)	73	88
1	Q	350/373 (94%)	341 (97%)	9 (3%)	59	79
1	S	349/373 (94%)	345 (99%)	4 (1%)	84	94
1	U	349/373 (94%)	344 (99%)	5 (1%)	78	91
1	W	349/373 (94%)	339 (97%)	10 (3%)	55	75
2	B	158/167 (95%)	154 (98%)	4 (2%)	60	79
2	D	158/167 (95%)	156 (99%)	2 (1%)	80	92
2	F	158/167 (95%)	150 (95%)	8 (5%)	33	50
2	H	160/167 (96%)	155 (97%)	5 (3%)	52	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	160/167 (96%)	156 (98%)	4 (2%)	60	79
2	L	160/167 (96%)	158 (99%)	2 (1%)	80	92
2	N	160/167 (96%)	154 (96%)	6 (4%)	44	64
2	P	160/167 (96%)	155 (97%)	5 (3%)	52	73
2	R	160/167 (96%)	154 (96%)	6 (4%)	44	64
2	T	160/167 (96%)	158 (99%)	2 (1%)	80	92
2	V	160/167 (96%)	156 (98%)	4 (2%)	60	79
2	X	160/167 (96%)	158 (99%)	2 (1%)	80	92
All	All	6108/6480 (94%)	5976 (98%)	132 (2%)	64	83

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	103	ARG
1	A	122	TYR
1	A	252	ASP
1	A	257	GLN
1	A	280	GLU
1	A	294	GLN
1	A	335	THR
1	A	340	ARG
1	A	410	ASN
2	B	22	GLU
2	B	94	ARG
2	B	158	ARG
2	B	179	LEU
1	C	103	ARG
1	C	122	TYR
1	C	280	GLU
1	C	335	THR
1	C	457	LEU
2	D	121	GLU
2	D	179	LEU
1	E	103	ARG
1	E	122	TYR
1	E	258	ILE
1	E	280	GLU
1	E	413	MET

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Mol	Chain	Res	Type
1	E	457	LEU
2	F	10	LYS
2	F	52	LYS
2	F	94	ARG
2	F	121	GLU
2	F	143	ARG
2	F	158	ARG
2	F	162	ASN
2	F	179	LEU
1	G	47	GLU
1	G	48	LEU
1	G	86	VAL
1	G	103	ARG
1	G	122	TYR
1	G	191	ARG
1	G	252	ASP
1	G	280	GLU
1	G	335	THR
1	G	358	VAL
1	G	410	ASN
1	G	419	GLN
1	G	424	ASP
2	H	9	PHE
2	H	67	ARG
2	H	143	ARG
2	H	169	LYS
2	H	179	LEU
1	I	122	TYR
1	I	280	GLU
1	I	340	ARG
1	I	457	LEU
2	J	8	PHE
2	J	17	LYS
2	J	67	ARG
2	J	179	LEU
1	K	103	ARG
1	K	122	TYR
1	K	191	ARG
1	K	252	ASP
1	K	340	ARG
1	K	407	GLN
2	L	95	LYS

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Mol	Chain	Res	Type
2	L	140	ARG
1	M	103	ARG
1	M	122	TYR
1	M	280	GLU
1	M	340	ARG
2	N	14	TRP
2	N	44	GLU
2	N	67	ARG
2	N	93	ILE
2	N	121	GLU
2	N	124	THR
1	O	122	TYR
1	O	255	GLN
1	O	261	LYS
1	O	280	GLU
1	O	340	ARG
1	O	418	SER
2	P	9	PHE
2	P	11	THR
2	P	17	LYS
2	P	51	ASP
2	P	94	ARG
1	Q	103	ARG
1	Q	116	LYS
1	Q	122	TYR
1	Q	255	GLN
1	Q	261	LYS
1	Q	280	GLU
1	Q	340	ARG
1	Q	358	VAL
1	Q	410	ASN
2	R	9	PHE
2	R	10	LYS
2	R	93	ILE
2	R	94	ARG
2	R	99	ASP
2	R	179	LEU
1	S	89	LYS
1	S	103	ARG
1	S	280	GLU
1	S	446	MET
2	T	94	ARG

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Mol	Chain	Res	Type
2	T	179	LEU
1	U	32	LYS
1	U	89	LYS
1	U	103	ARG
1	U	122	TYR
1	U	376	ARG
2	V	8	PHE
2	V	44	GLU
2	V	76	ASP
2	V	179	LEU
1	W	94	LYS
1	W	103	ARG
1	W	167	THR
1	W	243	ILE
1	W	307	GLN
1	W	335	THR
1	W	376	ARG
1	W	407	GLN
1	W	410	ASN
1	W	435	GLU
2	X	8	PHE
2	X	126	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	255	GLN
1	A	294	GLN
1	A	343	HIS
1	A	391	ASN
1	A	410	ASN
1	A	412	GLN
1	A	422	HIS
1	A	444	HIS
2	B	25	ASN
2	B	36	GLN
2	B	77	GLN
2	B	131	ASN
2	B	162	ASN
1	C	294	GLN
1	C	391	ASN

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Mol	Chain	Res	Type
1	C	410	ASN
1	C	412	GLN
1	C	422	HIS
1	C	444	HIS
2	D	36	GLN
2	D	162	ASN
1	E	18	ASN
1	E	257	GLN
1	E	263	ASN
1	E	391	ASN
1	E	410	ASN
1	E	412	GLN
1	E	422	HIS
2	F	25	ASN
2	F	36	GLN
2	F	131	ASN
2	F	162	ASN
1	G	257	GLN
1	G	391	ASN
1	G	410	ASN
1	G	422	HIS
1	G	444	HIS
2	H	36	GLN
2	H	131	ASN
1	I	264	GLN
1	I	391	ASN
1	I	410	ASN
1	I	422	HIS
1	I	444	HIS
2	J	25	ASN
2	J	36	GLN
2	J	131	ASN
1	K	212	GLN
1	K	343	HIS
1	K	391	ASN
1	K	410	ASN
1	K	422	HIS
2	L	25	ASN
2	L	36	GLN
2	L	131	ASN
1	M	212	GLN
1	M	257	GLN

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Mol	Chain	Res	Type
1	M	263	ASN
1	M	343	HIS
1	M	391	ASN
1	M	410	ASN
1	M	422	HIS
1	M	444	HIS
2	N	25	ASN
2	N	40	HIS
2	N	131	ASN
1	O	257	GLN
1	O	377	ASN
1	O	391	ASN
1	O	410	ASN
1	O	422	HIS
1	O	444	HIS
2	P	25	ASN
2	P	40	HIS
2	P	131	ASN
1	Q	255	GLN
1	Q	311	HIS
1	Q	391	ASN
1	Q	410	ASN
1	Q	422	HIS
2	R	25	ASN
2	R	40	HIS
2	R	131	ASN
2	R	162	ASN
1	S	212	GLN
1	S	255	GLN
1	S	391	ASN
1	S	410	ASN
1	S	422	HIS
1	S	444	HIS
2	T	25	ASN
2	T	36	GLN
2	T	131	ASN
1	U	212	GLN
1	U	255	GLN
1	U	264	GLN
1	U	343	HIS
1	U	422	HIS
2	V	25	ASN

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Mol	Chain	Res	Type
2	V	36	GLN
1	W	212	GLN
1	W	410	ASN
1	W	422	HIS
2	X	25	ASN
2	X	36	GLN
2	X	131	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	A	1462	-	13,13,13	0.52	0	16,16,16	0.59	0
3	FES	C	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	C	1462	-	13,13,13	0.52	0	16,16,16	0.48	0
3	FES	E	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	E	1462	-	13,13,13	0.53	0	16,16,16	0.54	0
3	FES	G	1460	1	0,4,4	0.00	-	0,4,4	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BNL	G	1462	-	13,13,13	0.51	0	16,16,16	0.52	0
3	FES	I	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	I	1462	-	13,13,13	0.50	0	16,16,16	0.63	0
3	FES	K	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	K	1462	-	13,13,13	0.54	0	16,16,16	0.45	0
3	FES	M	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	M	1462	-	13,13,13	0.51	0	16,16,16	0.52	0
3	FES	O	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	O	1462	-	13,13,13	0.53	0	16,16,16	0.50	0
3	FES	Q	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	Q	1462	-	13,13,13	0.57	0	16,16,16	0.46	0
3	FES	S	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	S	1462	-	13,13,13	0.52	0	16,16,16	0.58	0
3	FES	U	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	U	1462	-	13,13,13	0.50	0	16,16,16	0.55	0
3	FES	W	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	W	1462	-	13,13,13	0.52	0	16,16,16	0.57	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	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	A	1462	-	-	0/4/4/4	0/2/2/2
3	FES	C	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	C	1462	-	-	0/4/4/4	0/2/2/2
3	FES	E	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	E	1462	-	-	0/4/4/4	0/2/2/2
3	FES	G	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	G	1462	-	-	0/4/4/4	0/2/2/2
3	FES	I	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	I	1462	-	-	0/4/4/4	0/2/2/2
3	FES	K	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	K	1462	-	-	0/4/4/4	0/2/2/2
3	FES	M	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	M	1462	-	-	0/4/4/4	0/2/2/2
3	FES	O	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	O	1462	-	-	0/4/4/4	0/2/2/2
3	FES	Q	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	Q	1462	-	-	0/4/4/4	0/2/2/2
3	FES	S	1460	1	-	0/0/4/4	0/0/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BNL	S	1462	-	-	0/4/4/4	0/2/2/2
3	FES	U	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	U	1462	-	-	0/4/4/4	0/2/2/2
3	FES	W	1460	1	-	0/0/4/4	0/0/1/1
5	BNL	W	1462	-	-	0/4/4/4	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	432/459 (94%)	-0.03	9 (2%) 60 57	24, 41, 55, 61	17 (3%)
1	C	432/459 (94%)	0.07	12 (2%) 50 48	30, 44, 54, 58	17 (3%)
1	E	432/459 (94%)	-0.01	5 (1%) 75 75	23, 35, 47, 55	17 (3%)
1	G	432/459 (94%)	0.09	8 (1%) 64 61	35, 47, 60, 66	17 (3%)
1	I	432/459 (94%)	0.38	28 (6%) 18 16	39, 52, 64, 69	17 (3%)
1	K	432/459 (94%)	0.61	51 (11%) 5 4	42, 55, 65, 68	17 (3%)
1	M	432/459 (94%)	0.01	8 (1%) 64 61	26, 38, 58, 62	17 (3%)
1	O	432/459 (94%)	-0.12	4 (0%) 81 80	20, 34, 49, 57	17 (3%)
1	Q	432/459 (94%)	-0.24	2 (0%) 88 88	22, 31, 44, 61	17 (3%)
1	S	432/459 (94%)	0.27	18 (4%) 35 32	36, 47, 58, 67	17 (3%)
1	U	432/459 (94%)	0.61	37 (8%) 11 9	39, 57, 72, 74	17 (3%)
1	W	432/459 (94%)	0.84	60 (13%) 4 3	46, 59, 70, 74	17 (3%)
2	B	181/188 (96%)	0.03	3 (1%) 67 65	30, 38, 47, 58	4 (2%)
2	D	181/188 (96%)	-0.01	3 (1%) 67 65	28, 39, 51, 56	4 (2%)
2	F	181/188 (96%)	-0.22	1 (0%) 86 86	28, 33, 47, 60	4 (2%)
2	H	181/188 (96%)	0.20	6 (3%) 44 41	36, 45, 60, 66	4 (2%)
2	J	181/188 (96%)	0.29	9 (4%) 28 25	40, 50, 57, 63	4 (2%)
2	L	181/188 (96%)	0.37	5 (2%) 50 48	39, 48, 63, 70	4 (2%)
2	N	181/188 (96%)	0.00	6 (3%) 44 41	27, 38, 61, 75	4 (2%)
2	P	181/188 (96%)	-0.03	5 (2%) 50 48	24, 36, 64, 79	4 (2%)
2	R	181/188 (96%)	-0.21	0 100 100	24, 32, 52, 62	4 (2%)
2	T	181/188 (96%)	0.13	3 (1%) 67 65	33, 39, 55, 65	4 (2%)
2	V	181/188 (96%)	0.21	4 (2%) 59 56	45, 53, 59, 64	4 (2%)
2	X	181/188 (96%)	0.50	14 (7%) 13 11	42, 52, 59, 62	4 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	7356/7764 (94%)	0.18	301 (4%)	35	32	20, 44, 63, 79	252 (3%)

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	ALA	8.8
1	K	256	ALA	8.1
1	A	257	GLN	6.5
1	K	255	GLN	6.2
1	W	425	PHE	5.7
1	S	256	ALA	5.6
1	W	292	VAL	5.4
1	K	260	THR	5.4
1	U	314	MET	5.2
1	U	19	TRP	5.2
2	N	14	TRP	5.2
1	A	255	GLN	5.1
1	W	301	ALA	5.0
1	W	316	VAL	5.0
1	W	257	GLN	4.9
1	K	24	ILE	4.9
1	W	255	GLN	4.9
1	K	312	THR	4.8
1	K	314	MET	4.8
1	U	256	ALA	4.7
2	X	11	THR	4.7
1	I	320	VAL	4.6
2	X	8	PHE	4.5
1	S	255	GLN	4.4
1	K	203	ALA	4.3
1	U	415	LEU	4.3
1	I	415	LEU	4.2
1	W	317	ARG	4.2
1	G	142	ALA	4.2
1	S	138	PHE	4.2
2	N	12	PHE	4.1
2	H	27	ILE	4.1
1	W	315	PRO	4.1
1	I	256	ALA	4.0
1	W	416	GLY	4.0
1	K	316	VAL	4.0
1	E	257	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	W	302	ALA	4.0
1	W	22	GLU	3.9
1	W	21	PRO	3.9
1	W	455	ALA	3.9
1	W	283	SER	3.9
1	A	260	THR	3.9
1	W	19	TRP	3.9
1	I	366	ILE	3.9
1	E	256	ALA	3.8
1	K	186	TYR	3.8
1	U	255	GLN	3.8
1	S	257	GLN	3.8
1	I	153	PHE	3.8
2	P	14	TRP	3.7
1	S	153	PHE	3.7
1	U	260	THR	3.7
1	W	28	VAL	3.7
1	A	259	PRO	3.7
1	K	261	LYS	3.7
1	W	281	PRO	3.7
1	C	314	MET	3.7
2	J	8	PHE	3.7
1	S	259	PRO	3.7
1	W	256	ALA	3.7
1	K	259	PRO	3.7
1	U	315	PRO	3.7
1	U	292	VAL	3.6
1	I	431	TYR	3.6
1	U	257	GLN	3.6
1	W	153	PHE	3.6
1	W	24	ILE	3.6
1	W	158	TRP	3.6
1	K	457	LEU	3.5
1	I	297	THR	3.5
1	M	261	LYS	3.5
2	H	123	ALA	3.5
1	I	18	ASN	3.5
1	C	417	ARG	3.4
1	I	178	VAL	3.4
1	K	313	GLY	3.4
1	I	295	TYR	3.4
1	W	415	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	311	HIS	3.4
1	S	260	THR	3.3
1	W	314	MET	3.3
1	S	416	GLY	3.3
2	X	12	PHE	3.3
1	E	259	PRO	3.3
1	K	417	ARG	3.3
1	G	256	ALA	3.3
1	I	246	GLY	3.2
1	U	295	TYR	3.2
1	K	23	ALA	3.2
1	C	301	ALA	3.2
1	O	311	HIS	3.2
1	W	414	GLY	3.2
1	K	421	GLY	3.2
1	C	24	ILE	3.2
2	H	8	PHE	3.2
1	G	24	ILE	3.2
2	D	160	ASP	3.1
1	K	95	VAL	3.1
1	I	257	GLN	3.0
1	K	415	LEU	3.0
1	Q	257	GLN	3.0
1	C	260	THR	3.0
1	W	297	THR	3.0
1	K	454	TRP	3.0
1	U	296	TRP	3.0
1	W	296	TRP	3.0
1	U	118	PHE	3.0
2	V	9	PHE	3.0
1	O	257	GLN	3.0
1	U	18	ASN	3.0
2	J	128	PHE	3.0
1	G	260	THR	3.0
1	W	250	GLU	2.9
1	U	320	VAL	2.9
2	X	16	SER	2.9
2	V	37	LEU	2.9
1	I	19	TRP	2.9
1	I	277	TYR	2.9
2	X	14	TRP	2.9
1	W	290	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	W	311	HIS	2.9
1	W	298	GLU	2.9
1	K	257	GLN	2.9
1	G	19	TRP	2.9
1	K	158	TRP	2.9
1	K	159	GLY	2.9
1	U	70	THR	2.9
1	C	309	LEU	2.8
2	T	8	PHE	2.8
2	L	17	LYS	2.8
1	K	201	THR	2.8
1	C	316	VAL	2.8
1	I	276	TRP	2.8
1	I	454	TRP	2.8
1	O	153	PHE	2.8
1	K	269	TRP	2.8
1	W	18	ASN	2.8
1	U	134	VAL	2.7
2	X	119	VAL	2.7
1	E	18	ASN	2.7
1	W	376	ARG	2.7
1	U	413	MET	2.7
1	W	25	ARG	2.7
1	W	420	THR	2.7
1	W	142	ALA	2.7
1	W	424	ASP	2.7
1	K	372	ARG	2.7
2	H	119	VAL	2.7
2	J	119	VAL	2.7
1	C	257	GLN	2.7
1	K	434	ALA	2.7
1	U	299	GLY	2.7
1	K	131	GLY	2.6
1	G	433	TYR	2.6
1	K	425	PHE	2.6
1	W	389	GLY	2.6
1	U	297	THR	2.6
1	I	298	GLU	2.6
1	W	276	TRP	2.6
1	I	419	GLN	2.6
1	K	96	PHE	2.6
1	E	260	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	123	ALA	2.6
1	U	363	PRO	2.6
1	W	278	VAL	2.6
1	I	260	THR	2.6
1	U	153	PHE	2.6
1	S	312	THR	2.6
1	U	250	GLU	2.6
1	U	206	VAL	2.6
2	T	12	PHE	2.6
1	A	305	ALA	2.5
1	U	316	VAL	2.5
1	W	434	ALA	2.5
1	M	251	MET	2.5
1	M	259	PRO	2.5
2	D	162	ASN	2.5
1	U	247	ILE	2.5
2	J	130	VAL	2.5
2	L	145	VAL	2.5
1	K	309	LEU	2.5
1	U	34	LEU	2.5
2	X	128	PHE	2.5
1	G	292	VAL	2.5
2	L	119	VAL	2.5
1	W	20	THR	2.5
1	K	300	PRO	2.5
1	U	259	PRO	2.5
1	W	203	ALA	2.4
1	W	423	PRO	2.4
1	W	254	SER	2.4
2	L	8	PHE	2.4
1	C	258	ILE	2.4
1	S	415	LEU	2.4
2	N	15	PRO	2.4
2	B	9	PHE	2.4
2	F	8	PHE	2.4
1	S	93	ILE	2.4
1	K	142	ALA	2.4
1	I	365	GLU	2.4
1	W	48	LEU	2.4
1	W	96	PHE	2.4
2	J	165	PHE	2.4
2	P	12	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	U	246	GLY	2.4
2	P	58	MET	2.4
2	X	13	GLU	2.4
2	P	16	SER	2.4
1	S	18	ASN	2.3
1	M	316	VAL	2.3
1	U	277	TYR	2.3
2	J	160	ASP	2.3
1	I	296	TRP	2.3
1	W	125	TRP	2.3
1	W	117	ALA	2.3
2	P	18	ALA	2.3
1	A	309	LEU	2.3
1	K	153	PHE	2.3
1	W	433	TYR	2.3
1	C	105	MET	2.3
1	K	278	VAL	2.3
1	W	319	MET	2.3
1	W	27	LEU	2.3
1	O	256	ALA	2.3
1	U	200	ARG	2.2
1	S	105	MET	2.2
2	N	27	ILE	2.2
1	U	420	THR	2.2
2	X	120	LYS	2.2
1	I	423	PRO	2.2
2	B	8	PHE	2.2
1	U	263	ASN	2.2
1	W	442	TYR	2.2
1	K	361	ASP	2.2
1	U	361	ASP	2.2
1	I	294	GLN	2.2
1	Q	251	MET	2.2
1	S	19	TRP	2.2
1	K	93	ILE	2.2
2	V	147	ILE	2.2
2	X	27	ILE	2.2
1	K	414	GLY	2.2
2	J	164	GLY	2.2
1	I	319	MET	2.2
1	K	276	TRP	2.2
1	K	459	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	21	LEU	2.2
1	C	425	PHE	2.2
1	K	167	THR	2.2
1	K	427	GLY	2.2
1	M	257	GLN	2.2
2	T	9	PHE	2.1
1	K	107	ILE	2.1
1	W	259	PRO	2.1
1	K	127	TYR	2.1
1	W	35	LEU	2.1
1	W	253	LEU	2.1
2	J	156	LEU	2.1
1	K	413	MET	2.1
1	I	414	GLY	2.1
1	U	31	GLU	2.1
1	M	297	THR	2.1
1	W	417	ARG	2.1
2	B	147	ILE	2.1
1	K	187	LEU	2.1
1	S	304	LEU	2.1
1	W	445	TRP	2.1
1	U	251	MET	2.1
1	I	418	SER	2.1
1	M	307	GLN	2.1
2	J	9	PHE	2.1
1	W	258	ILE	2.1
1	U	431	TYR	2.1
2	H	125	PRO	2.1
1	S	417	ARG	2.1
1	I	263	ASN	2.1
1	U	275	GLY	2.1
2	X	123	ALA	2.1
1	C	253	LEU	2.1
2	H	16	SER	2.1
2	X	10	LYS	2.1
1	W	260	THR	2.0
2	X	145	VAL	2.0
2	X	43	TYR	2.0
2	L	165	PHE	2.0
1	K	258	ILE	2.0
1	A	261	LYS	2.0
1	S	89	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	18	ASN	2.0
2	N	8	PHE	2.0
2	V	57	PHE	2.0
1	K	319	MET	2.0
1	G	306	GLU	2.0
1	K	422	HIS	2.0
1	A	421	GLY	2.0
1	W	126	ALA	2.0
1	I	158	TRP	2.0
1	S	261	LYS	2.0
1	K	423	PRO	2.0
1	K	420	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	BNL	K	1462	12/12	0.35	11.04	86,86,87,87	0
5	BNL	W	1462	12/12	0.37	6.04	87,87,88,88	0
5	BNL	G	1462	12/12	0.30	5.72	63,64,64,64	0
5	BNL	I	1462	12/12	0.26	5.26	63,63,64,64	0
5	BNL	S	1462	12/12	0.35	4.72	82,82,82,82	0
5	BNL	C	1462	12/12	0.23	4.53	55,56,56,56	0
5	BNL	O	1462	12/12	0.22	3.92	44,44,45,45	0
5	BNL	A	1462	12/12	0.24	3.65	76,76,76,76	0
5	BNL	U	1462	12/12	0.31	3.23	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BNL	Q	1462	12/12	0.19	2.79	40,40,41,41	0
5	BNL	E	1462	12/12	0.19	2.09	49,49,49,49	0
5	BNL	M	1462	12/12	0.18	0.99	55,56,56,56	0
4	FE2	A	1461	1/1	0.15	0.41	53,53,53,53	0
4	FE2	C	1461	1/1	0.12	-0.05	44,44,44,44	0
4	FE2	O	1461	1/1	0.13	-0.14	34,34,34,34	0
4	FE2	I	1461	1/1	0.14	-0.28	58,58,58,58	0
3	FES	I	1460	4/4	0.12	-0.31	45,46,48,50	0
3	FES	E	1460	4/4	0.11	-0.33	44,46,47,50	0
3	FES	G	1460	4/4	0.13	-0.35	54,54,54,56	0
3	FES	O	1460	4/4	0.12	-0.42	44,45,46,48	0
4	FE2	Q	1461	1/1	0.12	-0.57	37,37,37,37	0
4	FE2	K	1461	1/1	0.14	-0.81	59,59,59,59	0
3	FES	C	1460	4/4	0.12	-0.83	43,44,45,46	0
4	FE2	E	1461	1/1	0.14	-0.85	41,41,41,41	0
3	FES	M	1460	4/4	0.09	-0.90	38,38,39,42	0
3	FES	Q	1460	4/4	0.09	-0.92	39,39,41,44	0
3	FES	A	1460	4/4	0.11	-0.99	43,44,46,48	0
3	FES	S	1460	4/4	0.10	-1.15	86,86,86,87	0
4	FE2	M	1461	1/1	0.12	-1.32	43,43,43,43	0
3	FES	K	1460	4/4	0.10	-1.33	74,75,75,76	0
4	FE2	S	1461	1/1	0.13	-1.33	51,51,51,51	0
3	FES	W	1460	4/4	0.09	-1.45	74,75,76,77	0
3	FES	U	1460	4/4	0.08	-1.81	48,48,49,49	0
4	FE2	W	1461	1/1	0.09	-2.22	68,68,68,68	0
4	FE2	U	1461	1/1	0.07	-2.42	57,57,57,57	0
4	FE2	G	1461	1/1	0.08	-2.47	52,52,52,52	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.