



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 AM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at 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.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

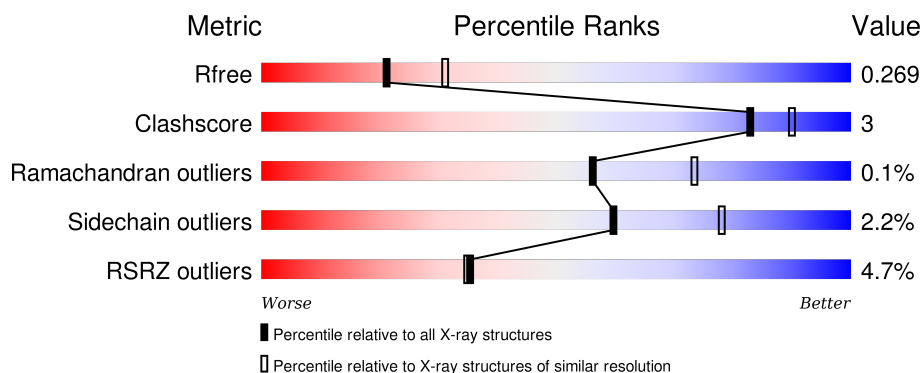
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (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 ≥ 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>3%</div> <div>84% 9% 6%</div> </div>
1	C	459	<div> <div>3%</div> <div>85% 9% 6%</div> </div>
1	E	459	<div> <div>2%</div> <div>87% 7% 6%</div> </div>
1	G	459	<div> <div>2%</div> <div>83% 11% 6%</div> </div>
1	I	459	<div> <div>8%</div> <div>87% 7% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
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
5	BNL	A	1462	-	-	-	X
5	BNL	G	1462	-	-	-	X
5	BNL	I	1462	-	-	-	X
5	BNL	K	1462	-	-	-	X
5	BNL	O	1462	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 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	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.

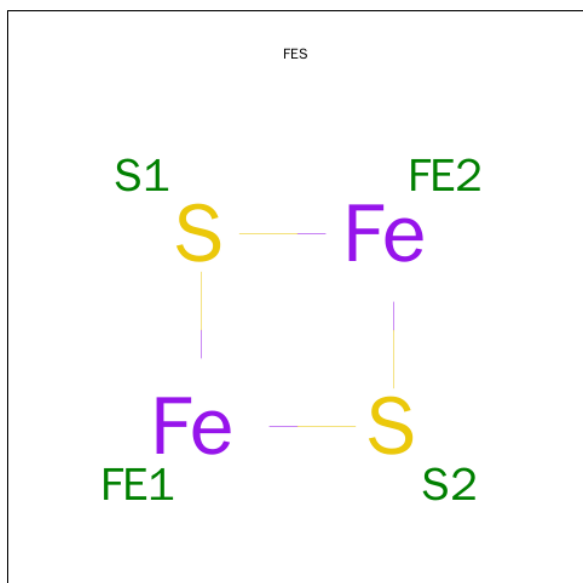
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			
2	D	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			

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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: Fe₂S₂).



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).

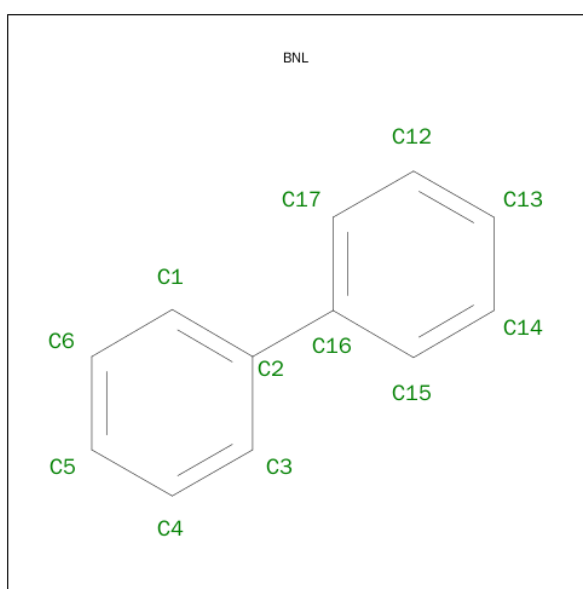
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Fe 1	0	0
4	Q	1	Total 1	Fe 1	0	0
4	K	1	Total 1	Fe 1	0	0
4	E	1	Total 1	Fe 1	0	0
4	I	1	Total 1	Fe 1	0	0
4	C	1	Total 1	Fe 1	0	0
4	W	1	Total 1	Fe 1	0	0
4	A	1	Total 1	Fe 1	0	0

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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: C₁₂H₁₀).



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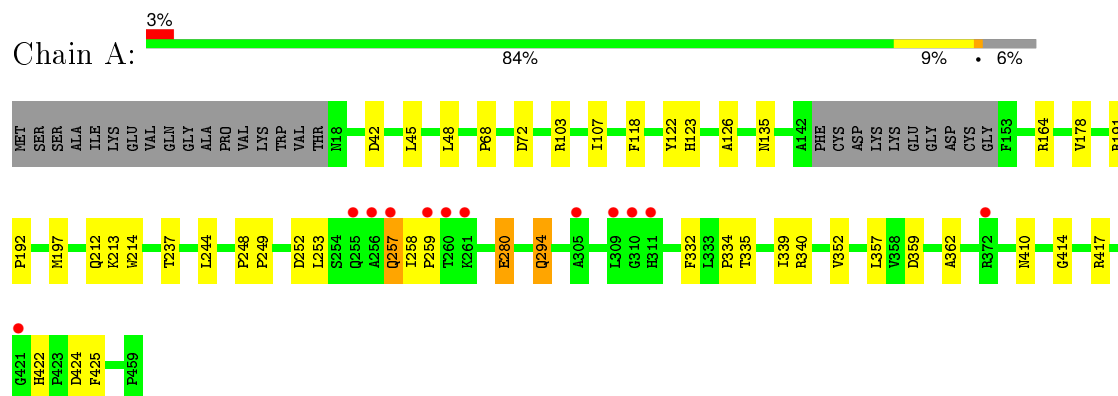
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	O	65	Total 65	O 65	0	0
6	P	26	Total 26	O 26	0	0
6	Q	83	Total 83	O 83	0	0
6	R	30	Total 30	O 30	0	0
6	S	33	Total 33	O 33	0	0
6	T	18	Total 18	O 18	0	0
6	U	25	Total 25	O 25	0	0
6	V	11	Total 11	O 11	0	0
6	W	30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

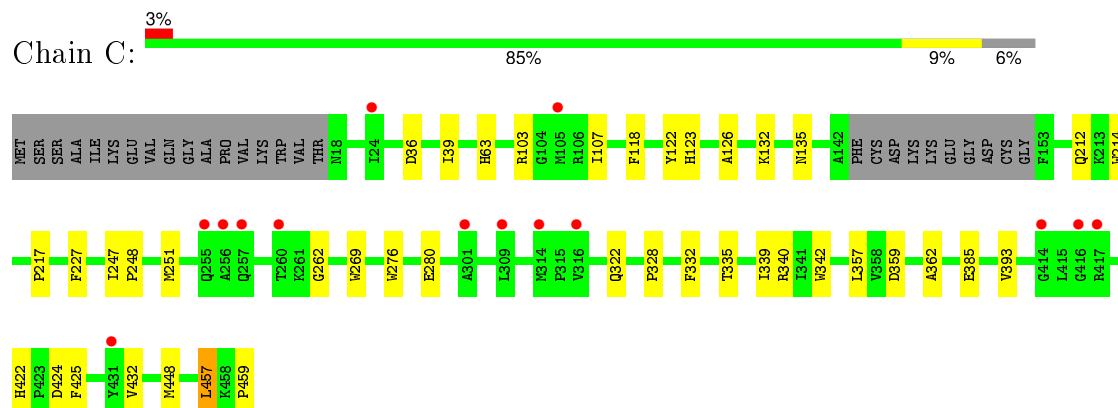
3 Residue-property plots [i](#)

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.

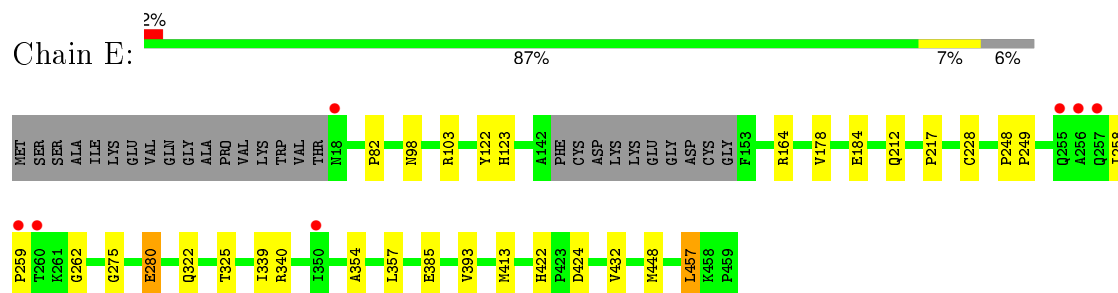
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



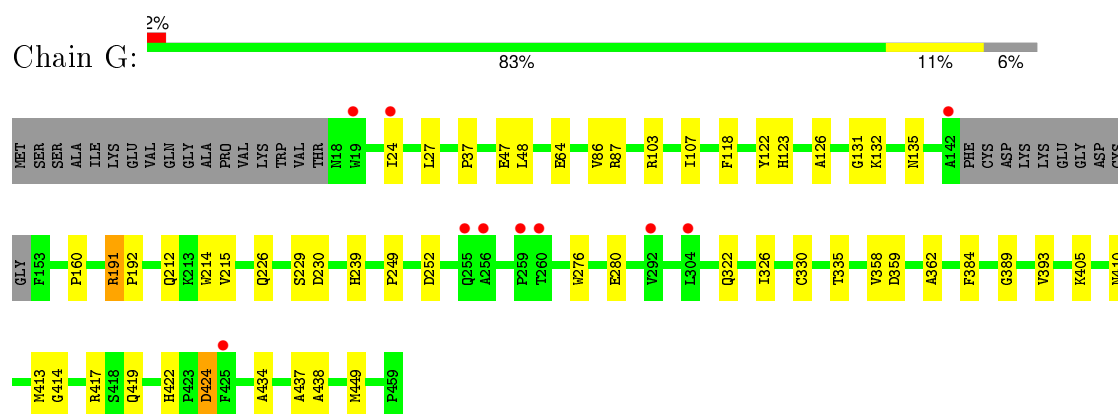
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



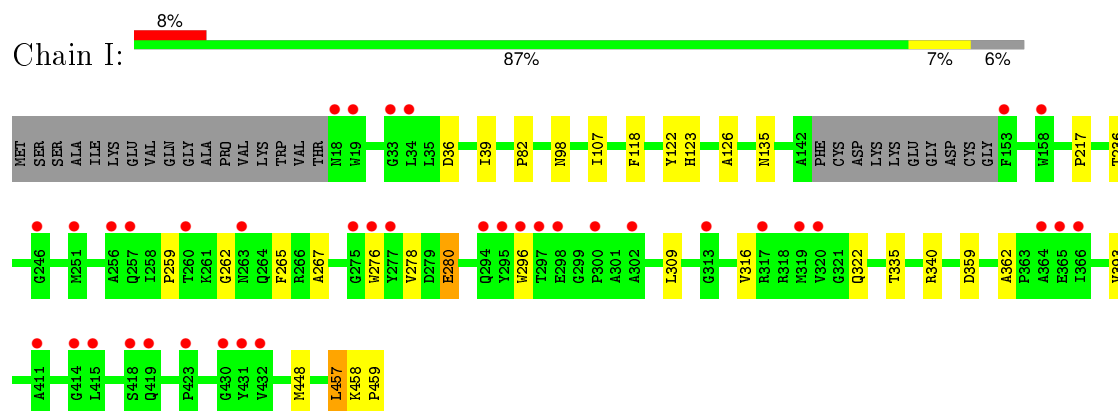
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



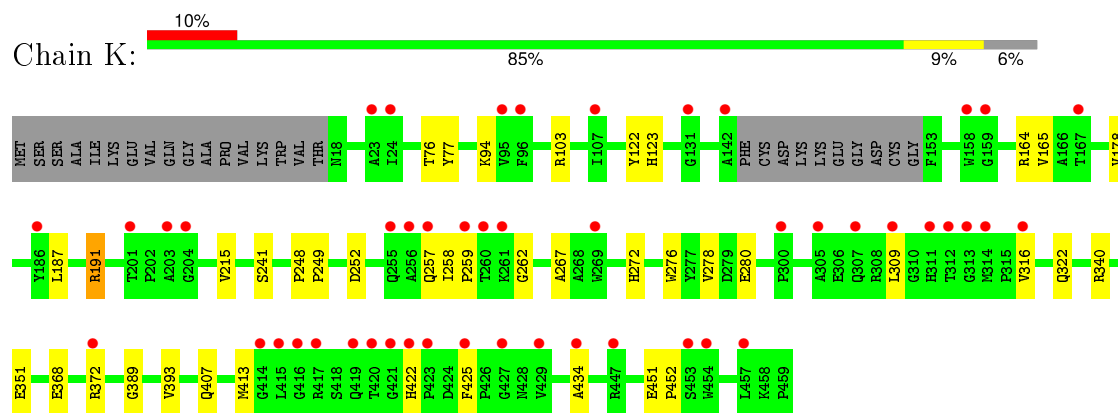
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



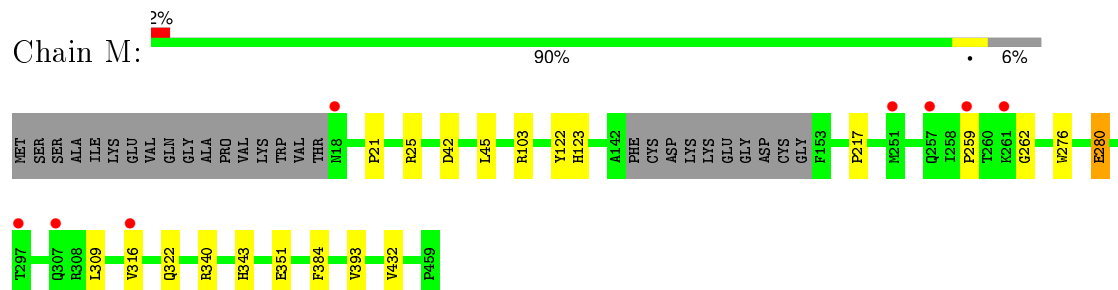
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



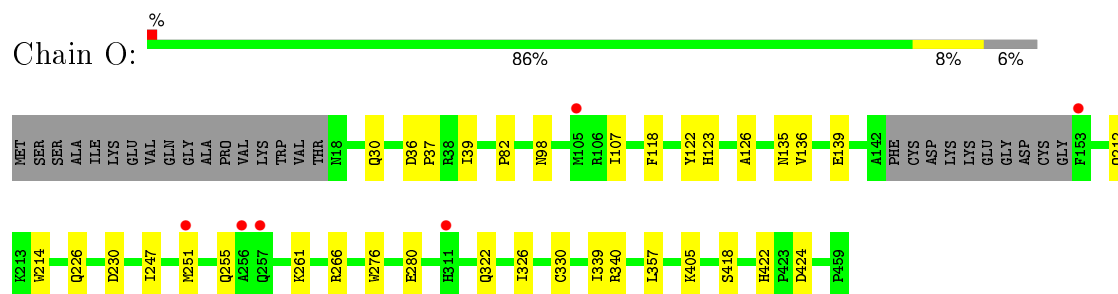
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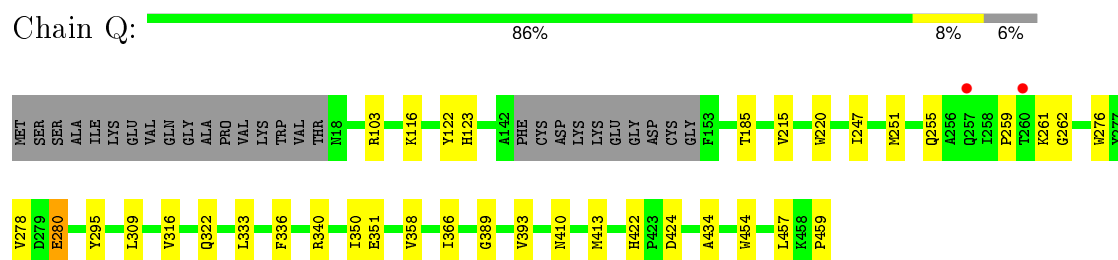
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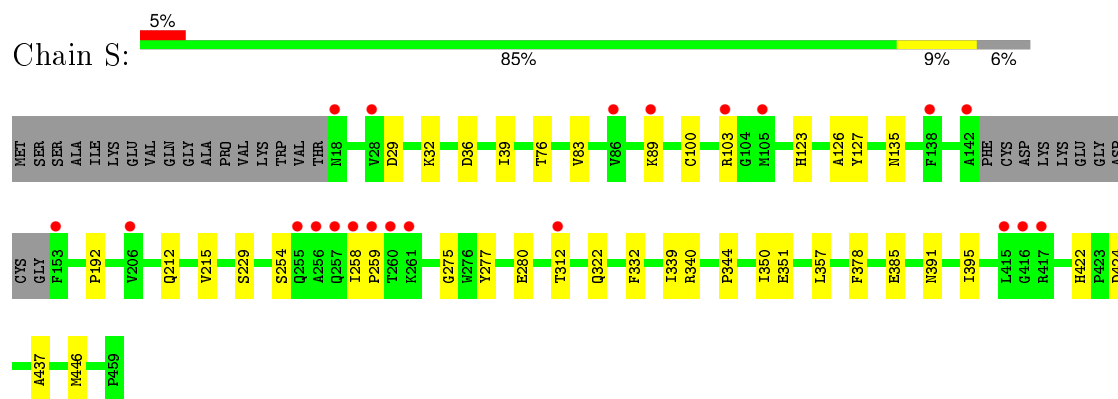
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



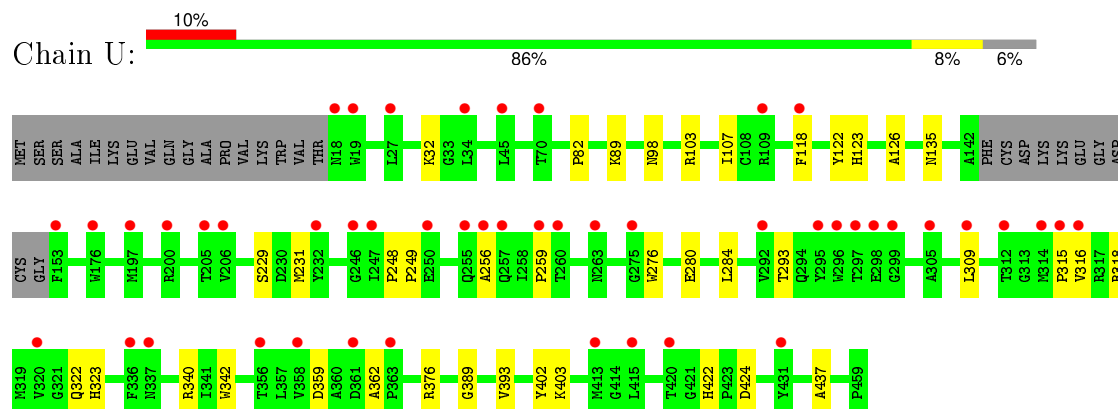
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



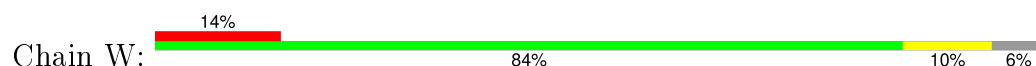
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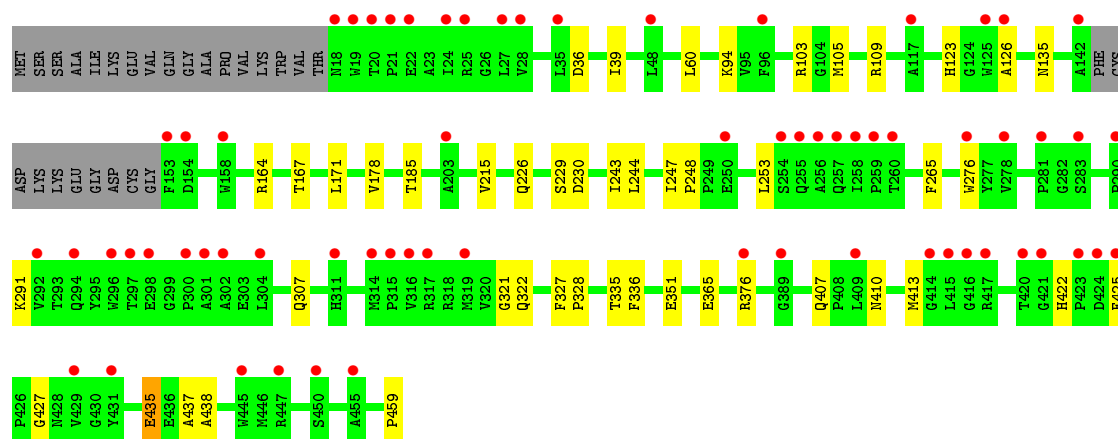


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

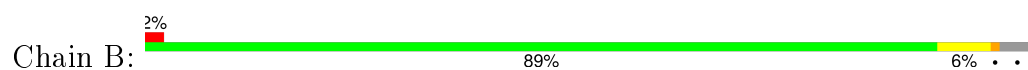


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

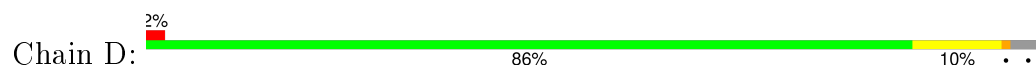




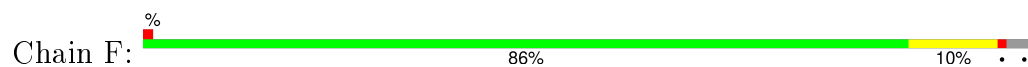
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



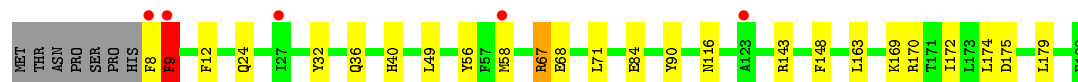
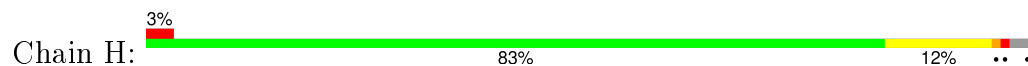
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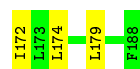
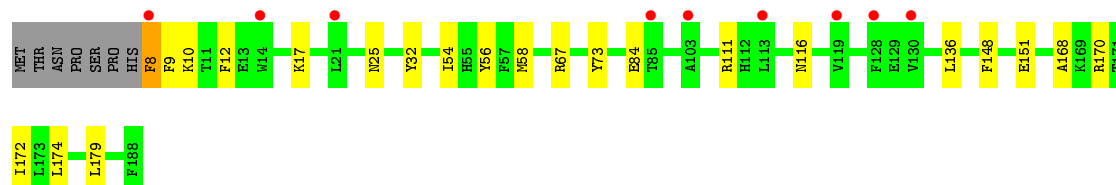
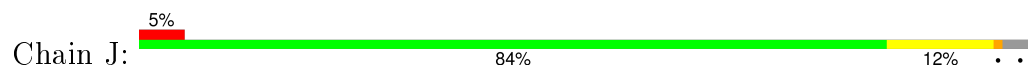
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



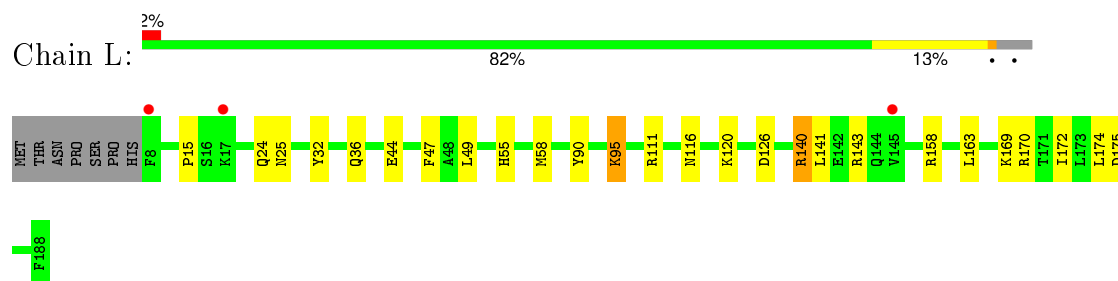
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



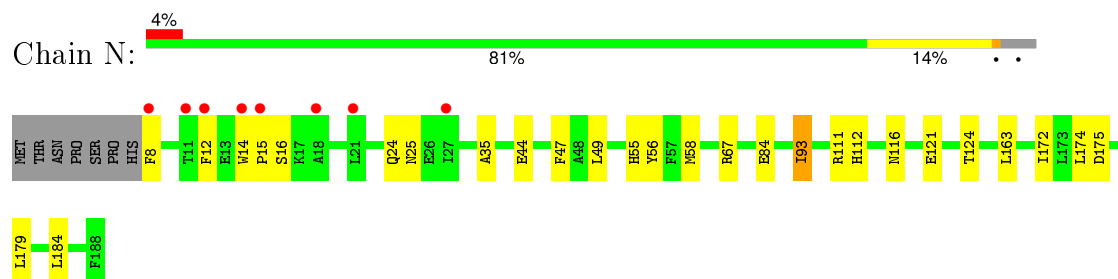
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



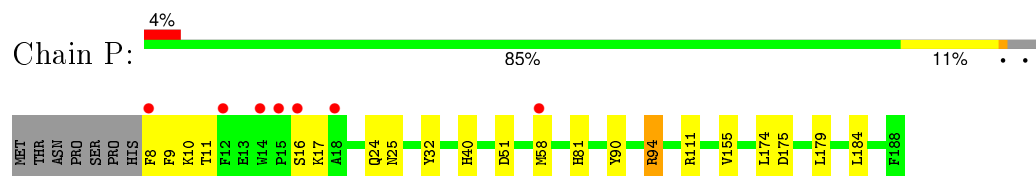
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



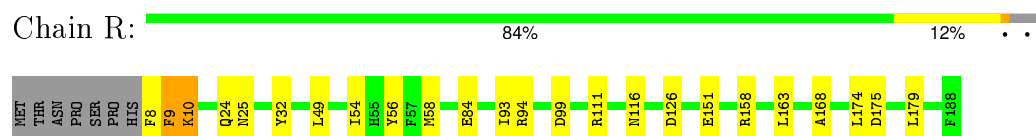
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



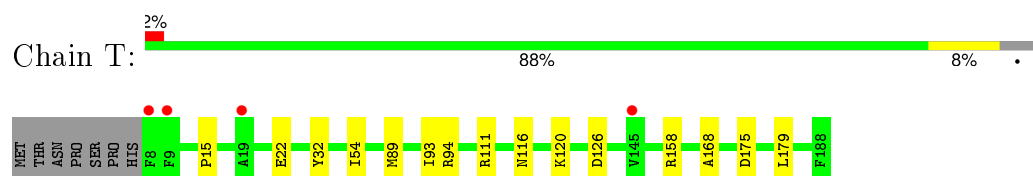
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



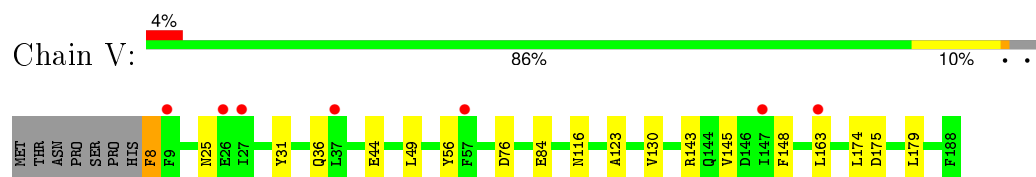
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



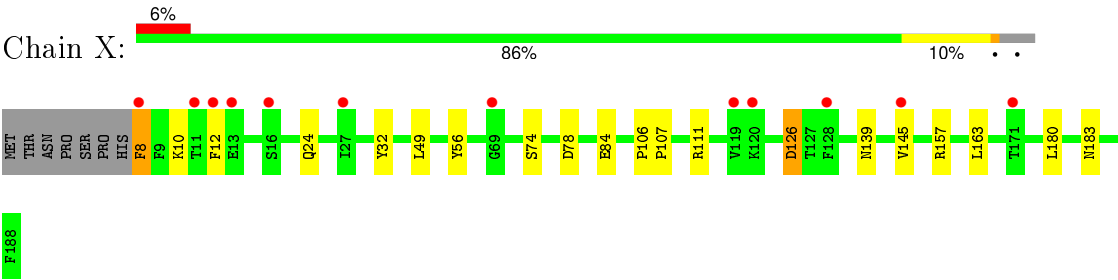
● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 76.1 (49.50-2.42)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.270 0.235 , 0.269	Depositor DCC
R_{free} test set	2608 reflections (1.03%)	DCC
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.7	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 ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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 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	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
3	W	4	0	0	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	R	30	0	0	0	0
6	S	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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

All (362) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:226:GLN:HA	1:W:230:ASP:HB2	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	428/459 (93%)	414 (97%)	14 (3%)	0	100	100
1	C	428/459 (93%)	411 (96%)	16 (4%)	1 (0%)	52	69
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%)	52	69
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%)	52	69
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%)	30	41
2	F	179/188 (95%)	171 (96%)	7 (4%)	1 (1%)	30	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	30	41
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%)	17	24
2	P	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	30	41
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%)	30	41
All	All	7284/7764 (94%)	6982 (96%)	292 (4%)	10 (0%)	56	73

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%)	50	70
1	C	350/373 (94%)	345 (99%)	5 (1%)	74	88
1	E	350/373 (94%)	344 (98%)	6 (2%)	68	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	349/373 (94%)	336 (96%)	13 (4%)	41	61
1	I	349/373 (94%)	345 (99%)	4 (1%)	80	91
1	K	349/373 (94%)	343 (98%)	6 (2%)	68	84
1	M	350/373 (94%)	346 (99%)	4 (1%)	80	91
1	O	350/373 (94%)	344 (98%)	6 (2%)	68	84
1	Q	350/373 (94%)	341 (97%)	9 (3%)	54	74
1	S	349/373 (94%)	345 (99%)	4 (1%)	80	91
1	U	349/373 (94%)	344 (99%)	5 (1%)	74	88
1	W	349/373 (94%)	339 (97%)	10 (3%)	50	70
2	B	158/167 (95%)	154 (98%)	4 (2%)	55	75
2	D	158/167 (95%)	156 (99%)	2 (1%)	76	89
2	F	158/167 (95%)	150 (95%)	8 (5%)	29	46
2	H	160/167 (96%)	155 (97%)	5 (3%)	47	68
2	J	160/167 (96%)	156 (98%)	4 (2%)	55	75
2	L	160/167 (96%)	158 (99%)	2 (1%)	76	89
2	N	160/167 (96%)	154 (96%)	6 (4%)	40	59
2	P	160/167 (96%)	155 (97%)	5 (3%)	47	68
2	R	160/167 (96%)	154 (96%)	6 (4%)	40	59
2	T	160/167 (96%)	158 (99%)	2 (1%)	76	89
2	V	160/167 (96%)	156 (98%)	4 (2%)	55	75
2	X	160/167 (96%)	158 (99%)	2 (1%)	76	89
All	All	6108/6480 (94%)	5976 (98%)	132 (2%)	60	78

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	0.56	0	16,16,16	0.58	0
3	FES	C	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	C	1462	-	13,13,13	0.56	0	16,16,16	0.47	0
3	FES	E	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	E	1462	-	13,13,13	0.57	0	16,16,16	0.54	0
3	FES	G	1460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	G	1462	-	13,13,13	0.55	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	0.54	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	0.58	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	0.55	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	0.57	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	0.62	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	0.56	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	0.54	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	0.56	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	0/1/1/1
5	BNL	A	1462	-	-	0/4/4/4	0/2/2/2
3	FES	C	1460	1	-	0/0/4/4	0/1/1/1
5	BNL	C	1462	-	-	0/4/4/4	0/2/2/2
3	FES	E	1460	1	-	0/0/4/4	0/1/1/1
5	BNL	E	1462	-	-	0/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	G	1460	1	-	0/0/4/4	0/1/1/1
5	BNL	G	1462	-	-	0/4/4/4	0/2/2/2
3	FES	I	1460	1	-	0/0/4/4	0/1/1/1
5	BNL	I	1462	-	-	0/4/4/4	0/2/2/2
3	FES	K	1460	1	-	0/0/4/4	0/1/1/1
5	BNL	K	1462	-	-	0/4/4/4	0/2/2/2
3	FES	M	1460	1	-	0/0/4/4	0/1/1/1
5	BNL	M	1462	-	-	0/4/4/4	0/2/2/2
3	FES	O	1460	1	-	0/0/4/4	0/1/1/1
5	BNL	O	1462	-	-	0/4/4/4	0/2/2/2
3	FES	Q	1460	1	-	0/0/4/4	0/1/1/1
5	BNL	Q	1462	-	-	0/4/4/4	0/2/2/2
3	FES	S	1460	1	-	0/0/4/4	0/1/1/1
5	BNL	S	1462	-	-	0/4/4/4	0/2/2/2
3	FES	U	1460	1	-	0/0/4/4	0/1/1/1
5	BNL	U	1462	-	-	0/4/4/4	0/2/2/2
3	FES	W	1460	1	-	0/0/4/4	0/1/1/1
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.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1460	FES	1	0
3	C	1460	FES	1	0
3	E	1460	FES	1	0
3	G	1460	FES	1	0
3	I	1460	FES	1	0
3	K	1460	FES	1	0
3	M	1460	FES	1	0
5	M	1462	BNL	1	0
3	O	1460	FES	1	0
3	Q	1460	FES	1	0
3	S	1460	FES	1	0
3	U	1460	FES	1	0
3	W	1460	FES	1	0

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, 95th 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 ²)	Q<0.9
1	A	432/459 (94%)	0.00	12 (2%) 56 55	24, 41, 55, 61	17 (3%)
1	C	432/459 (94%)	0.07	14 (3%) 51 50	30, 44, 54, 58	17 (3%)
1	E	432/459 (94%)	-0.03	7 (1%) 74 74	23, 35, 47, 55	17 (3%)
1	G	432/459 (94%)	0.08	10 (2%) 64 63	35, 47, 60, 66	17 (3%)
1	I	432/459 (94%)	0.39	38 (8%) 12 12	39, 52, 64, 69	17 (3%)
1	K	432/459 (94%)	0.62	48 (11%) 7 7	42, 55, 65, 68	17 (3%)
1	M	432/459 (94%)	0.00	8 (1%) 70 69	26, 38, 58, 62	17 (3%)
1	O	432/459 (94%)	-0.14	6 (1%) 78 77	20, 34, 49, 57	17 (3%)
1	Q	432/459 (94%)	-0.25	2 (0%) 91 91	22, 31, 44, 61	17 (3%)
1	S	432/459 (94%)	0.31	21 (4%) 33 33	36, 47, 58, 67	17 (3%)
1	U	432/459 (94%)	0.68	48 (11%) 7 7	39, 57, 72, 74	17 (3%)
1	W	432/459 (94%)	0.89	66 (15%) 3 3	46, 59, 70, 74	17 (3%)
2	B	181/188 (96%)	0.06	4 (2%) 65 64	30, 38, 47, 58	4 (2%)
2	D	181/188 (96%)	0.01	3 (1%) 73 72	28, 39, 51, 56	4 (2%)
2	F	181/188 (96%)	-0.20	1 (0%) 90 90	28, 33, 47, 60	4 (2%)
2	H	181/188 (96%)	0.23	5 (2%) 56 55	36, 45, 60, 66	4 (2%)
2	J	181/188 (96%)	0.28	9 (4%) 32 32	40, 50, 57, 63	4 (2%)
2	L	181/188 (96%)	0.41	3 (1%) 73 72	39, 48, 63, 70	4 (2%)
2	N	181/188 (96%)	0.04	8 (4%) 38 38	27, 38, 61, 75	4 (2%)
2	P	181/188 (96%)	0.02	7 (3%) 43 43	24, 36, 64, 79	4 (2%)
2	R	181/188 (96%)	-0.16	0 100 100	24, 32, 52, 62	4 (2%)
2	T	181/188 (96%)	0.22	4 (2%) 65 64	33, 39, 55, 65	4 (2%)
2	V	181/188 (96%)	0.25	7 (3%) 43 43	45, 53, 59, 64	4 (2%)
2	X	181/188 (96%)	0.58	12 (6%) 22 21	42, 52, 59, 62	4 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	7356/7764 (94%)	0.20	343 (4%)	35	35	20, 44, 63, 79	252 (3%)

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	ALA	10.3
1	K	256	ALA	9.7
1	S	256	ALA	7.5
1	A	257	GLN	7.1
1	K	255	GLN	6.9
1	U	256	ALA	6.9
1	U	314	MET	6.0
1	K	260	THR	5.9
1	A	255	GLN	5.9
1	W	257	GLN	5.7
1	W	425	PHE	5.7
1	I	320	VAL	5.5
1	W	301	ALA	5.4
1	U	19	TRP	5.3
1	W	292	VAL	5.2
1	S	255	GLN	5.1
2	N	14	TRP	5.0
1	W	455	ALA	5.0
1	W	316	VAL	5.0
1	S	257	GLN	4.9
1	I	256	ALA	4.8
1	W	255	GLN	4.7
1	K	203	ALA	4.7
2	X	11	THR	4.7
1	U	257	GLN	4.7
1	G	256	ALA	4.6
1	K	259	PRO	4.6
1	W	416	GLY	4.6
1	K	24	ILE	4.6
1	A	260	THR	4.6
1	K	312	THR	4.6
1	I	415	LEU	4.5
2	X	8	PHE	4.5
1	W	315	PRO	4.4
1	K	314	MET	4.3
1	W	21	PRO	4.3
1	W	389	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	246	GLY	4.3
1	W	283	SER	4.2
2	H	123	ALA	4.1
1	E	259	PRO	4.1
1	E	257	GLN	4.1
1	U	415	LEU	4.1
1	S	259	PRO	4.1
1	W	302	ALA	4.1
1	E	256	ALA	4.0
1	M	261	LYS	4.0
1	C	301	ALA	4.0
1	A	259	PRO	4.0
1	U	260	THR	4.0
1	K	316	VAL	3.9
1	W	256	ALA	3.9
1	W	415	LEU	3.9
1	W	22	GLU	3.9
2	H	27	ILE	3.9
1	W	298	GLU	3.8
1	K	417	ARG	3.8
1	G	142	ALA	3.8
1	I	297	THR	3.8
1	U	315	PRO	3.8
2	D	160	ASP	3.8
1	C	257	GLN	3.7
1	S	260	THR	3.7
1	S	138	PHE	3.7
1	K	95	VAL	3.7
1	K	457	LEU	3.7
1	K	311	HIS	3.6
1	K	421	GLY	3.6
1	K	427	GLY	3.6
1	I	153	PHE	3.6
1	W	317	ARG	3.6
1	W	314	MET	3.6
1	W	24	ILE	3.6
1	S	153	PHE	3.6
1	C	314	MET	3.6
2	P	14	TRP	3.6
1	I	366	ILE	3.5
1	C	417	ARG	3.5
1	U	206	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	U	263	ASN	3.5
1	W	281	PRO	3.5
1	U	292	VAL	3.5
1	U	297	THR	3.4
1	U	34	LEU	3.4
1	I	418	SER	3.4
1	W	28	VAL	3.4
1	C	260	THR	3.4
2	N	12	PHE	3.4
2	P	16	SER	3.4
1	G	260	THR	3.4
1	U	275	GLY	3.3
1	U	255	GLN	3.3
1	I	260	THR	3.3
1	K	23	ALA	3.3
1	W	158	TRP	3.3
1	W	414	GLY	3.3
1	I	419	GLN	3.3
2	V	37	LEU	3.3
1	I	431	TYR	3.3
1	U	70	THR	3.3
1	C	256	ALA	3.3
1	I	257	GLN	3.3
1	E	260	THR	3.2
1	K	201	THR	3.2
1	U	299	GLY	3.2
1	W	276	TRP	3.2
1	W	153	PHE	3.2
1	S	105	MET	3.2
2	T	8	PHE	3.2
1	K	261	LYS	3.2
2	X	12	PHE	3.2
1	K	309	LEU	3.2
1	K	415	LEU	3.2
2	H	8	PHE	3.1
1	W	19	TRP	3.1
1	A	305	ALA	3.1
1	W	420	THR	3.1
1	W	142	ALA	3.1
2	X	16	SER	3.1
2	P	8	PHE	3.1
1	K	313	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	U	118	PHE	3.1
1	I	295	TYR	3.0
1	U	316	VAL	3.0
1	I	319	MET	3.0
1	U	363	PRO	3.0
1	K	372	ARG	3.0
1	K	186	TYR	3.0
1	U	295	TYR	3.0
2	P	18	ALA	3.0
1	K	257	GLN	3.0
1	G	24	ILE	3.0
2	L	145	VAL	3.0
2	L	17	LYS	3.0
1	W	25	ARG	3.0
2	N	15	PRO	3.0
1	U	309	LEU	3.0
1	I	276	TRP	3.0
1	I	18	ASN	3.0
1	I	298	GLU	2.9
1	W	450	SER	2.9
1	Q	257	GLN	2.9
1	K	305	ALA	2.9
1	O	256	ALA	2.9
1	I	19	TRP	2.9
1	U	413	MET	2.9
1	U	232	TYR	2.9
1	W	125	TRP	2.9
1	K	96	PHE	2.9
2	J	8	PHE	2.9
1	K	434	ALA	2.9
1	K	425	PHE	2.8
1	W	290	PRO	2.8
1	O	311	HIS	2.8
1	K	131	GLY	2.8
1	W	417	ARG	2.8
1	I	411	ALA	2.8
1	U	361	ASP	2.8
2	V	9	PHE	2.8
1	U	296	TRP	2.8
1	C	24	ILE	2.8
1	W	300	PRO	2.8
1	U	176	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	S	416	GLY	2.8
1	C	105	MET	2.7
1	S	312	THR	2.7
1	G	292	VAL	2.7
1	U	259	PRO	2.7
2	J	130	VAL	2.7
1	C	309	LEU	2.7
1	I	34	LEU	2.7
2	T	19	ALA	2.7
2	B	147	ILE	2.7
1	C	414	GLY	2.7
1	K	416	GLY	2.7
1	U	200	ARG	2.7
1	W	259	PRO	2.7
2	B	8	PHE	2.6
1	W	35	LEU	2.6
1	W	297	THR	2.6
1	U	298	GLU	2.6
1	K	269	TRP	2.6
1	A	309	LEU	2.6
2	V	147	ILE	2.6
2	P	15	PRO	2.6
1	U	246	GLY	2.6
2	P	58	MET	2.6
1	K	414	GLY	2.6
1	M	297	THR	2.6
2	N	18	ALA	2.6
1	U	109	ARG	2.5
1	U	320	VAL	2.5
1	I	251	MET	2.5
1	W	311	HIS	2.5
1	I	263	ASN	2.5
1	W	48	LEU	2.5
1	U	337	ASN	2.5
1	S	86	VAL	2.5
1	W	18	ASN	2.5
2	X	171	THR	2.5
1	I	313	GLY	2.5
2	P	12	PHE	2.5
1	K	423	PRO	2.5
1	A	311	HIS	2.5
2	N	27	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	277	TYR	2.5
1	U	250	GLU	2.5
1	W	250	GLU	2.5
2	D	162	ASN	2.5
2	F	8	PHE	2.4
1	I	423	PRO	2.4
1	U	27	LEU	2.4
1	W	319	MET	2.4
2	X	128	PHE	2.4
1	W	429	VAL	2.4
1	U	18	ASN	2.4
2	J	85	THR	2.4
1	K	159	GLY	2.4
1	W	304	LEU	2.4
2	X	27	ILE	2.4
1	S	103	ARG	2.4
1	G	425	PHE	2.4
1	W	296	TRP	2.4
2	J	128	PHE	2.4
1	I	275	GLY	2.4
1	I	158	TRP	2.4
1	K	158	TRP	2.4
1	O	153	PHE	2.4
1	A	261	LYS	2.4
1	S	415	LEU	2.4
1	W	424	ASP	2.4
2	X	145	VAL	2.4
1	K	420	THR	2.4
1	I	300	PRO	2.3
1	W	376	ARG	2.3
1	I	294	GLN	2.3
1	M	257	GLN	2.3
2	N	11	THR	2.3
1	O	251	MET	2.3
1	M	259	PRO	2.3
1	W	423	PRO	2.3
1	G	19	TRP	2.3
1	K	167	THR	2.3
1	W	20	THR	2.3
1	I	364	ALA	2.3
1	K	142	ALA	2.3
1	M	251	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	257	GLN	2.3
1	Q	260	THR	2.3
2	T	145	VAL	2.3
1	W	117	ALA	2.3
1	U	197	MET	2.3
1	U	336	PHE	2.3
2	L	8	PHE	2.3
1	I	365	GLU	2.3
1	M	307	GLN	2.3
1	S	206	VAL	2.3
1	W	421	GLY	2.3
2	B	145	VAL	2.3
1	O	105	MET	2.3
1	K	419	GLN	2.3
1	G	304	LEU	2.3
2	J	21	LEU	2.3
1	K	300	PRO	2.3
1	G	255	GLN	2.2
1	A	421	GLY	2.2
1	C	316	VAL	2.2
1	K	307	GLN	2.2
1	W	409	LEU	2.2
1	I	432	VAL	2.2
2	B	58	MET	2.2
1	C	416	GLY	2.2
1	I	414	GLY	2.2
2	T	9	PHE	2.2
1	S	28	VAL	2.2
1	K	454	TRP	2.2
1	U	45	LEU	2.2
1	W	431	TYR	2.2
1	W	447	ARG	2.2
2	H	58	MET	2.2
1	I	430	GLY	2.2
2	J	14	TRP	2.2
1	S	261	LYS	2.2
2	X	120	LYS	2.2
1	K	429	VAL	2.2
1	S	142	ALA	2.2
2	D	123	ALA	2.2
1	U	420	THR	2.2
2	V	26	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	V	57	PHE	2.1
1	M	316	VAL	2.1
1	U	358	VAL	2.1
1	W	254	SER	2.1
2	X	69	GLY	2.1
2	X	119	VAL	2.1
2	V	27	ILE	2.1
1	U	312	THR	2.1
1	W	260	THR	2.1
1	I	33	GLY	2.1
1	K	447	ARG	2.1
1	W	154	ASP	2.1
1	E	255	GLN	2.1
1	W	445	TRP	2.1
1	I	302	ALA	2.1
1	W	278	VAL	2.1
1	U	431	TYR	2.1
1	C	255	GLN	2.1
1	W	294	GLN	2.1
1	W	96	PHE	2.1
2	V	163	LEU	2.1
1	K	204	GLY	2.1
1	I	296	TRP	2.1
2	J	119	VAL	2.1
1	K	107	ILE	2.1
1	S	258	ILE	2.1
1	S	417	ARG	2.1
2	H	9	PHE	2.1
2	J	113	LEU	2.1
1	E	18	ASN	2.1
1	I	317	ARG	2.1
1	W	258	ILE	2.1
1	A	310	GLY	2.1
1	C	431	TYR	2.1
1	S	89	LYS	2.1
1	A	372	ARG	2.0
1	W	126	ALA	2.0
2	J	103	ALA	2.0
1	G	259	PRO	2.0
2	N	8	PHE	2.0
1	E	350	ILE	2.0
1	W	27	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	18	ASN	2.0
1	S	18	ASN	2.0
1	U	305	ALA	2.0
1	W	203	ALA	2.0
1	K	422	HIS	2.0
1	U	247	ILE	2.0
2	X	13	GLU	2.0
1	K	453	SER	2.0
2	N	21	LEU	2.0
1	U	153	PHE	2.0
1	U	205	THR	2.0
1	U	356	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
5	BNL	K	1462	12/12	0.78	0.33	8.49	86,86,87,87	0
5	BNL	G	1462	12/12	0.89	0.30	4.94	63,64,64,64	0
5	BNL	O	1462	12/12	0.93	0.24	4.68	44,44,45,45	0
5	BNL	A	1462	12/12	0.84	0.27	4.45	76,76,76,76	0
5	BNL	W	1462	12/12	0.78	0.34	4.20	87,87,88,88	0
5	BNL	S	1462	12/12	0.84	0.32	4.12	82,82,82,82	0
5	BNL	U	1462	12/12	0.84	0.30	3.19	86,86,86,86	0
5	BNL	I	1462	12/12	0.86	0.22	2.46	63,63,64,64	0
5	BNL	Q	1462	12/12	0.94	0.18	2.26	40,40,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	BNL	C	1462	12/12	0.93	0.18	1.87	55,56,56,56	0
5	BNL	M	1462	12/12	0.91	0.19	1.19	55,56,56,56	0
5	BNL	E	1462	12/12	0.92	0.17	0.98	49,49,49,49	0
4	FE2	A	1461	1/1	0.99	0.16	0.88	53,53,53,53	0
4	FE2	Q	1461	1/1	0.99	0.12	-0.06	37,37,37,37	0
4	FE2	E	1461	1/1	0.98	0.15	-0.34	41,41,41,41	0
3	FES	E	1460	4/4	0.90	0.11	-0.38	44,46,47,50	0
4	FE2	I	1461	1/1	0.98	0.14	-0.41	58,58,58,58	0
3	FES	O	1460	4/4	0.95	0.11	-0.55	44,45,46,48	0
3	FES	I	1460	4/4	0.92	0.11	-0.79	45,46,48,50	0
3	FES	G	1460	4/4	0.96	0.10	-0.85	54,54,54,56	0
3	FES	C	1460	4/4	0.96	0.10	-1.10	43,44,45,46	0
3	FES	M	1460	4/4	0.95	0.09	-1.15	38,38,39,42	0
3	FES	A	1460	4/4	0.93	0.10	-1.20	43,44,46,48	0
3	FES	Q	1460	4/4	0.94	0.09	-1.20	39,39,41,44	0
3	FES	S	1460	4/4	0.91	0.10	-1.21	86,86,86,87	0
4	FE2	M	1461	1/1	0.99	0.13	-1.27	43,43,43,43	0
3	FES	W	1460	4/4	0.91	0.09	-1.42	74,75,76,77	0
3	FES	K	1460	4/4	0.96	0.07	-1.93	74,75,75,76	0
3	FES	U	1460	4/4	0.97	0.08	-2.12	48,48,49,49	0
4	FE2	U	1461	1/1	0.98	0.08	-2.55	57,57,57,57	0
4	FE2	G	1461	1/1	0.99	0.07	-4.17	52,52,52,52	0
4	FE2	S	1461	1/1	0.98	0.14	-	51,51,51,51	0
4	FE2	W	1461	1/1	0.95	0.09	-	68,68,68,68	0
4	FE2	K	1461	1/1	0.96	0.14	-	59,59,59,59	0
4	FE2	C	1461	1/1	0.99	0.11	-	44,44,44,44	0
4	FE2	O	1461	1/1	1.00	0.13	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.