Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 06:25 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 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

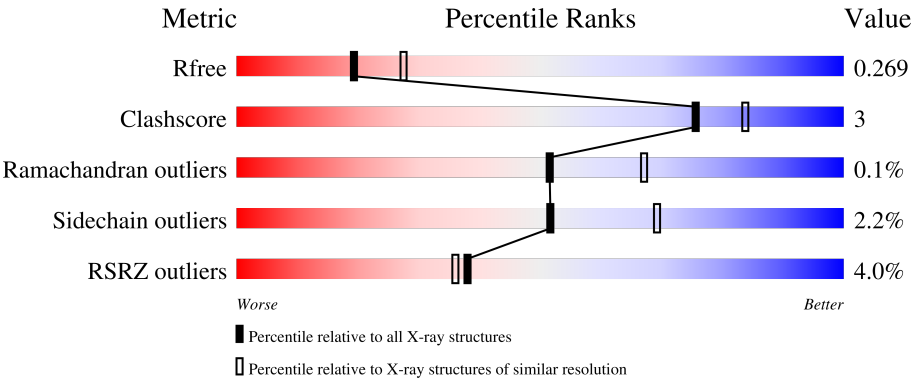
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.42 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}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	2% 84% 9% 6%
1	C	459	3% 85% 9% 6%
1	E	459	% 87% 7% 6%
1	G	459	2% 83% 11% 6%
1	I	459	7% 87% 7% 6%

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Mol	Chain	Length	Quality of chain
1	K	459	9% 85% 9% 6%
1	M	459	% 90% 6%
1	O	459	% 86% 8% 6%
1	Q	459	86% 8% 6%
1	S	459	4% 85% 9% 6%
1	U	459	9% 86% 8% 6%
1	W	459	13% 84% 10% 6%
2	B	188	2% 89% 6%
2	D	188	% 86% 10%
2	F	188	% 86% 10%
2	H	188	2% 83% 12%
2	J	188	3% 84% 12%
2	L	188	2% 82% 13%
2	N	188	3% 81% 14%
2	P	188	4% 85% 11%
2	R	188	84% 12%
2	T	188	2% 88% 8%
2	V	188	3% 86% 10%
2	X	188	5% 86% 10%

2 Entry composition (i)

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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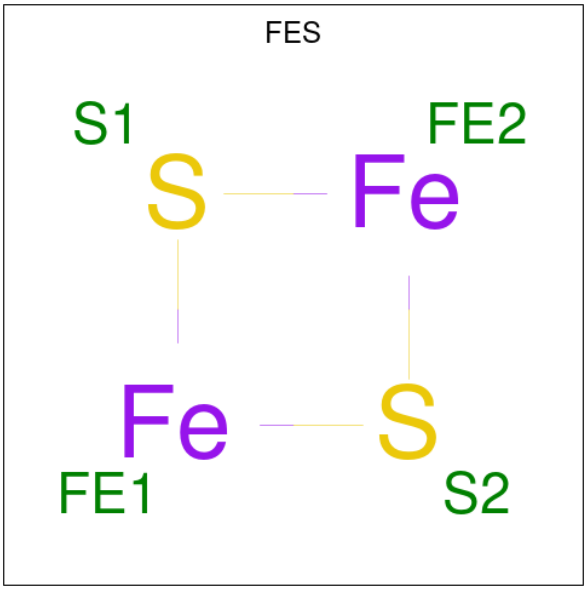
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			
2	H	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	J	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	L	181	Total	C	N	O	S	0	0	0
			1507	957	266	280	4			
2	N	181	Total	C	N	O	S	0	0	0
			1507	957	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: Fe_2S_2).



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 Fe S 4 2 2	0	0
3	E	1	Total Fe S 4 2 2	0	0
3	G	1	Total Fe S 4 2 2	0	0
3	I	1	Total Fe S 4 2 2	0	0
3	K	1	Total Fe S 4 2 2	0	0
3	M	1	Total Fe S 4 2 2	0	0
3	O	1	Total Fe S 4 2 2	0	0
3	Q	1	Total Fe S 4 2 2	0	0
3	S	1	Total Fe S 4 2 2	0	0
3	U	1	Total Fe S 4 2 2	0	0
3	W	1	Total Fe S 4 2 2	0	0

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

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

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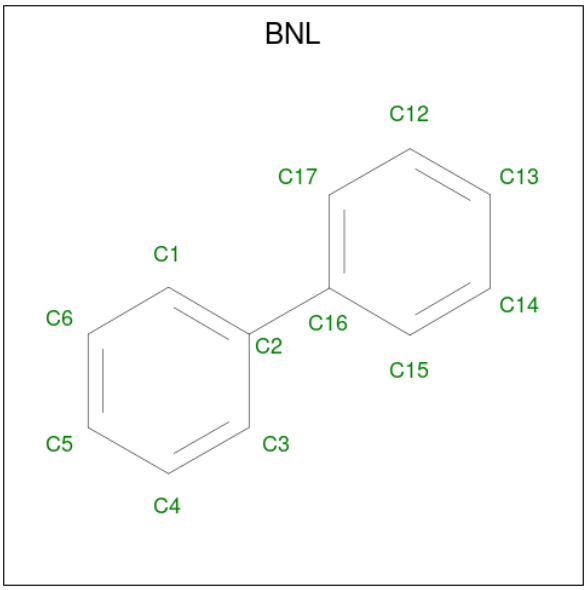
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Q	1	Total Fe 1 1	0	0
4	S	1	Total Fe 1 1	0	0
4	U	1	Total Fe 1 1	0	0
4	W	1	Total Fe 1 1	0	0

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



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

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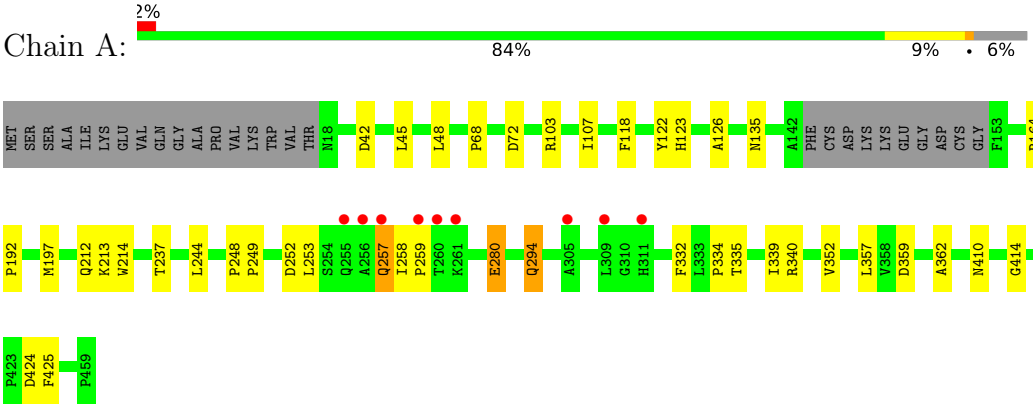
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	O	65	Total O 65 65	0	0
6	P	26	Total O 26 26	0	0
6	Q	83	Total O 83 83	0	0
6	R	30	Total O 30 30	0	0
6	S	33	Total O 33 33	0	0
6	T	18	Total O 18 18	0	0
6	U	25	Total O 25 25	0	0
6	V	11	Total O 11 11	0	0
6	W	30	Total O 30 30	0	0
6	X	14	Total O 14 14	0	0

3 Residue-property plots (i)

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

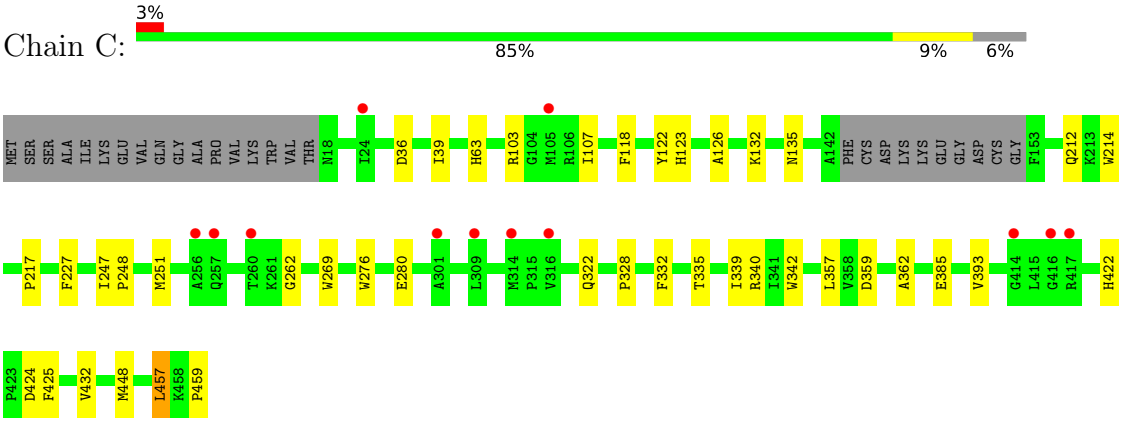
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain A:



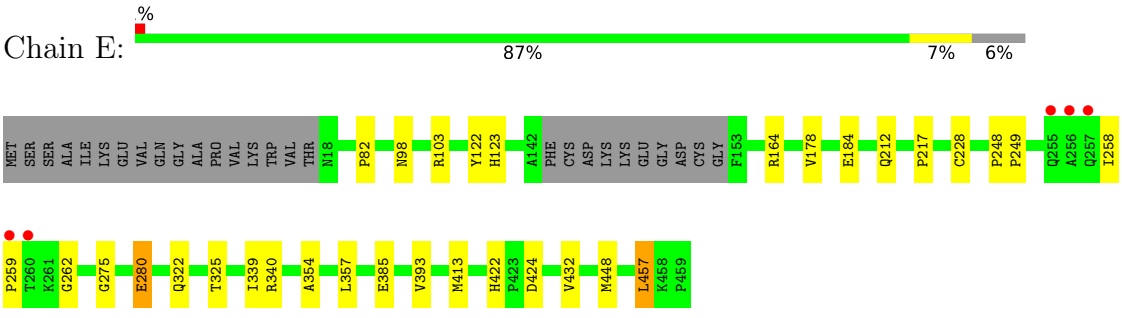
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain C:



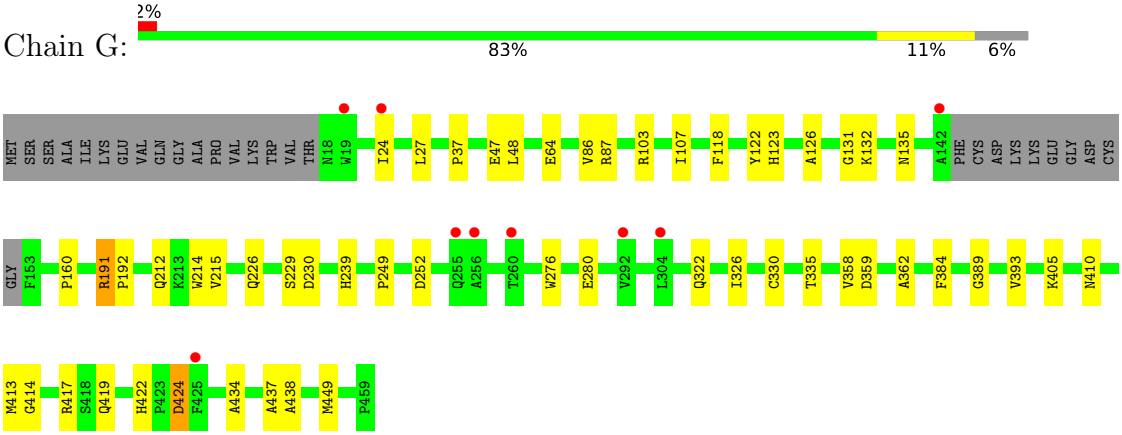
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain E:



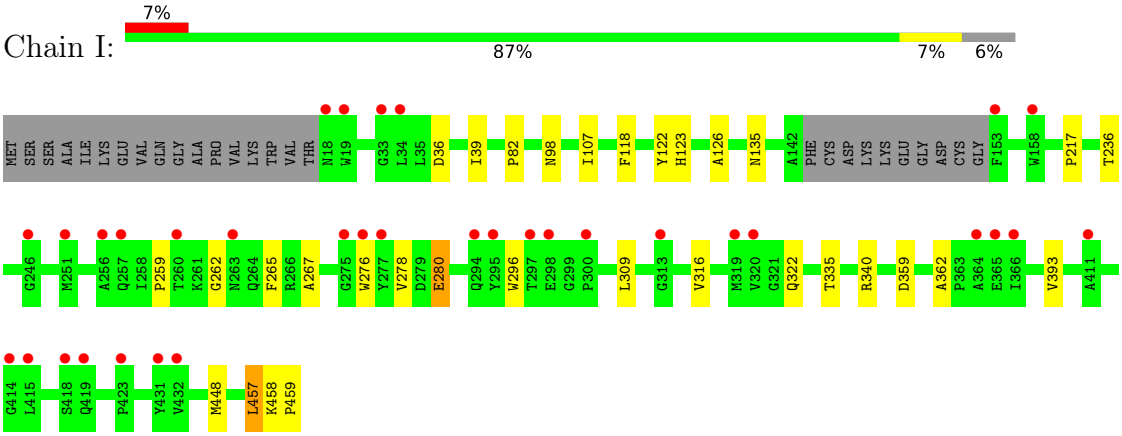
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain G:



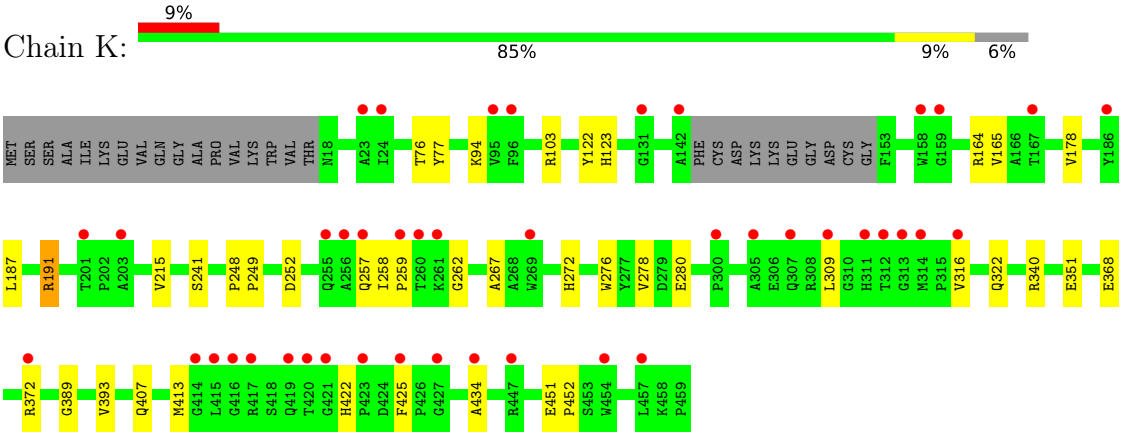
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain I:



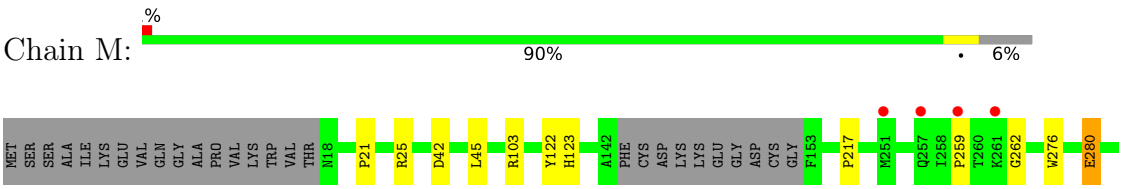
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

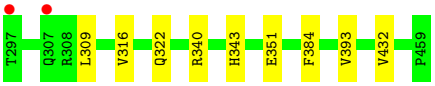
Chain K:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

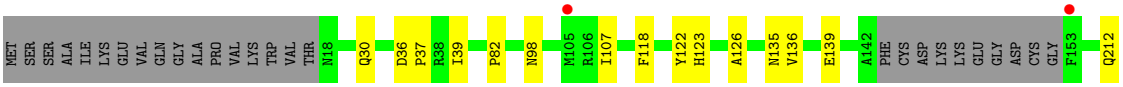
Chain M:





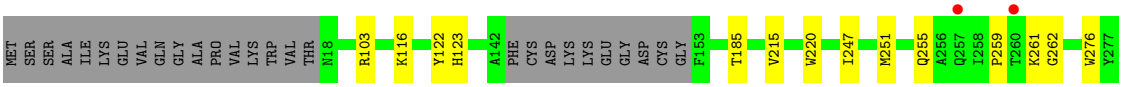
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

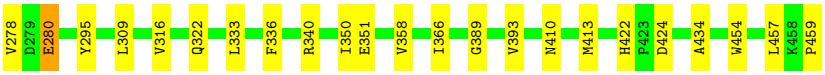
Chain O:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

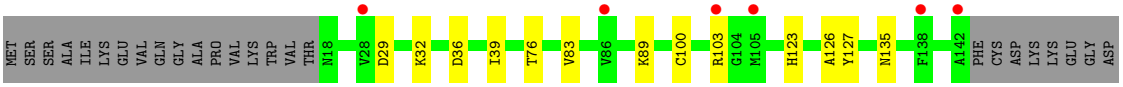
Chain Q:

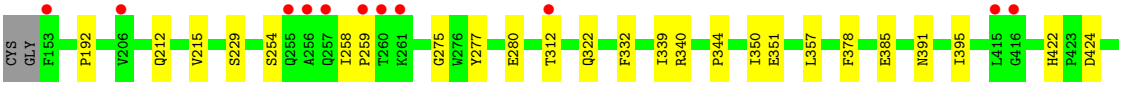




• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

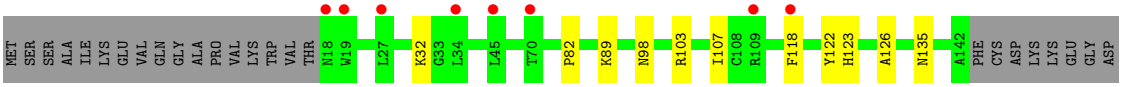
Chain S:

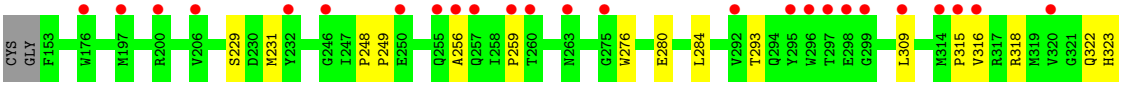


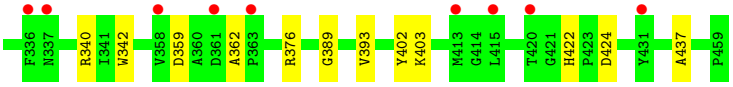


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

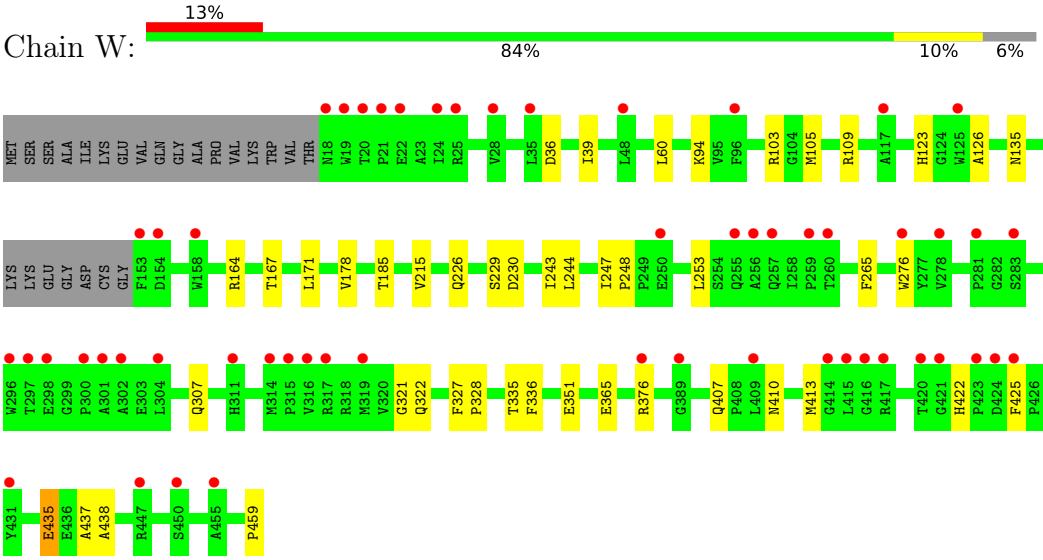
Chain U:



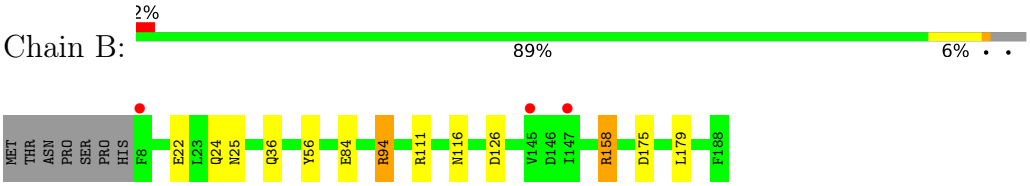




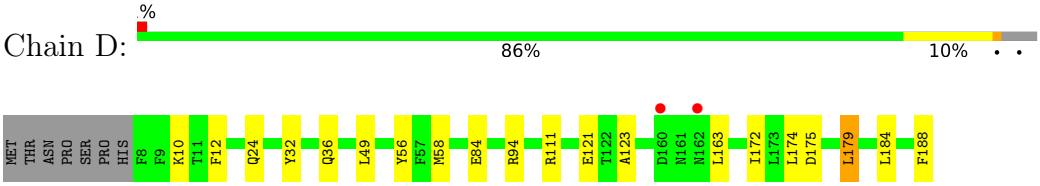
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



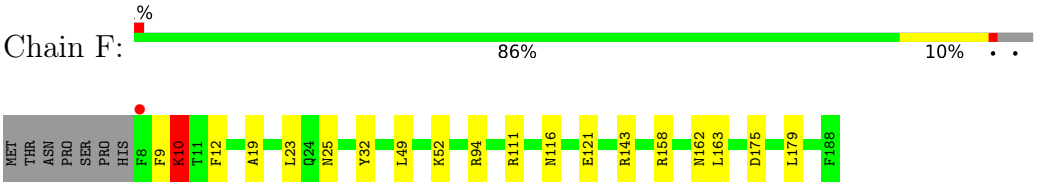
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



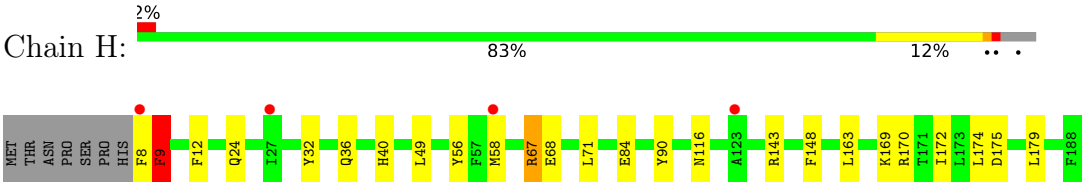
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

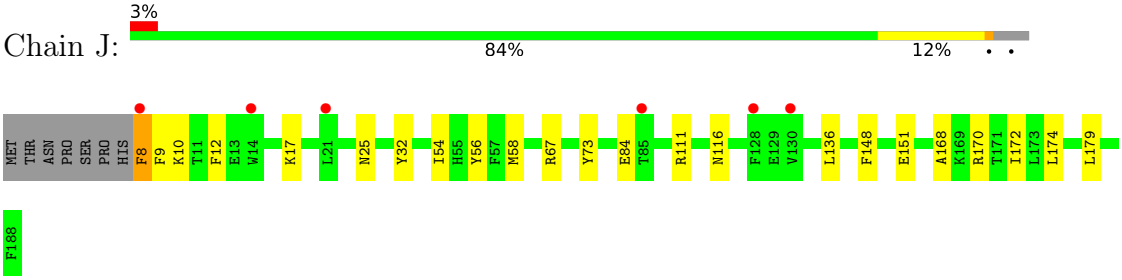


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



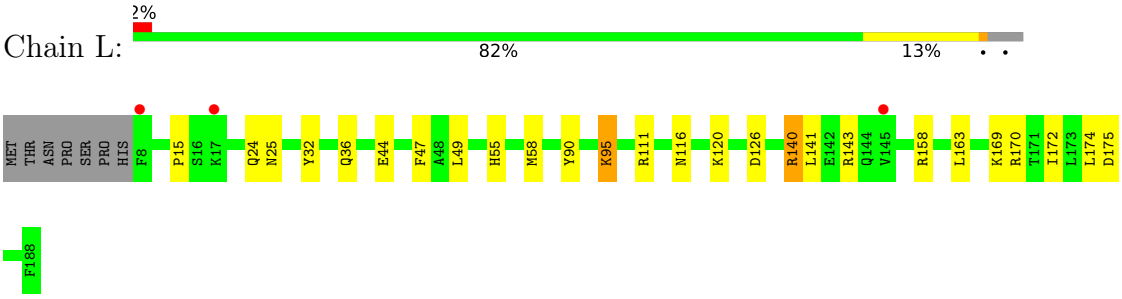
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain J:



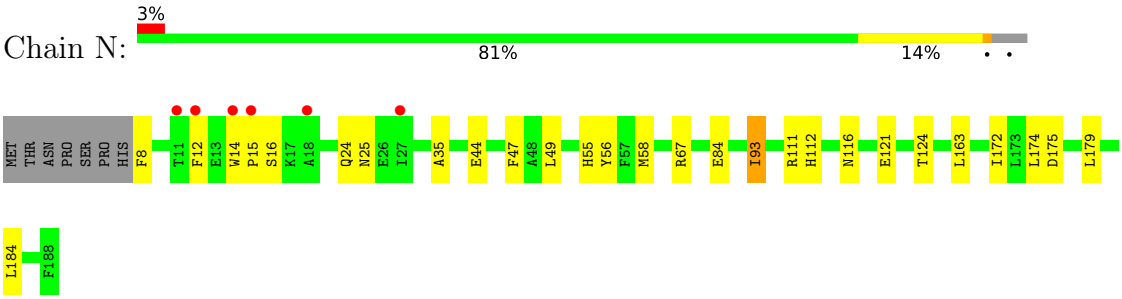
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain L:



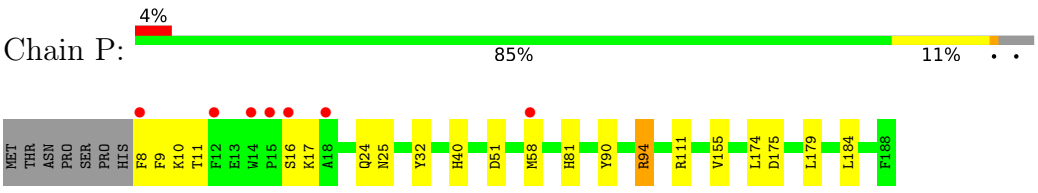
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain N:



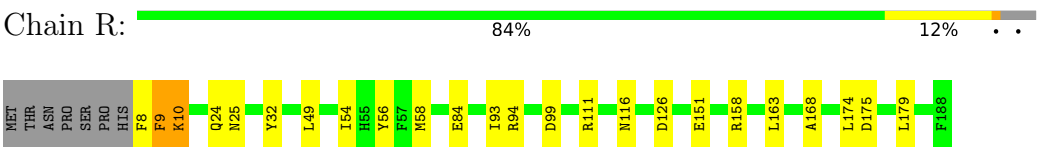
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain P:



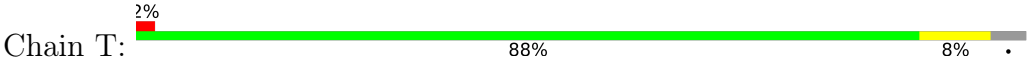
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain R:



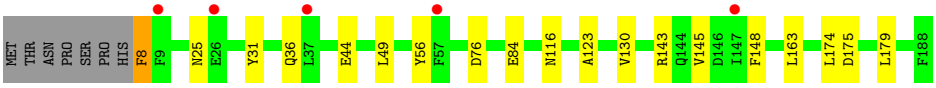
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain T:



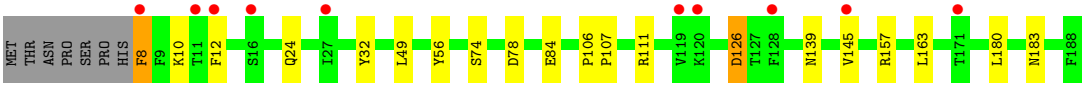
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain V:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain X:



4 Data and refinement statistics (i)

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) 82.5 (49.50-2.42)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	2612 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
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
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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:HG2	2:P:94:ARG:HH11	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:C:123:HIS:HB2	3:C:1460:FES:S2	2.27	0.74
1:Q:259:PRO:HB3	1:Q:280:GLU:HG2	1.68	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:HG2	2:P:94:ARG:NH1	2.07	0.67
2:B:94:ARG:HH11	2:B:94:ARG:HG2	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:CD1	2:V:8:PHE:N	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:H:148:PHE:HB3	2:H:174:LEU:HD11	1.80	0.63
2:V:143:ARG:HD3	1:W:215:VAL:HG21	1.80	0.63
2:X:8:PHE:O	2:X:8:PHE:CD1	2.44	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
1:K:257:GLN:NE2	2:P:8:PHE:HB3	2.18	0.57
2:V:8:PHE:N	2:V:8:PHE:HD1	2.01	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: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
2:R:58:MET:CE	2:R:174:LEU:HD22	2.36	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)
2:N:56:TYR:HB3	2:N:84:GLU:HB2	1.88	0.55
1:U:123:HIS:HB2	3:U:1460:FES:S2	2.47	0.55
1:U:359:ASP:HB2	1:U:362:ALA:HB2	1.89	0.55
1:W:226:GLN:HA	1:W:230:ASP:HB2	1.88	0.55
2:L:55:HIS:HB3	2:L:169:LYS:HG3	1.90	0.54
1:W:229:SER:HB3	1:W:437:ALA:HB3	1.89	0.54
2:B:94:ARG:HG2	2:B:94:ARG:NH1	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:I:359:ASP:HB2	1:I:362:ALA:HB2	1.90	0.53
1:W:226:GLN:HA	1:W:230:ASP:CB	2.39	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
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: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
1:U:309:LEU:HD13	1:U:316:VAL:HG11	1.89	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:E:448:MET:HA	1:E:457:LEU:HD11	1.90	0.52
2:P:25:ASN:HD21	2:R:24:GLN:HG2	1.74	0.52
1:W:422:HIS:HD2	1:W:425:PHE:H	1.56	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: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: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: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
2:H:36:GLN:HE21	2:J:12:PHE:H	1.57	0.51
1:I:309:LEU:HD13	1:I:316:VAL:HG11	1.91	0.51
1:K:262:GLY:HA2	1:K:278:VAL:HG23	1.92	0.51
1:M:259:PRO:HB3	1:M:280:GLU:HG2	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
2:B:25:ASN:HD21	2:D:24:GLN:HG2	1.76	0.50
1:C:340:ARG:HH12	1:C:385:GLU:CD	2.15	0.50
1:G:131:GLY:O	1:G:160:PRO:HD2	2.12	0.50
1:Q:309:LEU:HD22	1:Q:316:VAL:HG11	1.94	0.50
2:J:32:TYR:CD1	2:L:116:ASN:HA	2.46	0.50
1:A:414:GLY:HA2	1:A:417:ARG:HD2	1.94	0.50
1:G:229:SER:HB3	1:G:437:ALA:HB3	1.92	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:J:170:ARG:HD3	2:J:172:ILE:HD11	1.94	0.49
2:N:58:MET:HE1	2:N:174:LEU:HD22	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:B:116:ASN:HA	2:F:32:TYR:CD1	2.48	0.49
2:N:111:ARG:HB2	2:P:175:ASP:OD2	2.12	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
2:N:35:ALA:HB1	2:N:112:HIS:HB2	1.95	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
1:S:332:PHE:HB3	1:S:339:ILE:HG23	1.96	0.48
1:E:422:HIS:HD2	1:E:424:ASP:H	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:309:LEU:HD13	1:K:316:VAL:HG11	1.95	0.48
2:J:54:ILE:HA	2:J:168:ALA:O	2.14	0.48
1:O:37:PRO:HG2	1:O:405:LYS:HA	1.94	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:M:42:ASP:HB3	1:M:45:LEU:HB2	1.96	0.47
1:O:82:PRO:HB2	1:O:98:ASN:HB3	1.96	0.47
2:P:40:HIS:HE1	2:R:151:GLU:OE2	1.97	0.47
1:S:126:ALA:HB3	1:S:135:ASN:HB3	1.96	0.47
1:U:389:GLY:O	1:U:393:VAL:HG23	2.15	0.47
1:U:402:TYR:CE2	1:U:403:LYS:HE3	2.49	0.47
1:C:359:ASP:HB2	1:C:362:ALA:HB2	1.95	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:G:359:ASP:HB2	1:G:362:ALA:HB2	1.97	0.47
1:M:217:PRO:HG2	1:M:393:VAL:HG22	1.96	0.47
2:N:55:HIS:HB3	6:N:2014:HOH:O	2.14	0.47
2:R:56:TYR:HB3	2:R:84:GLU:HB2	1.96	0.47
1:W:126:ALA:HB3	1:W:135:ASN:HB3	1.96	0.47
1:G:107:ILE:HG22	1:G:118:PHE:HB3	1.95	0.47
1:S:36:ASP:O	1:S:39:ILE:HG12	2.14	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
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:175:ASP:OD2	2:X:111:ARG:HB2	2.16	0.45
1:E:82:PRO:HB2	1:E:98:ASN:HB3	1.98	0.45
1:O:136:VAL:O	1:O:139:GLU:HB2	2.17	0.45
2:T:32:TYR:CD1	2:V:116:ASN:HA	2.51	0.45
1:G:24:ILE:CD1	1:G:449:MET:HB3	2.47	0.45
1:U:276:TRP:HB3	1:U:322:GLN:HG3	1.98	0.45
6:W:2026:HOH:O	2:X:183:ASN:HB3	2.16	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: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
2:V:145:VAL:HG21	2:X:180:LEU:HD11	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
1:W:244:LEU:HD13	1:W:253:LEU:HG	1.99	0.45
1:K:187:LEU:HB2	1:K:191:ARG:HD3	1.99	0.44
2:N:116:ASN:HA	2:R:32:TYR:CG	2.52	0.44
2:B:24:GLN:HG2	2:F:25:ASN:HD21	1.82	0.44
1:Q:454:TRP:HA	1:Q:457:LEU:HB2	1.99	0.44
1:W:164:ARG:HD2	1:W:178:VAL:HA	1.99	0.44
2:H:170:ARG:HD3	2:H:172:ILE:HD11	1.99	0.44
2:N:58:MET:HG3	2:N:172:ILE:HB	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:H	2:T:22:GLU:CD	2.21	0.44
1:E:212:GLN:HG3	1:E:354:ALA:HB3	2.00	0.44
1:G:37:PRO:HG2	1:G:405:LYS:HA	1.99	0.44
1:G:422:HIS:HD2	1:G:424:ASP:H	1.65	0.44
1:S:76:THR:HG23	1:S:83:VAL:HG23	1.99	0.44
1:U:422:HIS:CD2	1:U:424:ASP:H	2.36	0.44
1:W:105:MET:CE	1:W:109:ARG:HD2	2.47	0.44
1:G:276:TRP:HB3	1:G:322:GLN:HG3	1.98	0.44
1:U:422:HIS:HD2	1:U:424:ASP:H	1.66	0.44
1:M:343:HIS:HB2	1:M:351:GLU:HB2	2.00	0.43
2:R:9:PHE:H	1:S:258:ILE:HD11	1.83	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
1:E:248:PRO:HA	1:E:249:PRO:HD3	1.93	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
2:T:116:ASN:HA	2:X:32:TYR:CG	2.54	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:K:389:GLY:O	1:K:393:VAL:HG23	2.19	0.43
1:K:422:HIS:HD2	1:K:425:PHE:H	1.64	0.43
2:L:49:LEU:HD21	2:L:163:LEU:HD13	2.01	0.43
1:M:262:GLY:C	1:M:432:VAL:HB	2.38	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
1:A:244:LEU:HD13	1:A:253:LEU:HG	1.99	0.43
2:B:94:ARG:HH11	2:B:94:ARG:CG	2.29	0.43
1:C:63:HIS:CD2	1:C:357:LEU:HD21	2.53	0.43
2:H:58:MET:HE1	2:H:174:LEU:HD22	2.00	0.43
1:I:107:ILE:HG22	1:I:118:PHE:HB3	2.01	0.43
2:L:170:ARG:HD3	2:L:172:ILE:HD11	2.01	0.43
2:P:179:LEU:HD21	2:P:184:LEU:HD11	2.01	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
2:H:116:ASN:HA	2:L:32:TYR:CD1	2.54	0.43
1:A:294:GLN:HE21	1:A:294:GLN:HA	1.84	0.43
1:E:184:GLU:HB2	6:E:2022:HOH:O	2.19	0.43
1:G:414:GLY:HA2	1:G:417:ARG:HD2	2.01	0.43
1:K:215:VAL:HG22	1:K:351:GLU:HG2	1.99	0.43
1:U:229:SER:HB2	1:U:437:ALA:HB3	2.00	0.43
1:W:185:THR:HG22	1:W:459:PRO:HG2	2.00	0.43
1:C:132:LYS:HD2	2:V:123:ALA:HA	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:O:226:GLN:HA	1:O:230:ASP:HB3	2.01	0.43
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
1:U:126:ALA:HB3	1:U:135:ASN:HB3	2.00	0.42
1:W:229:SER:OG	1:W:438:ALA:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:111:ARG:HB2	2:R:175:ASP:OD2	2.20	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: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:Q:247:ILE:HD12	1:Q:251:MET:HB3	2.02	0.42
1:C:126:ALA:HB3	1:C:135:ASN:HB3	2.01	0.42
1:G:212:GLN:HG3	1:G:214:TRP:HZ3	1.85	0.42
1:K:257:GLN:HE22	2:P:8:PHE:HB3	1.81	0.42
1:K:368:GLU:O	1:K:372:ARG:HG3	2.20	0.42
1:W:247:ILE:HG13	1:W:248:PRO:HD2	2.00	0.42
1:A:42:ASP:HB3	1:A:45:LEU:HB2	2.01	0.42
2:B:36:GLN:NE2	2:D:12:PHE:H	2.18	0.42
1:G:191:ARG:N	1:G:192:PRO:HD2	2.35	0.42
2:J:58:MET:HE1	2:J:174:LEU:HD22	2.01	0.42
1:Q:333:LEU:HD13	1:Q:336:PHE:HD1	1.84	0.42
2:V:143:ARG:NH2	6:V:2011:HOH:O	2.53	0.42
1:A:257:GLN:HB2	6:A:2030:HOH:O	2.19	0.42
1:Q:295:TYR:CD1	1:Q:366:ILE:HD13	2.54	0.42
2:L:15:PRO:HG3	2:L:120:LYS:HG3	2.01	0.42
1:O:126:ALA:HB3	1:O:135:ASN:HB3	2.02	0.42
2:P:58:MET:HE1	2:P:174:LEU:HD22	2.02	0.42
1:S:100:CYS:SG	1:S:127:TYR:OH	2.78	0.42
1:U:248:PRO:HA	1:U:249:PRO:HD3	1.90	0.42
1:I:296:TRP:CE2	1:I:335:THR:HG23	2.55	0.42
1:I:458:LYS:HB2	1:I:459:PRO:HD2	2.00	0.42
1:M:276:TRP:HB3	1:M:322:GLN:HG3	2.02	0.42
1:G:422:HIS:CD2	1:G:424:ASP:H	2.37	0.41
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:A:422:HIS:HD2	1:A:425:PHE:H	1.67	0.41
1:C:340:ARG:HD3	1:C:342:TRP:CH2	2.55	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)
1:I:36:ASP:O	1:I:39:ILE:HG12	2.20	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
2:P:58:MET:HE2	2:P:81:HIS:CB	2.50	0.41
2:B:56:TYR:HB3	2:B:84:GLU:HB2	2.02	0.41
2:R:54:ILE:HA	2:R:168:ALA:O	2.20	0.41
1:S:212:GLN:HE21	1:S:212:GLN:HB2	1.67	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: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
1:U:231:MET:HB2	1:U:323:HIS:NE2	2.35	0.41
1:A:197:MET:HB2	1:A:334:PRO: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:G:226:GLN:HA	1:G:230:ASP:HB3	2.03	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:V:31:TYR:HE2	2:V:130:VAL:HG11	1.86	0.41
1:W:60:LEU:HD11	1:W:171:LEU:HD22	2.02	0.41
1:W:321:GLY:HA2	1:W:336:PHE:CZ	2.56	0.41
1:K:248:PRO:HA	1:K:249:PRO:HD3	1.93	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:C:422:HIS:CD2	1:C:424:ASP:H	2.38	0.40
2:H:24:GLN:HG2	2:L:25:ASN:ND2	2.35	0.40
1:O:422:HIS:CD2	1:O:424:ASP:H	2.40	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:S:275:GLY:O	1:S:322:GLN:HA	2.22	0.40
1:A:68:PRO:HD2	1:A:72:ASP:OD2	2.21	0.40
2:D:179:LEU:HD21	2:D:184:LEU:HD11	2.03	0.40
2:J:136:LEU:HB3	2:J:148:PHE:HB2	2.03	0.40
1:K:258:ILE:HA	1:K:259:PRO:HD2	1.93	0.40
2:N:179:LEU:HD21	2:N:184:LEU:HD11	2.03	0.40
1:Q:389:GLY:O	1:Q:393:VAL:HG23	2.22	0.40
1:G:326:ILE:HB	1:G:330:CYS:HB3	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:GLN:NE2	2:F:12:PHE:H	2.19	0.40
2:F:9:PHE:O	2:F:10:LYS:HG3	2.22	0.40
1:G:239:HIS:CE1	1:G:384:PHE:O	2.74	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:U:107:ILE:CG2	1:U:118:PHE:HB3	2.52	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%)	47	61
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%)	47	61
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%)	47	61
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%)	25	35
2	F	179/188 (95%)	171 (96%)	7 (4%)	1 (1%)	25	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	25 35
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%)	14 19
2	P	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	25 35
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%)	25 35
All	All	7284/7764 (94%)	6982 (96%)	292 (4%)	10 (0%)	51 67

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 (i)

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%)	42 61
1	C	350/373 (94%)	345 (99%)	5 (1%)	67 81
1	E	350/373 (94%)	344 (98%)	6 (2%)	60 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	349/373 (94%)	336 (96%)	13 (4%)	34 51
1	I	349/373 (94%)	345 (99%)	4 (1%)	73 86
1	K	349/373 (94%)	343 (98%)	6 (2%)	60 77
1	M	350/373 (94%)	346 (99%)	4 (1%)	73 86
1	O	350/373 (94%)	344 (98%)	6 (2%)	60 77
1	Q	350/373 (94%)	341 (97%)	9 (3%)	46 64
1	S	349/373 (94%)	345 (99%)	4 (1%)	73 86
1	U	349/373 (94%)	344 (99%)	5 (1%)	67 81
1	W	349/373 (94%)	339 (97%)	10 (3%)	42 61
2	B	158/167 (95%)	154 (98%)	4 (2%)	47 66
2	D	158/167 (95%)	156 (99%)	2 (1%)	69 83
2	F	158/167 (95%)	150 (95%)	8 (5%)	24 37
2	H	160/167 (96%)	155 (97%)	5 (3%)	40 58
2	J	160/167 (96%)	156 (98%)	4 (2%)	47 66
2	L	160/167 (96%)	158 (99%)	2 (1%)	69 83
2	N	160/167 (96%)	154 (96%)	6 (4%)	33 50
2	P	160/167 (96%)	155 (97%)	5 (3%)	40 58
2	R	160/167 (96%)	154 (96%)	6 (4%)	33 50
2	T	160/167 (96%)	158 (99%)	2 (1%)	69 83
2	V	160/167 (96%)	156 (98%)	4 (2%)	47 66
2	X	160/167 (96%)	158 (99%)	2 (1%)	69 83
All	All	6108/6480 (94%)	5976 (98%)	132 (2%)	52 69

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	BNL	C	1462	-	12,13,13	1.01	0	12,16,16	0.39	0
5	BNL	I	1462	-	12,13,13	1.02	0	12,16,16	0.65	0
5	BNL	M	1462	-	12,13,13	1.00	0	12,16,16	0.47	0
3	FES	A	1460	1	0,4,4	-	-	-		
5	BNL	Q	1462	-	12,13,13	1.05	0	12,16,16	0.36	0
3	FES	K	1460	1	0,4,4	-	-	-		
3	FES	E	1460	1	0,4,4	-	-	-		
3	FES	W	1460	1	0,4,4	-	-	-		
5	BNL	K	1462	-	12,13,13	1.01	0	12,16,16	0.36	0
5	BNL	E	1462	-	12,13,13	1.01	0	12,16,16	0.49	0
5	BNL	G	1462	-	12,13,13	1.01	0	12,16,16	0.48	0
3	FES	Q	1460	1	0,4,4	-	-	-		
5	BNL	S	1462	-	12,13,13	1.00	0	12,16,16	0.57	0
3	FES	O	1460	1	0,4,4	-	-	-		
3	FES	C	1460	1	0,4,4	-	-	-		
5	BNL	U	1462	-	12,13,13	1.00	0	12,16,16	0.52	0
3	FES	S	1460	1	0,4,4	-	-	-		
3	FES	I	1460	1	0,4,4	-	-	-		
3	FES	U	1460	1	0,4,4	-	-	-		
5	BNL	W	1462	-	12,13,13	1.02	0	12,16,16	0.55	0
3	FES	M	1460	1	0,4,4	-	-	-		
5	BNL	A	1462	-	12,13,13	1.01	0	12,16,16	0.57	0
5	BNL	O	1462	-	12,13,13	1.02	0	12,16,16	0.44	0
3	FES	G	1460	1	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BNL	C	1462	-	-	0/0/4/4	0/2/2/2
5	BNL	I	1462	-	-	0/0/4/4	0/2/2/2
5	BNL	M	1462	-	-	0/0/4/4	0/2/2/2
3	FES	A	1460	1	-	-	0/1/1/1
5	BNL	Q	1462	-	-	0/0/4/4	0/2/2/2
3	FES	K	1460	1	-	-	0/1/1/1

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

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
5	M	1462	BNL	1	0
3	A	1460	FES	1	0
3	K	1460	FES	1	0
3	E	1460	FES	1	0
3	W	1460	FES	1	0
3	Q	1460	FES	1	0
3	O	1460	FES	1	0
3	C	1460	FES	1	0
3	S	1460	FES	1	0
3	I	1460	FES	1	0
3	U	1460	FES	1	0
3	M	1460	FES	1	0
3	G	1460	FES	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.06	10 (2%) 60 57	24, 41, 55, 61	17 (3%)
1	C	432/459 (94%)	-0.00	12 (2%) 53 50	30, 44, 54, 58	17 (3%)
1	E	432/459 (94%)	-0.10	5 (1%) 79 76	23, 35, 47, 55	17 (3%)
1	G	432/459 (94%)	0.01	9 (2%) 63 60	35, 47, 60, 66	17 (3%)
1	I	432/459 (94%)	0.32	34 (7%) 12 11	39, 52, 64, 69	17 (3%)
1	K	432/459 (94%)	0.54	43 (9%) 7 6	42, 55, 65, 68	17 (3%)
1	M	432/459 (94%)	-0.06	6 (1%) 75 73	26, 38, 58, 62	17 (3%)
1	O	432/459 (94%)	-0.20	6 (1%) 75 73	20, 34, 49, 57	17 (3%)
1	Q	432/459 (94%)	-0.31	2 (0%) 91 89	22, 31, 44, 61	17 (3%)
1	S	432/459 (94%)	0.23	17 (3%) 39 37	36, 47, 58, 67	17 (3%)
1	U	432/459 (94%)	0.60	42 (9%) 7 6	39, 57, 72, 74	17 (3%)
1	W	432/459 (94%)	0.80	59 (13%) 3 2	46, 59, 70, 74	17 (3%)
2	B	181/188 (96%)	-0.01	3 (1%) 70 67	30, 38, 47, 58	4 (2%)
2	D	181/188 (96%)	-0.07	2 (1%) 80 78	28, 39, 51, 56	4 (2%)
2	F	181/188 (96%)	-0.27	1 (0%) 89 88	28, 33, 47, 60	4 (2%)
2	H	181/188 (96%)	0.17	4 (2%) 62 59	36, 45, 60, 66	4 (2%)
2	J	181/188 (96%)	0.22	6 (3%) 46 44	40, 50, 57, 63	4 (2%)
2	L	181/188 (96%)	0.33	3 (1%) 70 67	39, 48, 63, 70	4 (2%)
2	N	181/188 (96%)	-0.03	6 (3%) 46 44	27, 38, 61, 75	4 (2%)
2	P	181/188 (96%)	-0.05	7 (3%) 39 37	24, 36, 64, 79	4 (2%)
2	R	181/188 (96%)	-0.23	0 100 100	24, 32, 52, 62	4 (2%)
2	T	181/188 (96%)	0.14	4 (2%) 62 59	33, 39, 55, 65	4 (2%)
2	V	181/188 (96%)	0.18	5 (2%) 53 50	45, 53, 59, 64	4 (2%)
2	X	181/188 (96%)	0.50	10 (5%) 25 23	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%)	0.12	296 (4%)	38	36	20, 44, 63, 79	252 (3%)

All (296) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	ALA	9.8
1	K	256	ALA	9.2
1	A	257	GLN	7.3
1	S	256	ALA	7.0
1	K	255	GLN	6.8
1	U	256	ALA	6.6
1	U	314	MET	5.8
1	K	260	THR	5.6
1	A	255	GLN	5.5
1	W	425	PHE	5.5
1	W	257	GLN	5.5
1	W	301	ALA	5.2
1	U	19	TRP	5.2
1	I	320	VAL	5.2
1	W	292	VAL	5.1
1	S	255	GLN	5.0
2	N	14	TRP	4.9
1	I	256	ALA	4.7
1	S	257	GLN	4.7
1	W	455	ALA	4.7
1	W	316	VAL	4.6
1	W	255	GLN	4.5
1	G	256	ALA	4.5
1	U	257	GLN	4.4
1	K	24	ILE	4.4
2	X	11	THR	4.4
1	K	203	ALA	4.3
1	K	312	THR	4.3
1	K	259	PRO	4.3
1	W	416	GLY	4.3
2	X	8	PHE	4.3
1	I	415	LEU	4.2
1	W	389	GLY	4.2
1	K	314	MET	4.2
1	W	315	PRO	4.2
1	A	260	THR	4.2
1	W	21	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	W	283	SER	4.1
1	E	257	GLN	4.0
1	I	246	GLY	4.0
1	U	415	LEU	3.9
2	H	123	ALA	3.9
1	E	259	PRO	3.9
1	K	316	VAL	3.8
1	W	302	ALA	3.8
1	M	261	LYS	3.8
1	U	260	THR	3.8
1	S	259	PRO	3.8
1	E	256	ALA	3.7
1	W	256	ALA	3.7
1	C	301	ALA	3.7
1	W	415	LEU	3.7
1	W	22	GLU	3.7
1	A	259	PRO	3.7
2	H	27	ILE	3.7
1	W	298	GLU	3.7
1	K	417	ARG	3.6
1	G	142	ALA	3.6
1	I	297	THR	3.6
1	U	315	PRO	3.6
2	D	160	ASP	3.5
1	C	257	GLN	3.5
1	K	311	HIS	3.5
1	K	457	LEU	3.5
1	S	260	THR	3.5
1	S	138	PHE	3.5
2	P	14	TRP	3.5
1	I	153	PHE	3.4
1	C	417	ARG	3.4
1	K	421	GLY	3.4
1	W	314	MET	3.4
1	W	317	ARG	3.4
1	S	153	PHE	3.4
1	K	427	GLY	3.4
1	U	255	GLN	3.3
1	W	24	ILE	3.3
1	K	95	VAL	3.3
1	U	206	VAL	3.3
1	U	297	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	366	ILE	3.3
1	U	263	ASN	3.3
1	C	314	MET	3.3
1	W	281	PRO	3.2
1	K	23	ALA	3.2
1	U	292	VAL	3.2
1	W	28	VAL	3.2
1	W	158	TRP	3.2
2	N	12	PHE	3.2
1	C	260	THR	3.2
1	I	260	THR	3.2
1	I	418	SER	3.2
2	P	16	SER	3.2
1	U	34	LEU	3.2
1	U	275	GLY	3.1
1	I	419	GLN	3.1
1	G	260	THR	3.1
1	K	261	LYS	3.1
1	I	257	GLN	3.1
1	W	414	GLY	3.1
1	K	201	THR	3.1
1	U	299	GLY	3.1
1	W	276	TRP	3.1
1	W	153	PHE	3.1
2	H	8	PHE	3.1
2	X	12	PHE	3.1
2	V	37	LEU	3.1
1	I	431	TYR	3.0
1	A	305	ALA	3.0
2	T	8	PHE	3.0
1	E	260	THR	3.0
1	K	309	LEU	3.0
1	U	70	THR	3.0
1	K	257	GLN	3.0
1	C	256	ALA	3.0
1	W	420	THR	3.0
1	U	118	PHE	3.0
1	K	415	LEU	3.0
1	U	295	TYR	3.0
1	K	313	GLY	3.0
2	X	16	SER	2.9
1	W	19	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	U	316	VAL	2.9
1	G	24	ILE	2.9
2	P	8	PHE	2.9
1	U	363	PRO	2.9
1	S	105	MET	2.9
2	P	18	ALA	2.9
1	I	295	TYR	2.9
1	I	18	ASN	2.8
1	I	319	MET	2.8
1	K	372	ARG	2.8
1	W	25	ARG	2.8
2	L	17	LYS	2.8
1	I	276	TRP	2.8
1	K	186	TYR	2.8
1	W	142	ALA	2.8
1	W	450	SER	2.8
1	I	19	TRP	2.8
1	I	298	GLU	2.8
1	U	309	LEU	2.8
2	N	15	PRO	2.8
1	W	125	TRP	2.8
2	L	145	VAL	2.7
1	K	425	PHE	2.7
1	O	311	HIS	2.7
1	K	305	ALA	2.7
1	O	256	ALA	2.7
2	J	8	PHE	2.7
1	Q	257	GLN	2.7
1	W	417	ARG	2.7
1	U	232	TYR	2.7
1	U	176	TRP	2.7
1	U	296	TRP	2.7
1	U	361	ASP	2.6
1	U	413	MET	2.6
1	C	24	ILE	2.6
1	K	131	GLY	2.6
2	V	9	PHE	2.6
1	K	434	ALA	2.6
1	C	309	LEU	2.6
1	K	96	PHE	2.6
1	W	290	PRO	2.6
1	S	416	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	T	19	ALA	2.5
1	W	300	PRO	2.5
1	U	200	ARG	2.5
1	C	414	GLY	2.5
1	S	312	THR	2.5
2	P	15	PRO	2.5
1	I	34	LEU	2.5
2	B	8	PHE	2.5
1	C	105	MET	2.5
1	W	297	THR	2.5
1	K	269	TRP	2.5
1	U	259	PRO	2.5
2	J	130	VAL	2.5
1	K	416	GLY	2.5
1	U	298	GLU	2.5
1	I	411	ALA	2.5
1	W	259	PRO	2.5
1	U	320	VAL	2.5
2	B	147	ILE	2.5
2	V	147	ILE	2.5
1	G	292	VAL	2.4
1	A	309	LEU	2.4
1	I	313	GLY	2.4
1	W	35	LEU	2.4
1	I	277	TYR	2.4
1	U	109	ARG	2.4
1	U	246	GLY	2.4
2	P	58	MET	2.4
1	W	250	GLU	2.4
1	W	311	HIS	2.4
2	F	8	PHE	2.4
1	S	86	VAL	2.4
1	A	311	HIS	2.4
2	P	12	PHE	2.4
1	M	297	THR	2.4
1	I	263	ASN	2.3
1	I	251	MET	2.3
1	K	423	PRO	2.3
2	N	18	ALA	2.3
1	K	414	GLY	2.3
1	W	18	ASN	2.3
1	W	429	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	U	250	GLU	2.3
1	W	296	TRP	2.3
1	U	337	ASN	2.3
2	X	171	THR	2.3
1	W	304	LEU	2.3
1	I	423	PRO	2.3
1	U	18	ASN	2.3
2	D	162	ASN	2.3
2	X	128	PHE	2.3
1	K	159	GLY	2.3
1	I	275	GLY	2.3
1	W	48	LEU	2.3
1	W	319	MET	2.3
1	G	19	TRP	2.3
2	N	27	ILE	2.3
1	W	117	ALA	2.3
1	K	420	THR	2.3
1	I	300	PRO	2.2
2	X	27	ILE	2.2
1	S	103	ARG	2.2
1	U	27	LEU	2.2
1	M	257	GLN	2.2
2	J	128	PHE	2.2
1	K	158	TRP	2.2
1	G	425	PHE	2.2
1	I	365	GLU	2.2
1	M	259	PRO	2.2
1	O	257	GLN	2.2
1	W	424	ASP	2.2
1	A	261	LYS	2.2
1	K	142	ALA	2.2
1	I	294	GLN	2.2
1	O	153	PHE	2.2
1	S	415	LEU	2.2
1	W	421	GLY	2.2
1	I	158	TRP	2.2
1	W	376	ARG	2.2
1	M	307	GLN	2.2
1	K	167	THR	2.2
1	W	20	THR	2.2
1	W	423	PRO	2.2
1	W	260	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	8	PHE	2.2
1	O	251	MET	2.1
2	X	145	VAL	2.1
1	A	421	GLY	2.1
2	J	21	LEU	2.1
1	C	316	VAL	2.1
1	I	432	VAL	2.1
1	U	420	THR	2.1
2	J	85	THR	2.1
1	U	197	MET	2.1
1	K	300	PRO	2.1
1	W	409	LEU	2.1
1	S	261	LYS	2.1
1	O	105	MET	2.1
1	I	364	ALA	2.1
1	K	419	GLN	2.1
1	S	206	VAL	2.1
2	N	11	THR	2.1
1	G	304	LEU	2.1
1	K	454	TRP	2.1
1	U	336	PHE	2.1
2	T	9	PHE	2.1
1	S	28	VAL	2.1
1	W	278	VAL	2.1
2	T	145	VAL	2.1
1	W	431	TYR	2.1
1	U	45	LEU	2.1
1	I	414	GLY	2.1
1	K	307	GLN	2.1
1	M	251	MET	2.1
1	S	142	ALA	2.1
2	X	119	VAL	2.1
1	C	416	GLY	2.1
1	E	255	GLN	2.1
1	Q	260	THR	2.0
1	I	33	GLY	2.0
1	W	96	PHE	2.0
2	V	57	PHE	2.0
2	X	120	LYS	2.0
2	J	14	TRP	2.0
2	H	58	MET	2.0
2	V	26	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	U	431	TYR	2.0
1	W	447	ARG	2.0
1	W	154	ASP	2.0
1	U	358	VAL	2.0
2	B	145	VAL	2.0
1	K	447	ARG	2.0
1	G	255	GLN	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
5	BNL	W	1462	12/12	0.77	0.34	87,87,88,88	0
5	BNL	K	1462	12/12	0.79	0.33	86,86,87,87	0
5	BNL	S	1462	12/12	0.83	0.33	82,82,82,82	0
5	BNL	A	1462	12/12	0.83	0.26	76,76,76,76	0
5	BNL	U	1462	12/12	0.84	0.30	86,86,86,86	0
5	BNL	I	1462	12/12	0.86	0.22	63,63,64,64	0
5	BNL	G	1462	12/12	0.90	0.30	63,64,64,64	0
3	FES	E	1460	4/4	0.90	0.11	44,46,47,50	0
3	FES	W	1460	4/4	0.91	0.09	74,75,76,77	0
3	FES	S	1460	4/4	0.91	0.10	86,86,86,87	0
3	FES	I	1460	4/4	0.92	0.11	45,46,48,50	0
5	BNL	E	1462	12/12	0.92	0.17	49,49,49,49	0
5	BNL	O	1462	12/12	0.93	0.24	44,44,45,45	0
3	FES	A	1460	4/4	0.93	0.10	43,44,46,48	0
5	BNL	C	1462	12/12	0.93	0.18	55,56,56,56	0
5	BNL	M	1462	12/12	0.93	0.18	55,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BNL	Q	1462	12/12	0.94	0.18	40,40,41,41	0
3	FES	Q	1460	4/4	0.94	0.09	39,39,41,44	0
3	FES	O	1460	4/4	0.95	0.11	44,45,46,48	0
3	FES	M	1460	4/4	0.95	0.09	38,38,39,42	0
4	FE2	W	1461	1/1	0.95	0.09	68,68,68,68	0
3	FES	G	1460	4/4	0.96	0.10	54,54,54,56	0
3	FES	C	1460	4/4	0.96	0.10	43,44,45,46	0
3	FES	K	1460	4/4	0.96	0.07	74,75,75,76	0
4	FE2	K	1461	1/1	0.97	0.14	59,59,59,59	0
3	FES	U	1460	4/4	0.97	0.08	48,48,49,49	0
4	FE2	E	1461	1/1	0.98	0.15	41,41,41,41	0
4	FE2	S	1461	1/1	0.98	0.14	51,51,51,51	0
4	FE2	U	1461	1/1	0.98	0.08	57,57,57,57	0
4	FE2	I	1461	1/1	0.98	0.14	58,58,58,58	0
4	FE2	G	1461	1/1	0.99	0.07	52,52,52,52	0
4	FE2	C	1461	1/1	0.99	0.11	44,44,44,44	0
4	FE2	A	1461	1/1	0.99	0.16	53,53,53,53	0
4	FE2	M	1461	1/1	0.99	0.13	43,43,43,43	0
4	FE2	Q	1461	1/1	0.99	0.12	37,37,37,37	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.