Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2026 – 05:53 am BST

PDB ID	:	2XRX / pdb_00002xrx
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 ⓘ 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 ⓘ) were used in the production of this report:

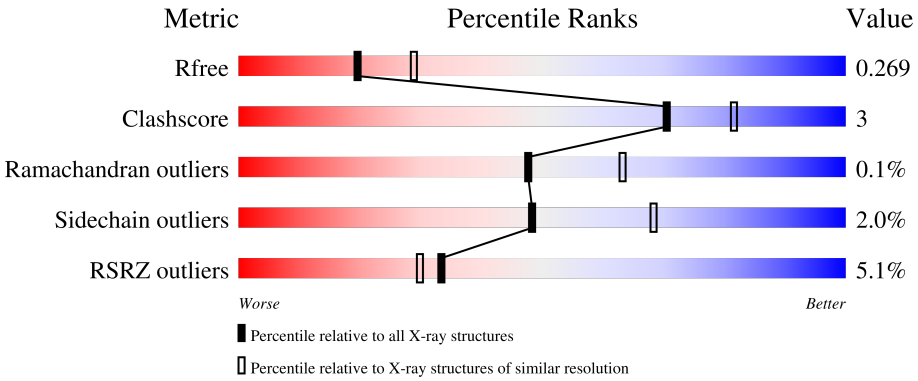
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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.



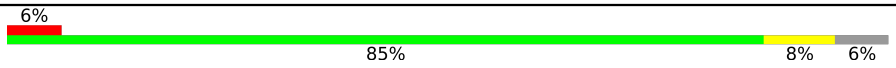
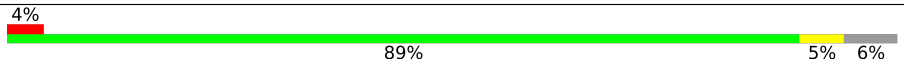
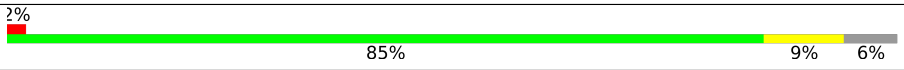
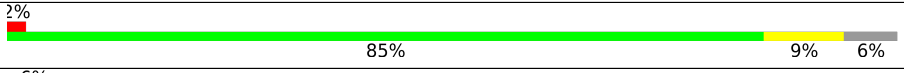
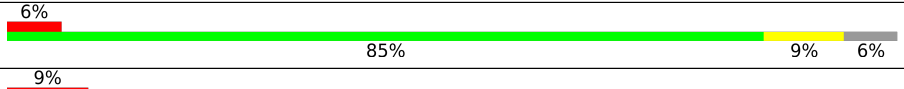
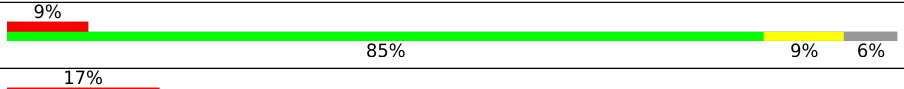
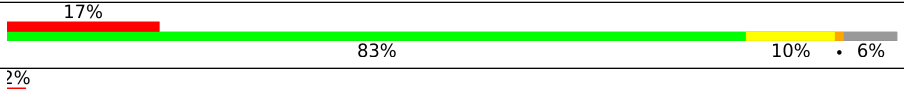
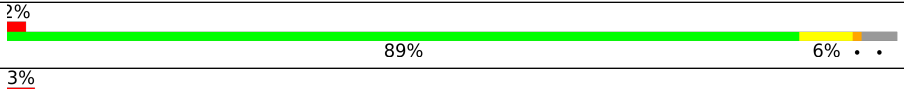
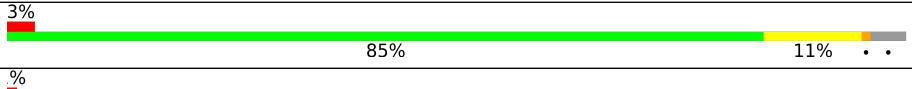
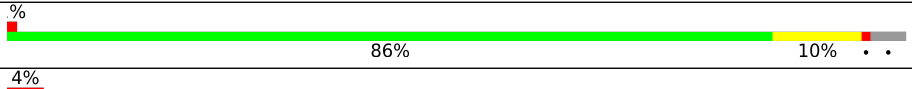
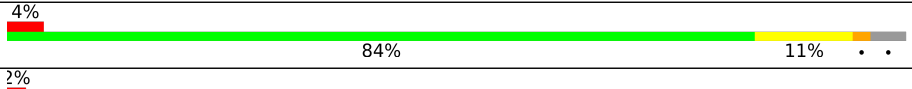
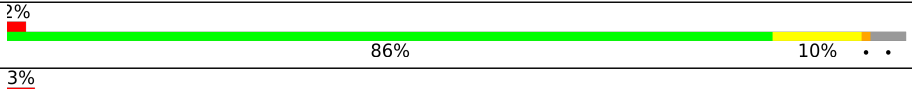
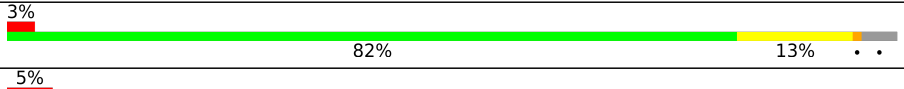
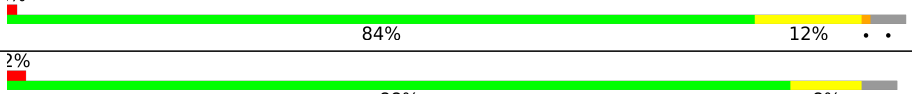
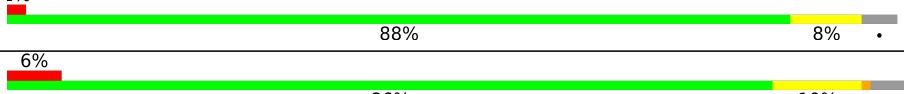
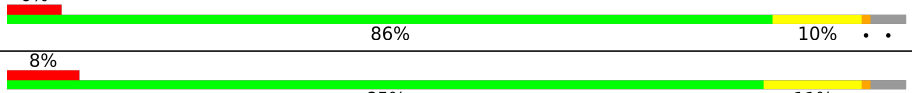
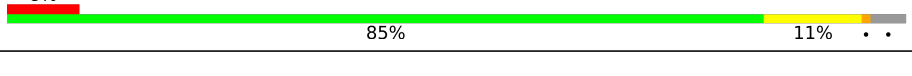
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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% 10% • 6%
1	C	459	4% 85% 9% 6%
1	E	459	2% 86% 7% 6%
1	G	459	3% 82% 12% 6%
1	I	459	7% 86% 7% 6%

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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	

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.

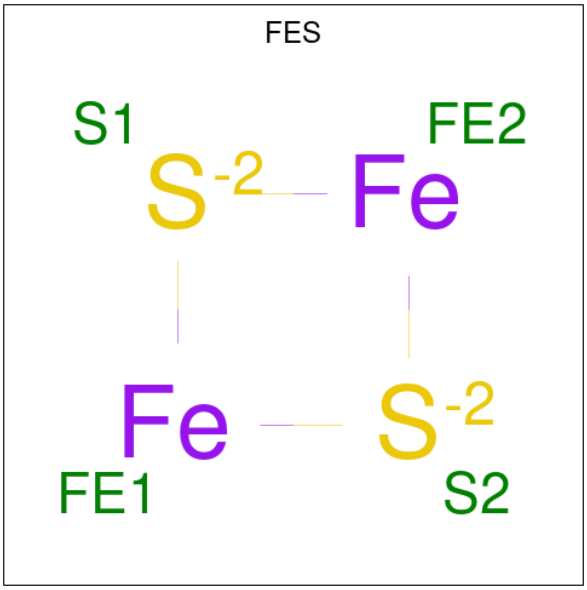
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			
2	D	181	Total	C	N	O	S	0	0	0
			1497	952	263	278	4			

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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 (CCD ID: 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 (CCD ID: FE2) (formula: Fe).

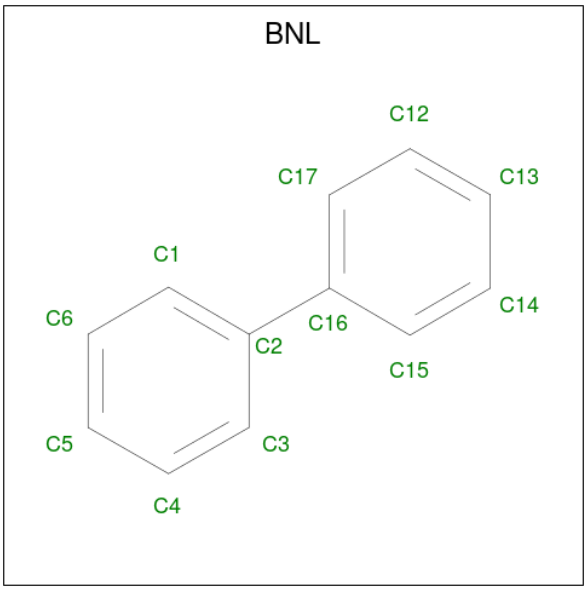
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe 1 1	0	0
4	C	1	Total Fe 1 1	0	0
4	E	1	Total Fe 1 1	0	0
4	G	1	Total Fe 1 1	0	0
4	I	1	Total Fe 1 1	0	0
4	K	1	Total Fe 1 1	0	0
4	M	1	Total Fe 1 1	0	0
4	O	1	Total Fe 1 1	0	0

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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 (CCD ID: 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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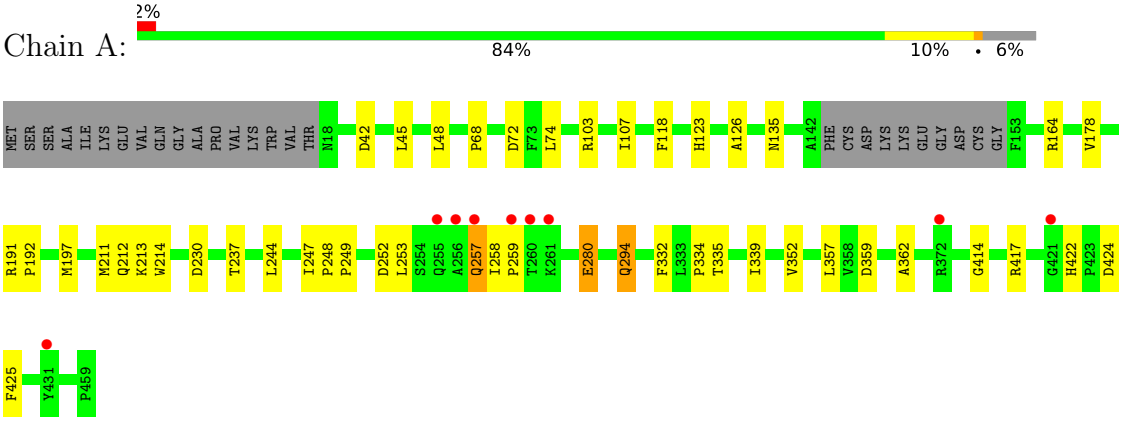
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6	P	26	Total O 26 26	0	0
6	Q	83	Total O 83 83	0	0
6	R	30	Total O 30 30	0	0
6	S	33	Total O 33 33	0	0
6	T	18	Total O 18 18	0	0
6	U	25	Total O 25 25	0	0
6	V	11	Total O 11 11	0	0
6	W	30	Total O 30 30	0	0
6	X	14	Total O 14 14	0	0

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.

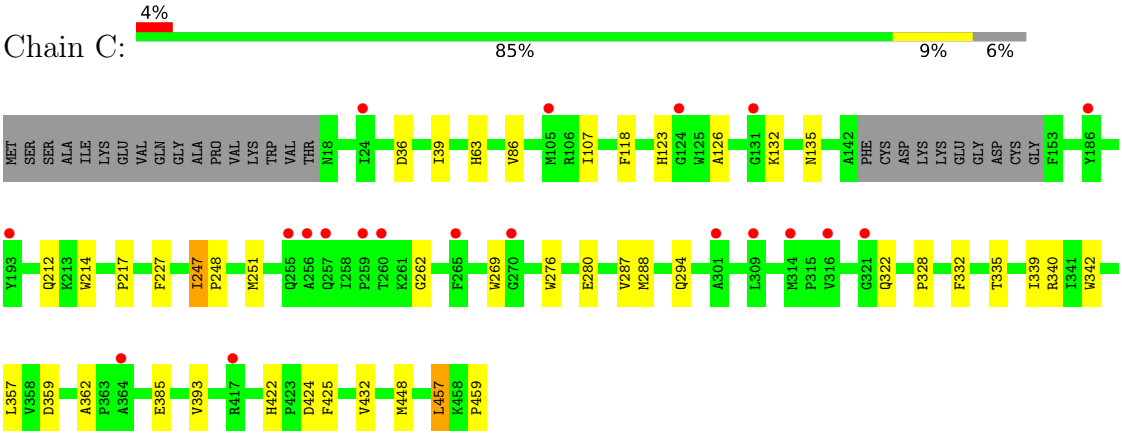
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain A:



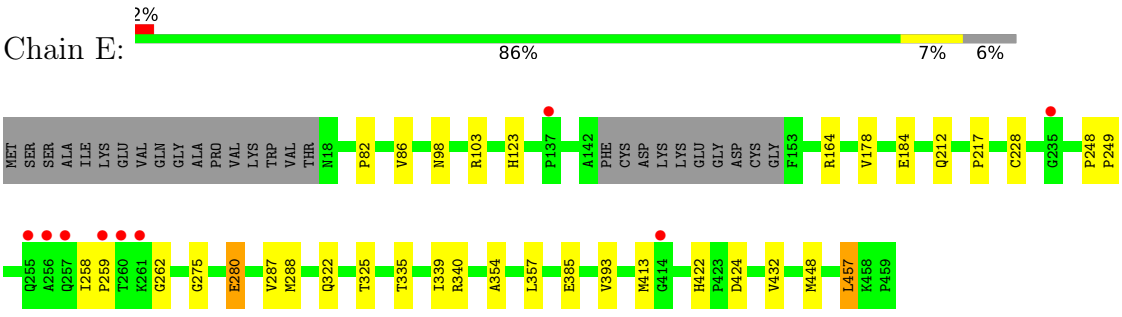
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Chain C:



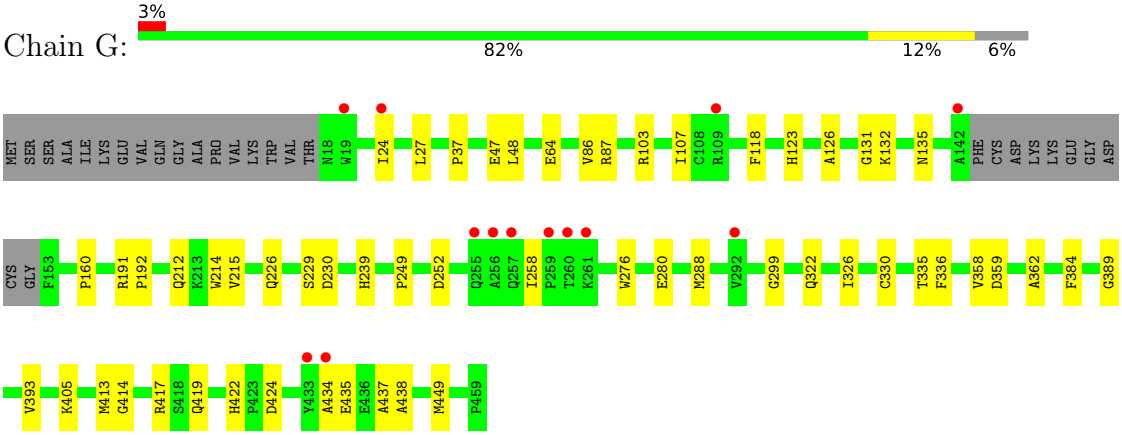
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain E:



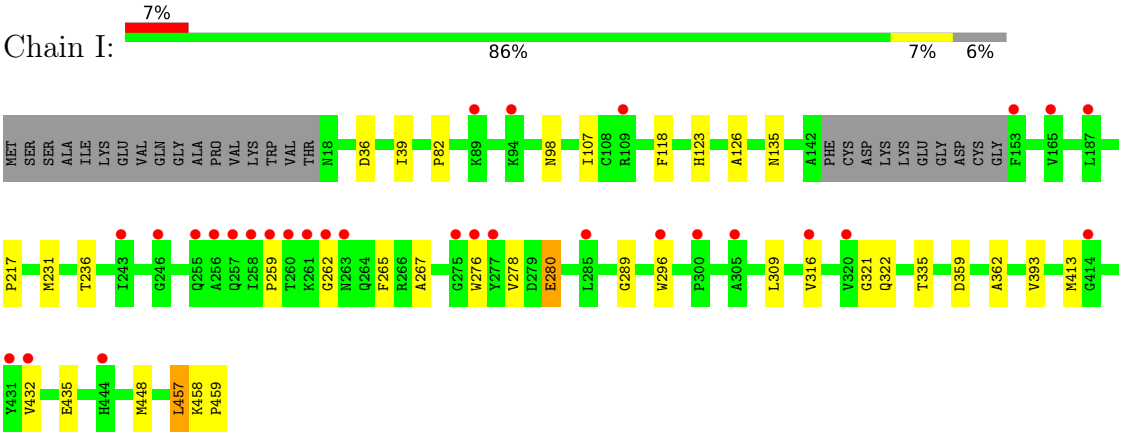
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain G:



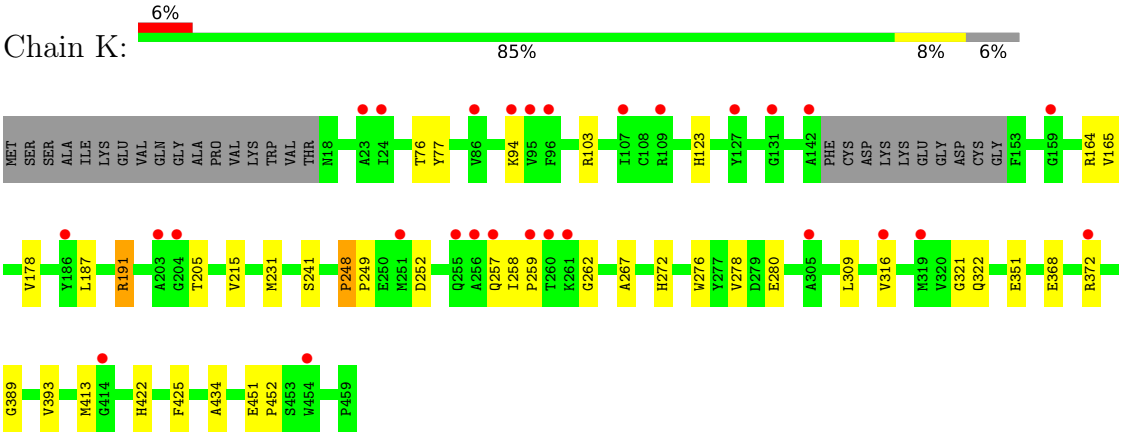
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain I:



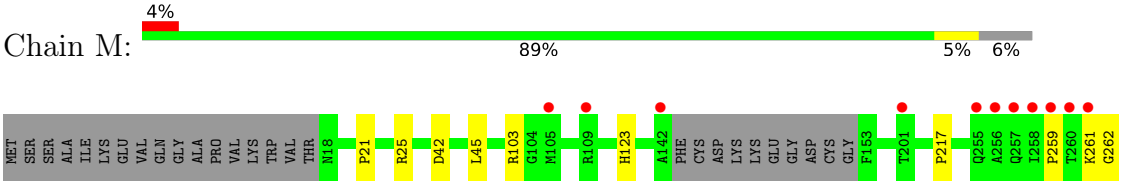
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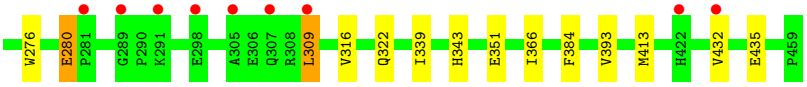
Chain K:



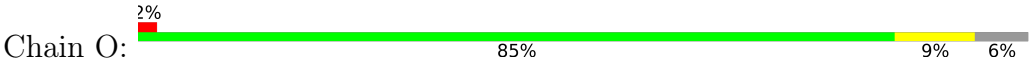
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

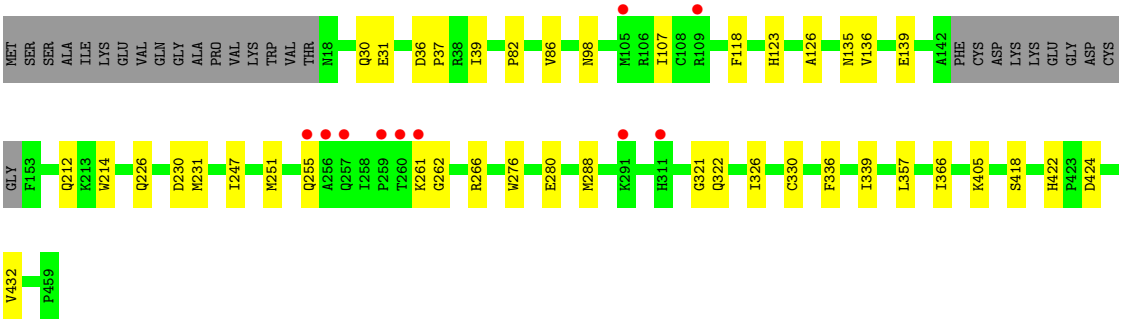
Chain M:



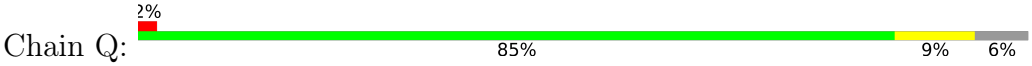


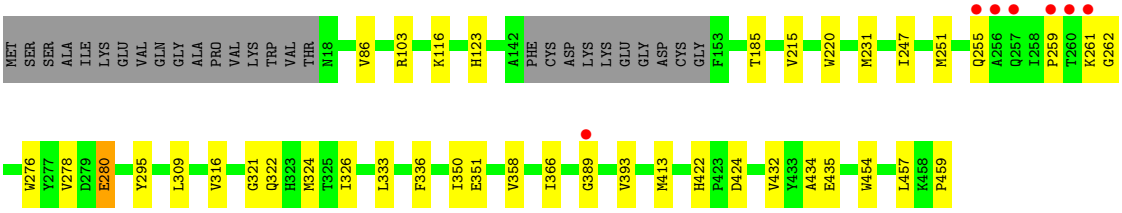
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



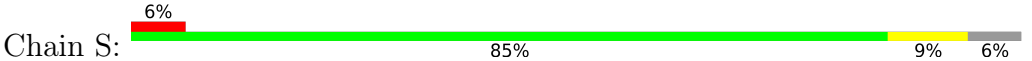


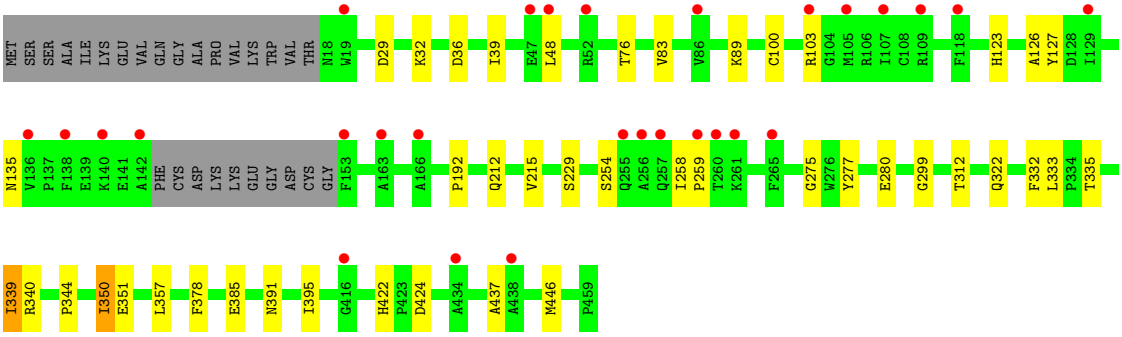
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



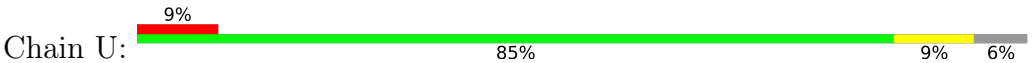


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

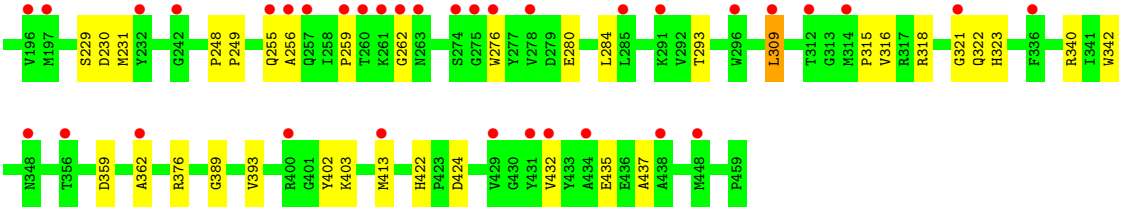




• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



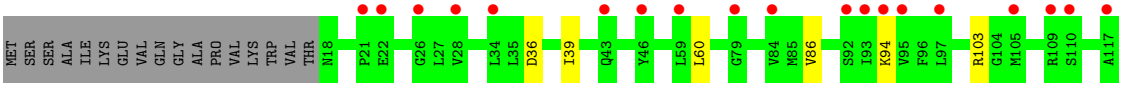




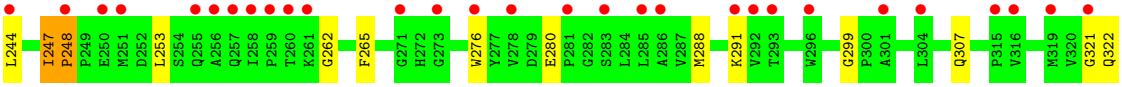
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

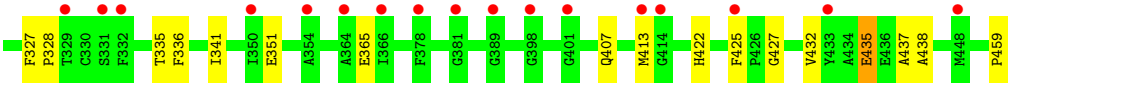
Chain W:







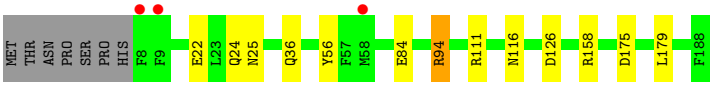




• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain B:





• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain D:

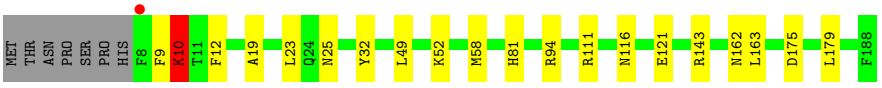




• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain F:

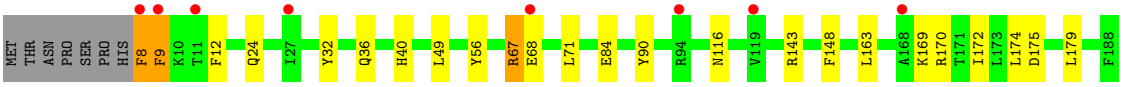




• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain H:

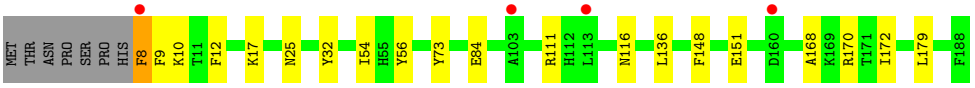




• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain J:

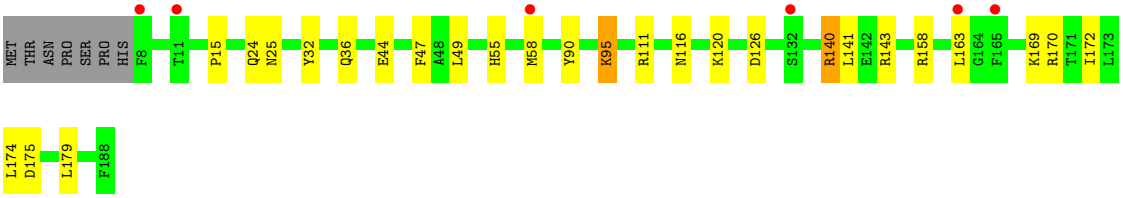




• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain L:

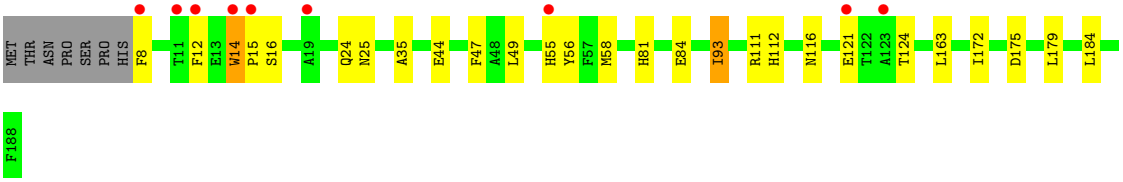




• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain N:

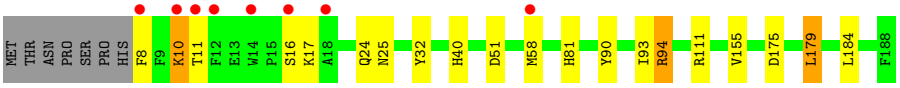




• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain P:

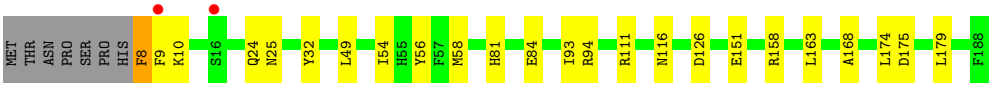




• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain R:

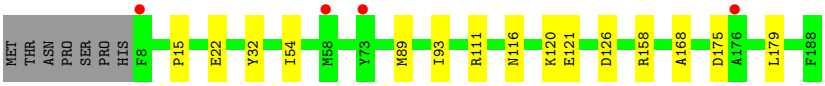




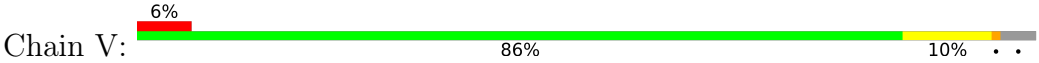
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

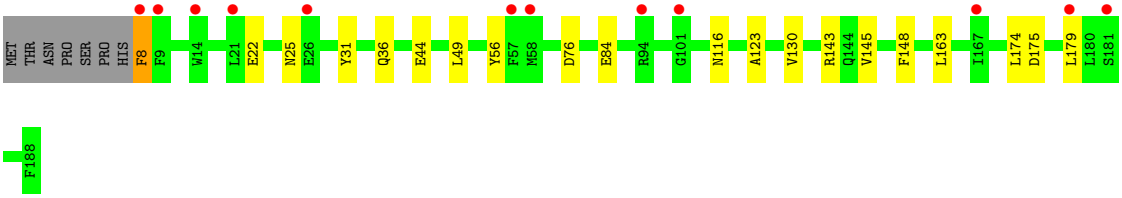
Chain T:



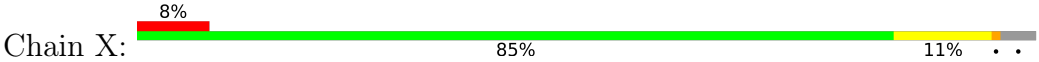


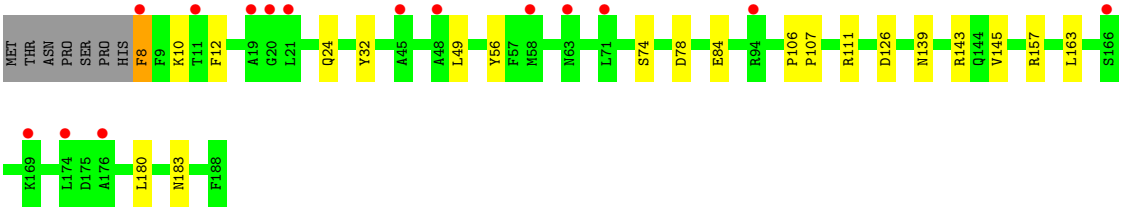
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA





• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA





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 – 2.42 119.52 – 2.42	Depositor EDS
% Data completeness (in resolution range)	95.0 (119.52-2.42) 82.8 (119.52-2.42)	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 (0.97%)	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 , 44.1	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: BNL, FE2, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/3523	0.77	0/4784
1	C	0.42	0/3523	0.77	0/4784
1	E	0.42	0/3523	0.79	0/4784
1	G	0.43	0/3518	0.78	2/4777 (0.0%)
1	I	0.42	0/3518	0.78	2/4777 (0.0%)
1	K	0.42	0/3518	0.78	2/4777 (0.0%)
1	M	0.42	0/3523	0.78	0/4784
1	O	0.42	0/3523	0.77	0/4784
1	Q	0.43	0/3523	0.77	0/4784
1	S	0.42	0/3519	0.77	4/4780 (0.1%)
1	U	0.44	0/3519	0.76	0/4780
1	W	0.46	0/3519	0.79	6/4780 (0.1%)
2	B	0.40	0/1532	0.68	0/2072
2	D	0.40	0/1532	0.72	0/2072
2	F	0.41	0/1532	0.70	0/2072
2	H	0.40	0/1542	0.73	2/2084 (0.1%)
2	J	0.41	0/1542	0.72	0/2084
2	L	0.40	0/1542	0.70	0/2084
2	N	0.41	0/1542	0.74	2/2084 (0.1%)
2	P	0.41	0/1542	0.74	0/2084
2	R	0.40	0/1542	0.75	2/2084 (0.1%)
2	T	0.41	0/1542	0.70	0/2084
2	V	0.42	0/1542	0.70	0/2084
2	X	0.41	0/1542	0.73	0/2084
All	All	0.42	0/60723	0.76	22/82347 (0.0%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	299	GLY	CA-C-N	6.62	126.12	119.24
1	S	299	GLY	C-N-CA	6.62	126.12	119.24
2	N	14	TRP	CA-C-N	6.36	127.79	119.84
2	N	14	TRP	C-N-CA	6.36	127.79	119.84
1	G	299	GLY	CA-C-N	6.35	125.84	119.24
1	G	299	GLY	C-N-CA	6.35	125.84	119.24
1	W	248	PRO	CA-C-N	6.21	125.89	119.56
1	W	248	PRO	C-N-CA	6.21	125.89	119.56
2	R	8	PHE	CA-C-N	5.47	131.55	121.70
2	R	8	PHE	C-N-CA	5.47	131.55	121.70
2	H	8	PHE	CA-C-N	5.46	131.53	121.70
2	H	8	PHE	C-N-CA	5.46	131.53	121.70
1	W	247	ILE	CA-C-N	5.29	125.83	120.38
1	W	247	ILE	C-N-CA	5.29	125.83	120.38
1	S	333	LEU	CA-C-N	5.07	125.10	119.32
1	S	333	LEU	C-N-CA	5.07	125.10	119.32
1	K	248	PRO	CA-C-N	5.03	125.31	119.47
1	K	248	PRO	C-N-CA	5.03	125.31	119.47
1	W	299	GLY	CA-C-N	5.03	124.52	119.19
1	W	299	GLY	C-N-CA	5.03	124.52	119.19
1	I	289	GLY	CA-C-N	5.01	124.31	118.85
1	I	289	GLY	C-N-CA	5.01	124.31	118.85

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	27	0
1	C	3421	0	3269	23	0
1	E	3421	0	3269	18	0
1	G	3416	0	3262	28	0
1	I	3416	0	3262	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3416	0	3262	22	0
1	M	3421	0	3269	11	0
1	O	3421	0	3269	18	0
1	Q	3421	0	3269	20	0
1	S	3417	0	3258	22	0
1	U	3417	0	3258	23	0
1	W	3417	0	3258	24	0
2	B	1497	0	1441	13	0
2	D	1497	0	1441	17	0
2	F	1497	0	1441	12	0
2	H	1507	0	1456	19	0
2	J	1507	0	1456	17	0
2	L	1507	0	1456	21	0
2	N	1507	0	1456	18	0
2	P	1507	0	1456	17	0
2	R	1507	0	1456	20	0
2	T	1507	0	1456	11	0
2	V	1507	0	1456	16	0
2	X	1507	0	1456	16	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	389	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 (389) 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
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:N:58:MET:HE2	2:N:81:HIS:HB2	1.75	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:W:288:MET:HE3	1:W:336:PHE:HB3	1.77	0.65
1:G:123:HIS:HB2	3:G:1460:FES:S2	2.37	0.64
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
2:D:58:MET:HE3	2:D:174:LEU:HD22	1.82	0.61
1:I:413:MET:HE2	1:I:435:GLU:HG3	1.83	0.60
1:I:448:MET:HG2	1:I:457:LEU:HD21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:217:PRO:HD2	1:I:393:VAL:HG22	1.83	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
2:N:58:MET:HE2	2:N:81:HIS:CB	2.32	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
1:S:340:ARG:HH12	1:S:385:GLU:CD	2.10	0.58
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:A:258:ILE:HD11	2:N:8:PHE:C	2.29	0.58
1:E:259:PRO:HB3	1:E:280:GLU:HG2	1.85	0.57
1:G:413:MET:HE2	1:G:435:GLU:HG3	1.86	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
2:P:58:MET:HE2	2:P:81:HIS:HB2	1.86	0.57
1:S:229:SER:HB2	1:S:437:ALA:HB3	1.87	0.56
2:R:58:MET:HE3	2:R:174:LEU:HD22	1.88	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
1:C:340:ARG:HH12	1:C:385:GLU:CD	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:340:ARG:HH12	1:E:385:GLU:CD	2.16	0.54
2:P:58:MET:HE2	2:P:81:HIS:CB	2.38	0.54
2:D:111:ARG:HB2	2:F:175:ASP:OD2	2.08	0.54
1:Q:324:MET:HE2	1:Q:326:ILE:HD11	1.89	0.53
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
2:J:8:PHE:CD1	2:J:8:PHE:C	2.87	0.53
2:N:24:GLN:HG2	2:R:25:ASN:HD21	1.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:L:58:MET:HE3	2:L:174:LEU:HD22	1.94	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
1:K:231:MET:HE1	1:K:321:GLY:O	2.12	0.49
2:J:170:ARG:HD3	2:J:172:ILE:HD11	1.94	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
1:G:288:MET:HE3	1:G:336:PHE:HB3	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
1:E:262:GLY:C	1:E:432:VAL:HB	2.38	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
2:T:22:GLU:H	2:T:22:GLU:CD	2.21	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
1:M:413:MET:HE2	1:M:435:GLU:HG3	1.95	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
1:K:309:LEU:HD13	1:K:316:VAL:HG11	1.95	0.48
1:M:262:GLY:C	1:M:432:VAL:HB	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:262:GLY:C	1:C:432:VAL:HB	2.40	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:I:231:MET:HE1	1:I:321:GLY:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:N	1:A:192:PRO:HD2	2.31	0.45
1:O:36:ASP:O	1:O:39:ILE:HG12	2.16	0.45
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: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
1:Q:413:MET:HE2	1:Q:435:GLU:HG3	1.98	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:L:58:MET:CE	2:L:174:LEU:HD22	2.46	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:E:287:VAL:HG12	1:E:288:MET:HE2	1.99	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:I:262:GLY:C	1:I:432:VAL:HB	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:9:PHE:H	1:S:258:ILE:HD11	1.83	0.43
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:W:262:GLY:C	1:W:432:VAL:HB	2.43	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: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
1:Q:262:GLY:C	1:Q:432:VAL:HB	2.44	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
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
1:A:74:LEU:HD21	1:A:211:MET:HE1	2.01	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)
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
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: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:Q:231:MET:HE1	1:Q:321:GLY:O	2.19	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
1:O:231:MET:HE1	1:O:321:GLY:O	2.20	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
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:U:231:MET:HE1	1:U:321:GLY:O	2.19	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:D:138:ARG:HD2	2:D:138:ARG:C	2.45	0.41
2:J:32:TYR:CG	2:L:116:ASN:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:340:ARG:HD3	1:U:342:TRP:CH2	2.55	0.41
1:W:265:PHE:HE1	1:W:427:GLY:HA3	1.84	0.41
1:K:267:ALA:HB2	1:K:272:HIS:HB2	2.02	0.41
2:F:58:MET:HE2	2:F:81:HIS:CB	2.50	0.41
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:R:58:MET:HE2	2:R:81:HIS:CD2	2.56	0.41
2:V:22:GLU:H	2:V:22:GLU:CD	2.27	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:U:413:MET:HE2	1:U:435:GLU:HG3	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: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
2:X:8:PHE:CD1	2:X:8:PHE:C	2.98	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:U:230:ASP:CG	1:W:123:HIS:HE2	2.28	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:262:GLY:C	1:O:432:VAL:HB	2.46	0.40
1:O:422:HIS:CD2	1:O:424:ASP:H	2.40	0.40
1:A:230:ASP:CG	1:C:123:HIS:HE2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:287:VAL:HG12	1:C:288:MET:HE3	2.03	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:O:288:MET:HE3	1:O:336:PHE:HB3	2.03	0.40
1:S:391:ASN:O	1:S:395:ILE:HG13	2.22	0.40
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
1:U:262:GLY:C	1:U:432:VAL:HB	2.47	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%)	43	57
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%)	43	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	43	57
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%)	21	30
2	F	179/188 (95%)	171 (96%)	7 (4%)	1 (1%)	21	30
2	H	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	21	30
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%)	11	16
2	P	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	21	30
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%)	21	30
All	All	7284/7764 (94%)	6982 (96%)	292 (4%)	10 (0%)	48	63

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%)	342 (98%)	8 (2%)	44	64
1	C	350/373 (94%)	344 (98%)	6 (2%)	53	73
1	E	350/373 (94%)	343 (98%)	7 (2%)	48	68
1	G	349/373 (94%)	339 (97%)	10 (3%)	37	57
1	I	349/373 (94%)	347 (99%)	2 (1%)	78	88
1	K	349/373 (94%)	345 (99%)	4 (1%)	65	81
1	M	350/373 (94%)	344 (98%)	6 (2%)	53	73
1	O	350/373 (94%)	343 (98%)	7 (2%)	48	68
1	Q	350/373 (94%)	343 (98%)	7 (2%)	48	68
1	S	349/373 (94%)	341 (98%)	8 (2%)	44	64
1	U	349/373 (94%)	345 (99%)	4 (1%)	65	81
1	W	349/373 (94%)	338 (97%)	11 (3%)	34	54
2	B	158/167 (95%)	155 (98%)	3 (2%)	50	70
2	D	158/167 (95%)	156 (99%)	2 (1%)	61	78
2	F	158/167 (95%)	151 (96%)	7 (4%)	25	41
2	H	160/167 (96%)	156 (98%)	4 (2%)	42	62
2	J	160/167 (96%)	157 (98%)	3 (2%)	50	70
2	L	160/167 (96%)	157 (98%)	3 (2%)	50	70
2	N	160/167 (96%)	155 (97%)	5 (3%)	35	55
2	P	160/167 (96%)	153 (96%)	7 (4%)	25	41
2	R	160/167 (96%)	157 (98%)	3 (2%)	50	70
2	T	160/167 (96%)	158 (99%)	2 (1%)	61	78
2	V	160/167 (96%)	156 (98%)	4 (2%)	42	62
2	X	160/167 (96%)	158 (99%)	2 (1%)	61	78
All	All	6108/6480 (94%)	5983 (98%)	125 (2%)	48	68

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	103	ARG
1	A	247	ILE
1	A	252	ASP
1	A	257	GLN
1	A	280	GLU
1	A	294	GLN
1	A	335	THR
2	B	22	GLU
2	B	94	ARG
2	B	179	LEU
1	C	86	VAL
1	C	247	ILE
1	C	280	GLU
1	C	294	GLN
1	C	335	THR
1	C	457	LEU
2	D	121	GLU
2	D	179	LEU
1	E	86	VAL
1	E	103	ARG
1	E	258	ILE
1	E	280	GLU
1	E	335	THR
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	162	ASN
2	F	179	LEU
1	G	47	GLU
1	G	48	LEU
1	G	86	VAL
1	G	103	ARG
1	G	252	ASP
1	G	258	ILE
1	G	280	GLU
1	G	335	THR
1	G	358	VAL
1	G	419	GLN

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Mol	Chain	Res	Type
2	H	67	ARG
2	H	143	ARG
2	H	169	LYS
2	H	179	LEU
1	I	280	GLU
1	I	457	LEU
2	J	8	PHE
2	J	17	LYS
2	J	179	LEU
1	K	103	ARG
1	K	191	ARG
1	K	205	THR
1	K	252	ASP
2	L	95	LYS
2	L	140	ARG
2	L	179	LEU
1	M	103	ARG
1	M	261	LYS
1	M	280	GLU
1	M	309	LEU
1	M	339	ILE
1	M	366	ILE
2	N	14	TRP
2	N	44	GLU
2	N	93	ILE
2	N	121	GLU
2	N	124	THR
1	O	31	GLU
1	O	86	VAL
1	O	255	GLN
1	O	261	LYS
1	O	280	GLU
1	O	366	ILE
1	O	418	SER
2	P	10	LYS
2	P	11	THR
2	P	17	LYS
2	P	51	ASP
2	P	93	ILE
2	P	94	ARG
2	P	179	LEU
1	Q	86	VAL

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Mol	Chain	Res	Type
1	Q	103	ARG
1	Q	116	LYS
1	Q	255	GLN
1	Q	261	LYS
1	Q	280	GLU
1	Q	358	VAL
2	R	93	ILE
2	R	94	ARG
2	R	179	LEU
1	S	48	LEU
1	S	89	LYS
1	S	103	ARG
1	S	280	GLU
1	S	335	THR
1	S	339	ILE
1	S	350	ILE
1	S	446	MET
2	T	121	GLU
2	T	179	LEU
1	U	103	ARG
1	U	255	GLN
1	U	309	LEU
1	U	376	ARG
2	V	8	PHE
2	V	44	GLU
2	V	76	ASP
2	V	179	LEU
1	W	86	VAL
1	W	94	LYS
1	W	103	ARG
1	W	167	THR
1	W	243	ILE
1	W	280	GLU
1	W	307	GLN
1	W	335	THR
1	W	341	ILE
1	W	407	GLN
1	W	435	GLU
2	X	8	PHE
2	X	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	88	GLN
1	A	99	GLN
1	A	226	GLN
1	A	255	GLN
1	A	294	GLN
1	A	311	HIS
1	A	343	HIS
1	A	391	ASN
1	A	410	ASN
1	A	422	HIS
1	A	443	HIS
1	A	444	HIS
2	B	25	ASN
2	B	36	GLN
2	B	77	GLN
2	B	144	GLN
2	B	162	ASN
1	C	43	GLN
1	C	294	GLN
1	C	386	GLN
1	C	391	ASN
1	C	410	ASN
1	C	412	GLN
1	C	422	HIS
1	C	443	HIS
1	C	444	HIS
2	D	36	GLN
2	D	162	ASN
1	E	18	ASN
1	E	43	GLN
1	E	257	GLN
1	E	294	GLN
1	E	391	ASN
1	E	410	ASN
1	E	412	GLN
1	E	422	HIS
1	E	443	HIS
2	F	25	ASN
2	F	131	ASN
2	F	162	ASN
1	G	43	GLN
1	G	257	GLN

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Mol	Chain	Res	Type
1	G	322	GLN
1	G	386	GLN
1	G	391	ASN
1	G	410	ASN
1	G	422	HIS
1	G	443	HIS
2	H	36	GLN
1	I	43	GLN
1	I	88	GLN
1	I	99	GLN
1	I	226	GLN
1	I	264	GLN
1	I	391	ASN
1	I	410	ASN
1	I	422	HIS
2	J	25	ASN
2	J	36	GLN
2	J	86	HIS
2	J	131	ASN
1	K	88	GLN
1	K	212	GLN
1	K	264	GLN
1	K	322	GLN
1	K	343	HIS
1	K	377	ASN
1	K	386	GLN
1	K	391	ASN
1	K	410	ASN
1	K	422	HIS
1	K	443	HIS
2	L	25	ASN
2	L	36	GLN
2	L	81	HIS
2	L	131	ASN
1	M	43	GLN
1	M	88	GLN
1	M	212	GLN
1	M	257	GLN
1	M	263	ASN
1	M	311	HIS
1	M	322	GLN
1	M	391	ASN

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Mol	Chain	Res	Type
1	M	410	ASN
2	N	25	ASN
2	N	77	GLN
2	N	131	ASN
1	O	43	GLN
1	O	226	GLN
1	O	257	GLN
1	O	322	GLN
1	O	391	ASN
1	O	407	GLN
1	O	410	ASN
1	O	422	HIS
2	P	25	ASN
2	P	40	HIS
2	P	77	GLN
2	P	86	HIS
1	Q	255	GLN
1	Q	377	ASN
1	Q	391	ASN
1	Q	410	ASN
1	Q	422	HIS
2	R	25	ASN
2	R	40	HIS
2	R	77	GLN
1	S	43	GLN
1	S	212	GLN
1	S	343	HIS
1	S	377	ASN
1	S	386	GLN
1	S	391	ASN
1	S	410	ASN
1	S	422	HIS
1	S	428	ASN
1	S	443	HIS
1	S	444	HIS
2	T	25	ASN
2	T	36	GLN
1	U	43	GLN
1	U	212	GLN
1	U	226	GLN
1	U	255	GLN
1	U	264	GLN

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Mol	Chain	Res	Type
1	U	322	GLN
1	U	343	HIS
1	U	386	GLN
1	U	410	ASN
1	U	422	HIS
1	U	443	HIS
2	V	25	ASN
2	V	36	GLN
2	V	81	HIS
1	W	212	GLN
1	W	264	GLN
1	W	386	GLN
1	W	391	ASN
1	W	410	ASN
1	W	422	HIS
1	W	443	HIS
2	X	25	ASN
2	X	86	HIS
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 oligosaccharides 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	I	1460	1	0,4,4	-	-	-		
3	FES	S	1460	1	0,4,4	-	-	-		
5	BNL	U	1462	-	13,13,13	0.52	0	16,16,16	0.54	0
3	FES	M	1460	1	0,4,4	-	-	-		
5	BNL	W	1462	-	13,13,13	0.55	0	16,16,16	0.55	0
5	BNL	S	1462	-	13,13,13	0.54	0	16,16,16	0.56	0
3	FES	U	1460	1	0,4,4	-	-	-		
3	FES	K	1460	1	0,4,4	-	-	-		
5	BNL	A	1462	-	13,13,13	0.54	0	16,16,16	0.57	0
5	BNL	G	1462	-	13,13,13	0.53	0	16,16,16	0.50	0
3	FES	C	1460	1	0,4,4	-	-	-		
3	FES	W	1460	1	0,4,4	-	-	-		
5	BNL	Q	1462	-	13,13,13	0.60	0	16,16,16	0.44	0
5	BNL	K	1462	-	13,13,13	0.57	0	16,16,16	0.43	0
3	FES	E	1460	1	0,4,4	-	-	-		
3	FES	A	1460	1	0,4,4	-	-	-		
3	FES	G	1460	1	0,4,4	-	-	-		
5	BNL	E	1462	-	13,13,13	0.55	0	16,16,16	0.53	0
5	BNL	C	1462	-	13,13,13	0.54	0	16,16,16	0.46	0
5	BNL	I	1462	-	13,13,13	0.52	0	16,16,16	0.62	0
5	BNL	O	1462	-	13,13,13	0.56	0	16,16,16	0.49	0
3	FES	Q	1460	1	0,4,4	-	-	-		
5	BNL	M	1462	-	13,13,13	0.53	0	16,16,16	0.50	0
3	FES	O	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
3	FES	I	1460	1	-	-	0/1/1/1
3	FES	S	1460	1	-	-	0/1/1/1
5	BNL	U	1462	-	-	0/4/4/4	0/2/2/2
3	FES	M	1460	1	-	-	0/1/1/1
5	BNL	W	1462	-	-	4/4/4/4	0/2/2/2
5	BNL	S	1462	-	-	0/4/4/4	0/2/2/2
3	FES	U	1460	1	-	-	0/1/1/1
3	FES	K	1460	1	-	-	0/1/1/1

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1462	BNL	C15-C16-C2-C1
5	I	1462	BNL	C17-C16-C2-C3
5	I	1462	BNL	C17-C16-C2-C1
5	I	1462	BNL	C15-C16-C2-C3
5	A	1462	BNL	C15-C16-C2-C1
5	A	1462	BNL	C17-C16-C2-C3
5	A	1462	BNL	C17-C16-C2-C1
5	A	1462	BNL	C15-C16-C2-C3
5	W	1462	BNL	C15-C16-C2-C1
5	W	1462	BNL	C17-C16-C2-C3
5	W	1462	BNL	C17-C16-C2-C1
5	W	1462	BNL	C15-C16-C2-C3

There are no ring outliers.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1460	FES	1	0
3	S	1460	FES	1	0
3	M	1460	FES	1	0
3	U	1460	FES	1	0
3	K	1460	FES	1	0
3	C	1460	FES	1	0
3	W	1460	FES	1	0
3	E	1460	FES	1	0
3	A	1460	FES	1	0
3	G	1460	FES	1	0
3	Q	1460	FES	1	0
5	M	1462	BNL	1	0
3	O	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%)	0.34	9 (2%)	63	60	22, 40, 55, 61	17 (3%)
1	C	432/459 (94%)	0.45	20 (4%)	37	33	25, 43, 54, 58	17 (3%)
1	E	432/459 (94%)	0.15	9 (2%)	63	60	21, 35, 46, 55	17 (3%)
1	G	432/459 (94%)	0.53	13 (3%)	52	49	29, 47, 60, 66	17 (3%)
1	I	432/459 (94%)	0.74	30 (6%)	23	19	29, 51, 63, 69	17 (3%)
1	K	432/459 (94%)	0.92	28 (6%)	25	21	27, 54, 65, 68	17 (3%)
1	M	432/459 (94%)	0.33	20 (4%)	37	33	22, 38, 58, 62	17 (3%)
1	O	432/459 (94%)	0.16	10 (2%)	61	57	20, 34, 49, 57	17 (3%)
1	Q	432/459 (94%)	-0.05	7 (1%)	70	67	17, 31, 42, 61	17 (3%)
1	S	432/459 (94%)	0.70	28 (6%)	25	21	19, 47, 58, 67	17 (3%)
1	U	432/459 (94%)	1.02	43 (9%)	12	9	31, 56, 72, 74	17 (3%)
1	W	432/459 (94%)	1.37	80 (18%)	3	3	34, 59, 70, 74	17 (3%)
2	B	181/188 (96%)	0.26	3 (1%)	69	66	26, 38, 47, 58	4 (2%)
2	D	181/188 (96%)	0.22	5 (2%)	55	51	28, 39, 51, 56	4 (2%)
2	F	181/188 (96%)	0.02	1 (0%)	85	84	23, 33, 47, 60	4 (2%)
2	H	181/188 (96%)	0.53	8 (4%)	39	34	32, 45, 60, 66	4 (2%)
2	J	181/188 (96%)	0.60	4 (2%)	62	59	35, 49, 57, 63	4 (2%)
2	L	181/188 (96%)	0.66	6 (3%)	49	45	35, 48, 63, 70	4 (2%)
2	N	181/188 (96%)	0.32	9 (4%)	34	30	25, 37, 61, 75	4 (2%)
2	P	181/188 (96%)	0.22	8 (4%)	39	34	24, 36, 64, 79	4 (2%)
2	R	181/188 (96%)	0.04	2 (1%)	78	75	21, 32, 52, 62	4 (2%)
2	T	181/188 (96%)	0.23	4 (2%)	62	59	28, 39, 55, 65	4 (2%)
2	V	181/188 (96%)	0.80	12 (6%)	24	20	40, 53, 59, 64	4 (2%)
2	X	181/188 (96%)	1.07	15 (8%)	17	14	37, 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%)	0.51	374 (5%)	33	30	17, 44, 63, 79	252 (3%)

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	ALA	10.0
1	K	256	ALA	8.9
1	W	256	ALA	8.4
1	M	256	ALA	8.3
1	Q	260	THR	7.8
1	I	256	ALA	7.6
1	K	255	GLN	7.4
1	E	256	ALA	6.8
1	G	256	ALA	6.7
1	U	260	THR	6.6
1	O	256	ALA	6.5
1	S	256	ALA	6.5
1	W	260	THR	5.8
1	A	255	GLN	5.8
1	I	260	THR	5.6
1	A	421	GLY	5.3
1	M	255	GLN	5.3
1	U	256	ALA	5.2
1	E	259	PRO	5.1
1	I	246	GLY	5.1
1	Q	256	ALA	5.1
1	W	257	GLN	4.9
1	K	142	ALA	4.9
1	S	255	GLN	4.9
1	O	255	GLN	4.8
1	G	259	PRO	4.8
1	S	259	PRO	4.7
1	K	260	THR	4.7
1	E	255	GLN	4.7
1	U	255	GLN	4.7
1	S	105	MET	4.6
1	Q	259	PRO	4.5
1	C	257	GLN	4.5
1	C	256	ALA	4.4
2	X	11	THR	4.4
1	M	260	THR	4.4
1	A	260	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	W	292	VAL	4.3
1	M	259	PRO	4.2
1	O	261	LYS	4.2
2	F	8	PHE	4.2
1	S	142	ALA	4.2
1	U	259	PRO	4.1
2	N	14	TRP	4.1
1	C	260	THR	4.0
1	S	257	GLN	4.0
2	N	12	PHE	3.9
1	W	389	GLY	3.9
1	S	260	THR	3.9
1	W	94	LYS	3.9
1	I	262	GLY	3.9
1	I	259	PRO	3.8
1	K	259	PRO	3.8
1	W	261	LYS	3.8
1	O	311	HIS	3.8
1	W	255	GLN	3.8
1	G	260	THR	3.7
1	C	259	PRO	3.7
1	W	259	PRO	3.7
1	G	261	LYS	3.7
1	G	24	ILE	3.7
2	N	19	ALA	3.6
2	H	9	PHE	3.6
1	A	259	PRO	3.6
1	E	260	THR	3.6
1	W	125	TRP	3.6
1	M	257	GLN	3.6
1	A	257	GLN	3.5
1	U	257	GLN	3.5
2	J	103	ALA	3.5
1	S	138	PHE	3.5
1	U	356	THR	3.5
1	U	285	LEU	3.5
1	K	316	VAL	3.5
1	Q	261	LYS	3.5
1	K	257	GLN	3.4
1	I	320	VAL	3.4
1	I	255	GLN	3.4
1	M	261	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	X	63	ASN	3.4
1	W	79	GLY	3.4
1	G	142	ALA	3.4
1	E	261	LYS	3.3
1	I	257	GLN	3.3
1	Q	257	GLN	3.3
2	P	14	TRP	3.3
1	G	292	VAL	3.3
1	U	262	GLY	3.3
1	G	257	GLN	3.3
1	O	259	PRO	3.3
1	W	286	ALA	3.3
2	J	8	PHE	3.2
1	K	186	TYR	3.2
1	K	131	GLY	3.2
2	N	8	PHE	3.2
1	S	261	LYS	3.2
1	M	142	ALA	3.2
1	W	250	GLU	3.2
1	S	129	ILE	3.2
1	Q	255	GLN	3.1
2	B	9	PHE	3.1
1	W	22	GLU	3.1
1	W	414	GLY	3.1
1	U	109	ARG	3.1
1	W	110	SER	3.1
1	W	316	VAL	3.1
1	E	257	GLN	3.1
2	V	9	PHE	3.1
1	U	187	LEU	3.1
2	X	174	LEU	3.1
1	I	275	GLY	3.1
1	U	400	ARG	3.1
2	D	123	ALA	3.1
1	W	285	LEU	3.1
2	J	113	LEU	3.1
1	S	109	ARG	3.1
1	W	196	VAL	3.1
1	W	236	THR	3.0
1	K	261	LYS	3.0
1	W	329	THR	3.0
1	I	261	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	276	TRP	3.0
2	X	176	ALA	3.0
1	U	28	VAL	3.0
1	W	142	ALA	3.0
1	W	433	TYR	3.0
1	W	34	LEU	3.0
1	W	244	LEU	3.0
1	U	314	MET	2.9
1	W	291	LYS	2.9
1	K	372	ARG	2.9
2	P	12	PHE	2.9
1	M	258	ILE	2.9
1	S	103	ARG	2.9
2	N	11	THR	2.9
1	W	183	LEU	2.9
1	C	105	MET	2.9
1	K	24	ILE	2.9
2	L	163	LEU	2.9
1	G	433	TYR	2.9
1	W	425	PHE	2.8
1	U	232	TYR	2.8
1	I	444	HIS	2.8
1	C	316	VAL	2.8
1	W	117	ALA	2.8
1	W	364	ALA	2.8
2	P	58	MET	2.8
1	K	95	VAL	2.8
1	W	28	VAL	2.8
1	O	260	THR	2.8
1	W	166	ALA	2.8
1	K	127	TYR	2.8
1	M	201	THR	2.8
1	O	105	MET	2.8
1	A	261	LYS	2.8
1	M	307	GLN	2.8
1	O	109	ARG	2.8
1	U	275	GLY	2.7
1	W	378	PHE	2.8
2	D	8	PHE	2.8
1	W	293	THR	2.7
2	H	27	ILE	2.7
1	C	193	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	316	VAL	2.7
1	U	196	VAL	2.7
1	O	291	LYS	2.7
2	V	58	MET	2.7
2	X	45	ALA	2.7
1	C	255	GLN	2.7
2	V	8	PHE	2.7
1	K	251	MET	2.7
2	H	94	ARG	2.7
1	E	235	GLY	2.7
1	K	414	GLY	2.7
1	U	291	LYS	2.7
1	W	109	ARG	2.7
1	W	190	ALA	2.7
1	U	261	LYS	2.6
1	W	258	ILE	2.6
1	W	278	VAL	2.6
1	C	314	MET	2.6
1	K	203	ALA	2.6
1	I	431	TYR	2.6
1	W	46	TYR	2.6
1	U	296	TRP	2.6
1	W	276	TRP	2.6
2	V	179	LEU	2.6
2	P	11	THR	2.6
1	W	248	PRO	2.6
1	I	285	LEU	2.6
2	X	21	LEU	2.6
1	U	274	SER	2.6
2	R	16	SER	2.6
2	V	94	ARG	2.5
2	L	165	PHE	2.5
2	X	8	PHE	2.5
1	C	309	LEU	2.5
1	I	432	VAL	2.5
1	W	92	SER	2.5
2	V	14	TRP	2.5
1	W	241	SER	2.5
1	W	105	MET	2.5
2	B	58	MET	2.5
1	W	315	PRO	2.5
1	S	416	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	24	ILE	2.5
2	V	57	PHE	2.5
1	O	257	GLN	2.5
1	I	305	ALA	2.5
1	K	109	ARG	2.5
1	W	331	SER	2.5
1	U	448	MET	2.5
1	C	131	GLY	2.5
1	S	107	ILE	2.5
1	K	94	LYS	2.5
1	K	454	TRP	2.5
2	H	119	VAL	2.5
1	G	109	ARG	2.5
1	U	434	ALA	2.5
1	W	174	ALA	2.5
1	K	204	GLY	2.4
1	U	118	PHE	2.4
1	U	336	PHE	2.4
2	B	8	PHE	2.4
1	W	296	TRP	2.4
1	W	84	VAL	2.4
1	W	251	MET	2.4
1	W	354	ALA	2.4
2	V	181	SER	2.4
1	C	321	GLY	2.4
1	W	59	LEU	2.4
2	H	8	PHE	2.4
2	X	94	ARG	2.4
1	G	434	ALA	2.4
1	W	126	ALA	2.4
1	U	321	GLY	2.4
1	U	348	ASN	2.4
1	S	434	ALA	2.4
1	I	94	LYS	2.4
2	H	11	THR	2.4
2	X	169	LYS	2.4
1	W	398	GLY	2.4
1	W	304	LEU	2.4
2	T	73	TYR	2.4
1	C	301	ALA	2.4
1	S	438	ALA	2.4
1	U	362	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	V	26	GLU	2.4
1	E	137	PRO	2.3
2	X	166	SER	2.3
1	W	97	LEU	2.3
1	W	198	LEU	2.3
2	D	160	ASP	2.3
1	W	193	TYR	2.3
1	S	19	TRP	2.3
1	I	414	GLY	2.3
1	M	289	GLY	2.3
2	V	101	GLY	2.3
1	I	187	LEU	2.3
1	W	366	ILE	2.3
2	N	55	HIS	2.3
1	W	448	MET	2.3
2	L	8	PHE	2.3
2	P	10	LYS	2.3
1	I	277	TYR	2.3
1	S	47	GLU	2.3
1	S	163	ALA	2.3
2	D	176	ALA	2.3
1	W	43	GLN	2.3
1	W	381	GLY	2.3
1	K	96	PHE	2.3
2	N	15	PRO	2.3
1	K	159	GLY	2.3
1	S	48	LEU	2.3
1	K	319	MET	2.3
1	I	153	PHE	2.3
1	S	265	PHE	2.3
2	P	8	PHE	2.3
1	U	432	VAL	2.3
1	I	263	ASN	2.2
2	H	168	ALA	2.2
2	T	176	ALA	2.2
2	X	48	ALA	2.2
1	W	189	ASP	2.2
1	W	332	PHE	2.2
2	R	9	PHE	2.2
1	C	417	ARG	2.2
1	M	109	ARG	2.2
1	M	422	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	270	GLY	2.2
1	W	401	GLY	2.2
2	V	167	ILE	2.2
1	U	276	TRP	2.2
1	I	300	PRO	2.2
1	U	429	VAL	2.2
2	P	18	ALA	2.2
1	I	89	LYS	2.2
1	M	291	LYS	2.2
1	U	431	TYR	2.2
1	C	124	GLY	2.2
1	M	105	MET	2.2
2	X	58	MET	2.2
1	M	309	LEU	2.2
1	K	107	ILE	2.2
1	U	24	ILE	2.2
1	M	298	GLU	2.2
1	W	223	ALA	2.2
1	G	255	GLN	2.2
1	U	413	MET	2.2
1	W	319	MET	2.2
1	Q	389	GLY	2.2
2	X	20	GLY	2.2
1	I	258	ILE	2.2
1	W	95	VAL	2.1
1	S	166	ALA	2.1
1	U	197	MET	2.1
1	U	263	ASN	2.1
1	W	301	ALA	2.1
1	U	242	GLY	2.1
1	W	271	GLY	2.1
1	W	350	ILE	2.1
2	H	68	GLU	2.1
1	C	265	PHE	2.1
1	G	19	TRP	2.1
1	S	153	PHE	2.1
1	S	136	VAL	2.1
1	U	438	ALA	2.1
2	X	71	LEU	2.1
1	A	372	ARG	2.1
2	N	121	GLU	2.1
1	W	283	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	281	PRO	2.1
1	W	21	PRO	2.1
1	W	281	PRO	2.1
1	K	86	VAL	2.1
1	U	19	TRP	2.1
2	N	123	ALA	2.1
1	U	312	THR	2.1
1	W	26	GLY	2.1
2	L	11	THR	2.1
1	S	140	LYS	2.1
1	W	413	MET	2.1
2	T	58	MET	2.1
1	M	432	VAL	2.1
1	S	86	VAL	2.1
1	U	278	VAL	2.1
2	T	8	PHE	2.1
1	C	364	ALA	2.1
1	K	305	ALA	2.1
2	X	19	ALA	2.1
1	I	296	TRP	2.1
1	I	109	ARG	2.1
1	S	52	ARG	2.1
1	U	62	GLY	2.1
1	W	273	GLY	2.1
1	A	431	TYR	2.1
1	C	186	TYR	2.1
2	J	160	ASP	2.1
1	I	165	VAL	2.0
1	W	222	PHE	2.0
2	V	21	LEU	2.0
1	E	414	GLY	2.0
1	U	176	TRP	2.0
1	I	243	ILE	2.0
2	L	58	MET	2.0
1	S	118	PHE	2.0
1	K	23	ALA	2.0
1	M	305	ALA	2.0
1	U	309	LEU	2.0
1	W	321	GLY	2.0
1	W	93	ILE	2.0
2	D	11	THR	2.0
2	L	132	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	P	16	SER	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 oligosaccharides 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	K	1462	12/12	0.82	0.22	86,86,87,87	0
5	BNL	G	1462	12/12	0.84	0.16	63,64,64,64	0
5	BNL	A	1462	12/12	0.86	0.19	76,76,76,76	0
5	BNL	W	1462	12/12	0.86	0.22	87,87,88,88	0
5	BNL	S	1462	12/12	0.87	0.23	82,82,82,82	0
5	BNL	U	1462	12/12	0.88	0.16	86,86,86,86	0
5	BNL	I	1462	12/12	0.89	0.15	63,63,64,64	0
5	BNL	O	1462	12/12	0.91	0.11	44,44,45,45	0
5	BNL	Q	1462	12/12	0.91	0.13	40,40,41,41	0
3	FES	S	1460	4/4	0.91	0.10	86,86,86,87	0
3	FES	E	1460	4/4	0.91	0.08	44,46,47,50	0
5	BNL	E	1462	12/12	0.91	0.13	49,49,49,49	0
5	BNL	M	1462	12/12	0.92	0.14	55,56,56,56	0
5	BNL	C	1462	12/12	0.92	0.14	55,56,56,56	0
3	FES	A	1460	4/4	0.93	0.09	43,44,46,48	0
3	FES	I	1460	4/4	0.94	0.08	45,46,48,50	0
3	FES	W	1460	4/4	0.94	0.11	74,75,76,77	0
3	FES	M	1460	4/4	0.95	0.06	38,38,39,42	0
3	FES	U	1460	4/4	0.95	0.08	48,48,49,49	0
3	FES	O	1460	4/4	0.95	0.07	44,45,46,48	0
4	FE2	W	1461	1/1	0.95	0.06	68,68,68,68	0
3	FES	G	1460	4/4	0.96	0.06	54,54,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FE2	U	1461	1/1	0.96	0.04	57,57,57,57	0
3	FES	Q	1460	4/4	0.96	0.08	39,39,41,44	0
4	FE2	I	1461	1/1	0.97	0.07	58,58,58,58	0
4	FE2	K	1461	1/1	0.97	0.07	59,59,59,59	0
3	FES	C	1460	4/4	0.97	0.06	43,44,45,46	0
3	FES	K	1460	4/4	0.97	0.06	74,75,75,76	0
4	FE2	A	1461	1/1	0.98	0.09	53,53,53,53	0
4	FE2	E	1461	1/1	0.98	0.06	41,41,41,41	0
4	FE2	S	1461	1/1	0.99	0.04	51,51,51,51	0
4	FE2	G	1461	1/1	0.99	0.04	52,52,52,52	0
4	FE2	M	1461	1/1	0.99	0.05	43,43,43,43	0
4	FE2	C	1461	1/1	1.00	0.05	44,44,44,44	0
4	FE2	O	1461	1/1	1.00	0.06	34,34,34,34	0
4	FE2	Q	1461	1/1	1.00	0.03	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.