



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:55 PM UTC

PDB ID : 5AEW / pdb_00005aew
Title : Crystal structure of II9 variant of Biphenyl dioxygenase from Burkholderia xenovorans LB400 in complex with biphenyl
Authors : Dhindwal, S.; Gomez-Gil, L.; Sylvestre, M.; Eltis, L.D.; Bolin, J.T.; Kumar, P.
Deposited on : 2015-01-10
Resolution : 1.88 Å(reported)

This is a 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

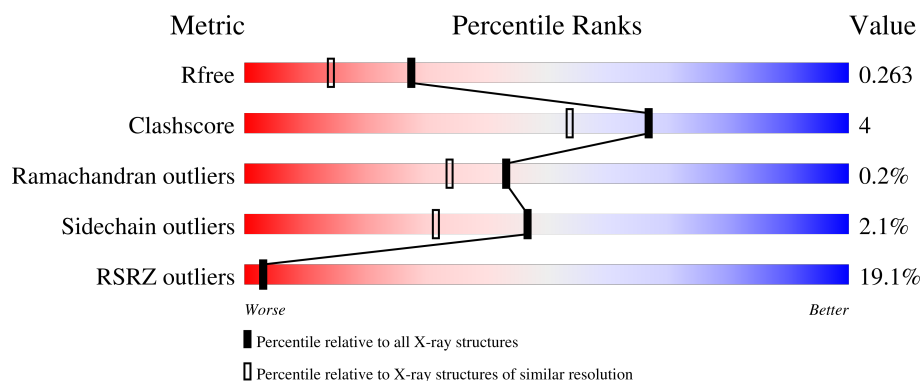
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	459	4% 86% 7% 6%
1	C	459	7% 89% 5% 6%
1	E	459	7% 88% 6% 6%
1	G	459	4% 88% 6% 6%
1	I	459	5% 83% 10% 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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	G	460	-	-	X	-
3	FES	Q	460	-	-	X	-
3	FES	W	460	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 63519 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BIPHENYL DIOXYGENASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	2	0
			3442	2189	604	625	24			
1	C	433	Total	C	N	O	S	0	2	0
			3444	2190	606	624	24			
1	E	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	G	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	I	433	Total	C	N	O	S	0	1	0
			3433	2184	602	623	24			
1	K	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	M	433	Total	C	N	O	S	0	1	0
			3434	2184	603	624	23			
1	O	433	Total	C	N	O	S	0	1	0
			3433	2184	602	623	24			
1	Q	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	S	433	Total	C	N	O	S	0	0	0
			3428	2180	602	623	23			
1	U	430	Total	C	N	O	S	0	0	0
			3405	2163	599	620	23			
1	W	432	Total	C	N	O	S	0	0	0
			3417	2171	601	622	23			

There are 48 discrepancies between the modelled and reference sequences:

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
W	341	THR	ILE	engineered mutation	UNP P37333

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

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

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

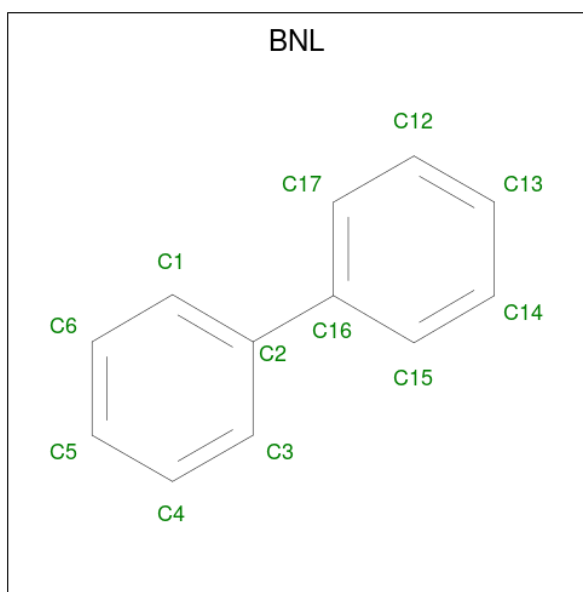


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		
3	M	1	Total	Fe	S	0	0
			4	2	2		
3	O	1	Total	Fe	S	0	0
			4	2	2		
3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

- Molecule 4 is FE (II) ION (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
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	C	1	Total C 12 12	0	0
5	E	1	Total C 12 12	0	0
5	I	1	Total C 12 12	0	0
5	K	1	Total C 12 12	0	0
5	M	1	Total C 12 12	0	0
5	O	1	Total C 12 12	0	0
5	Q	1	Total C 12 12	0	0
5	S	1	Total C 12 12	0	0
5	W	1	Total C 12 12	0	0

- Molecule 6 is water.

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

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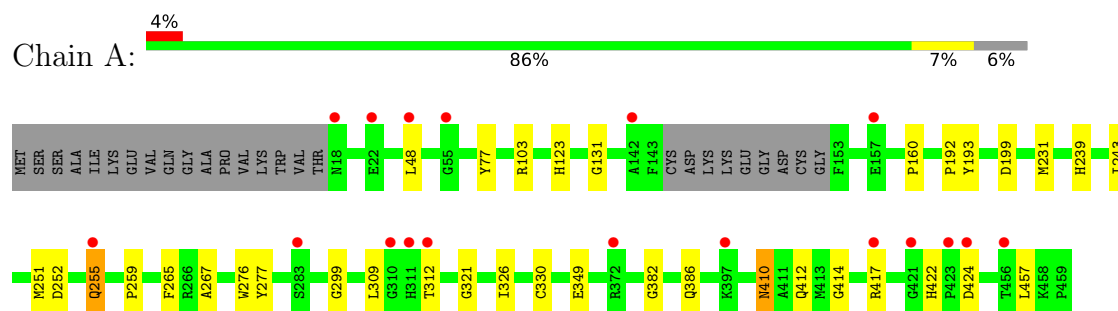
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	130	Total 130	O 130	0	0
6	M	204	Total 204	O 204	0	0
6	N	101	Total 101	O 101	0	0
6	O	205	Total 205	O 205	0	0
6	P	108	Total 108	O 108	0	0
6	Q	150	Total 150	O 150	0	0
6	R	124	Total 124	O 124	0	0
6	S	95	Total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

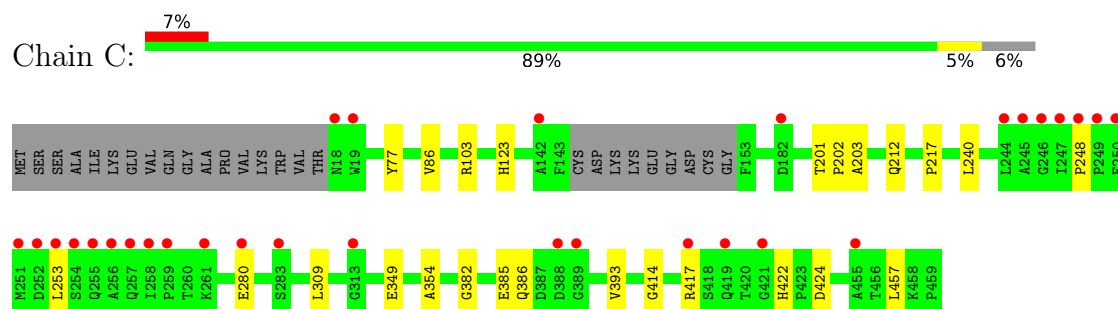
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

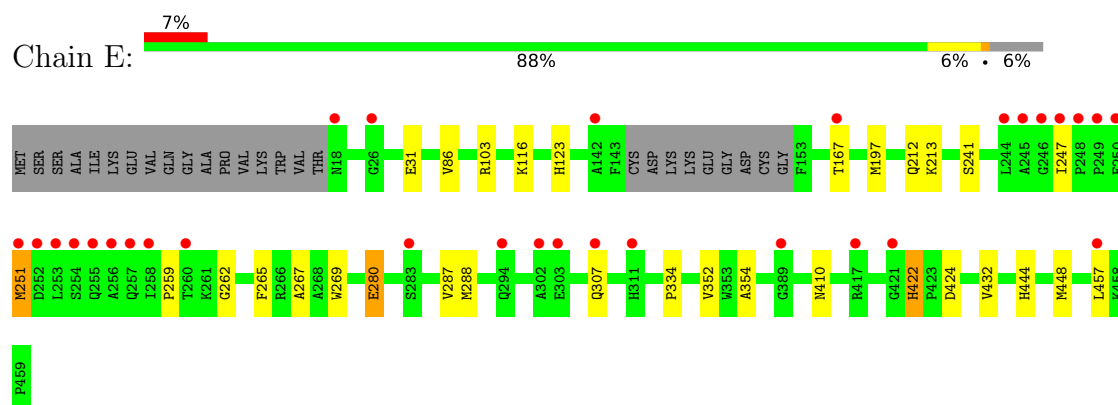
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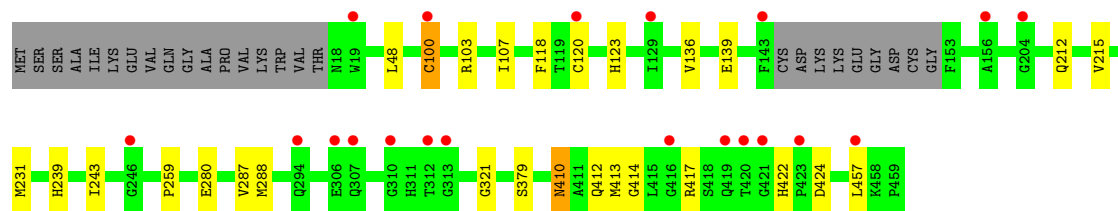


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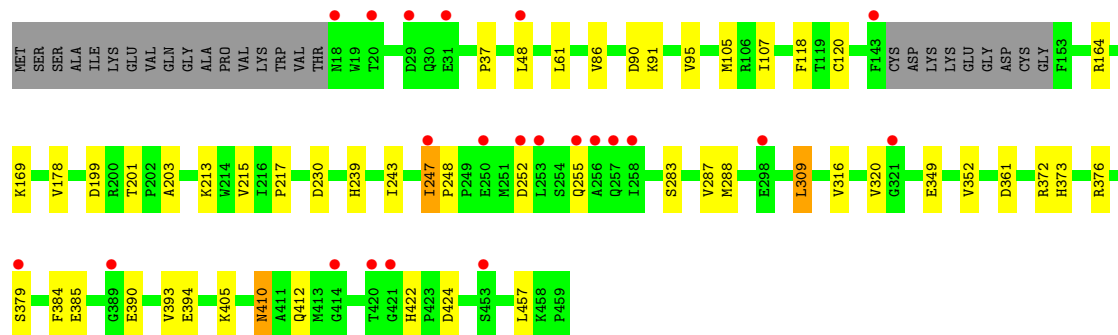
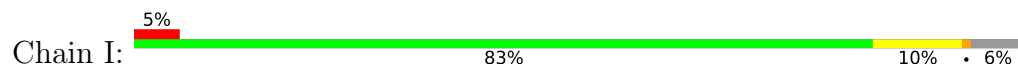


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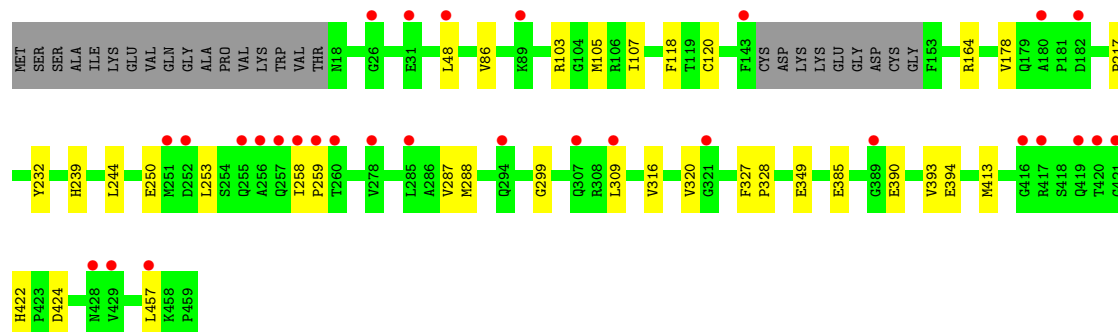
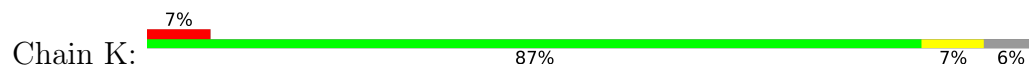




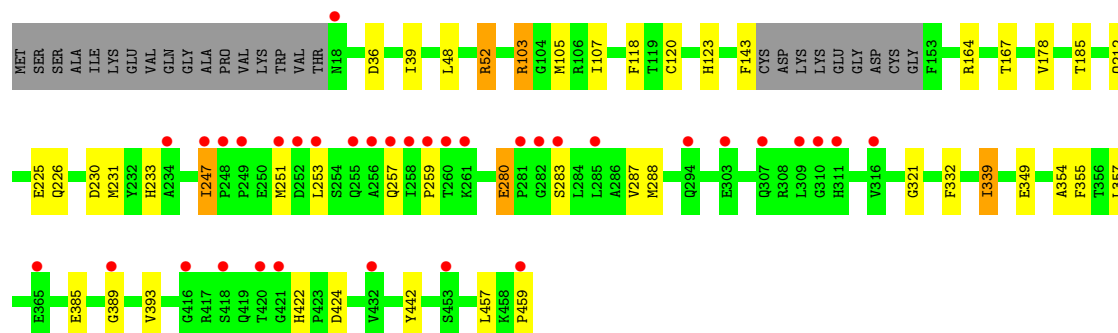
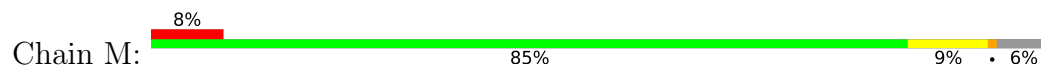
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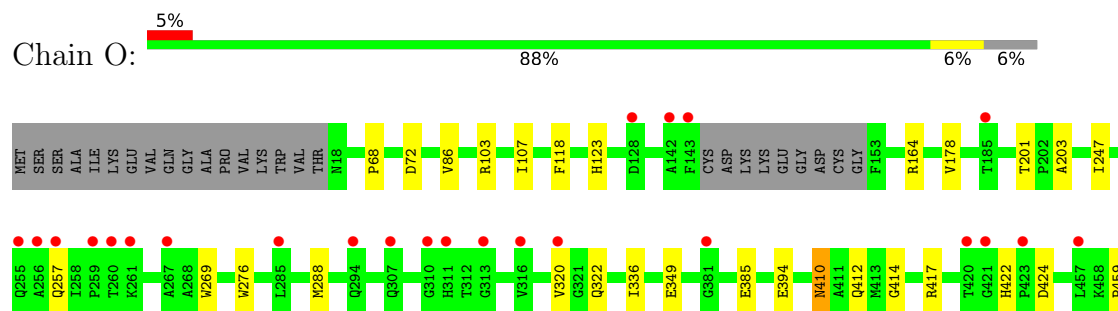
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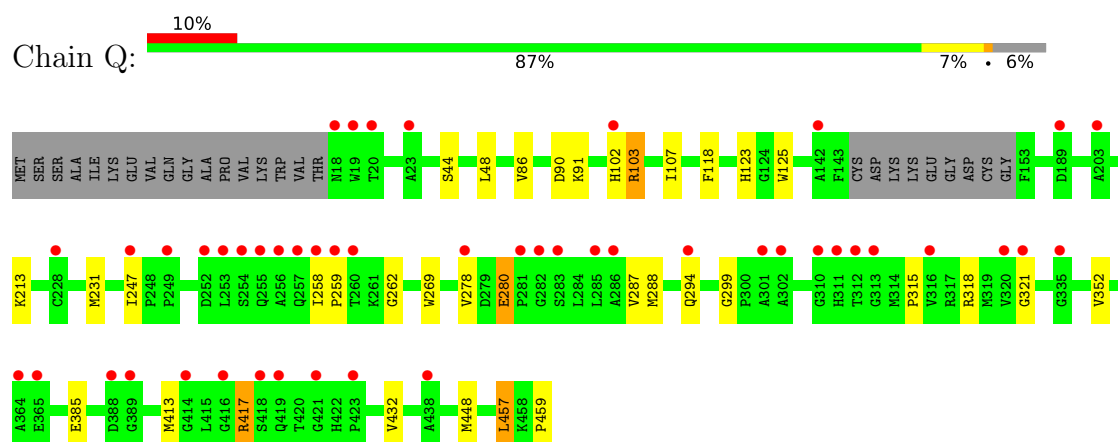
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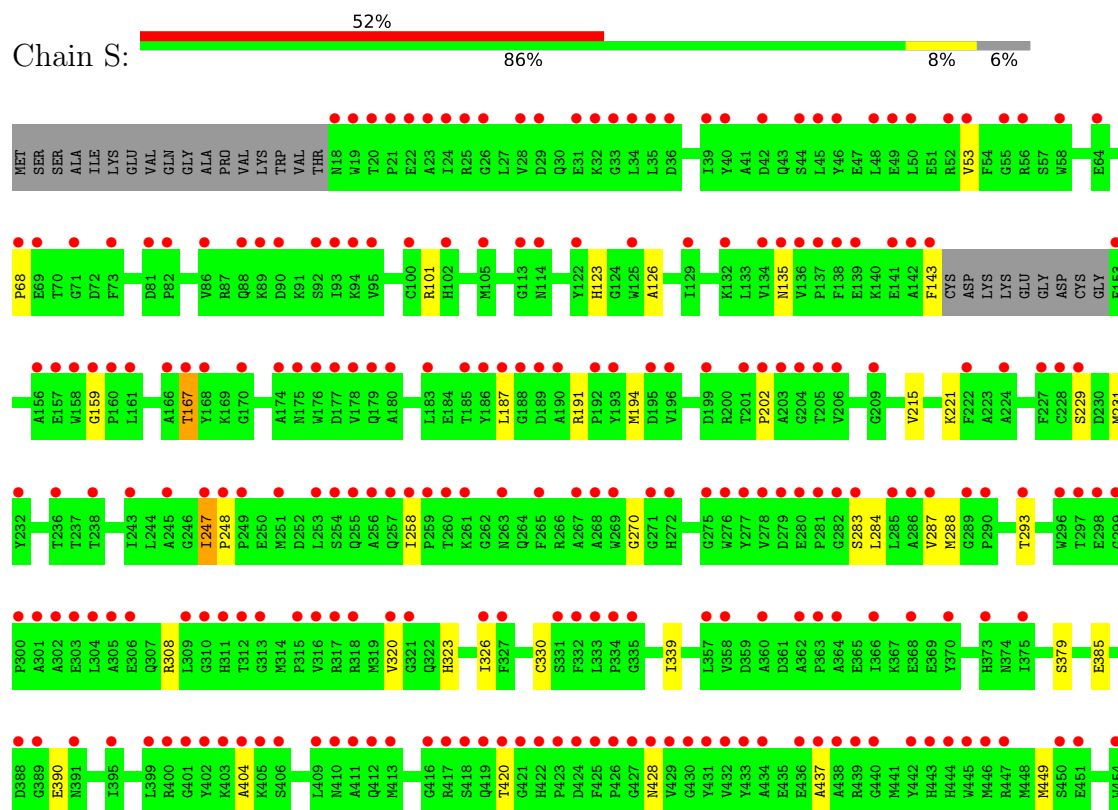
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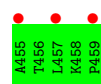


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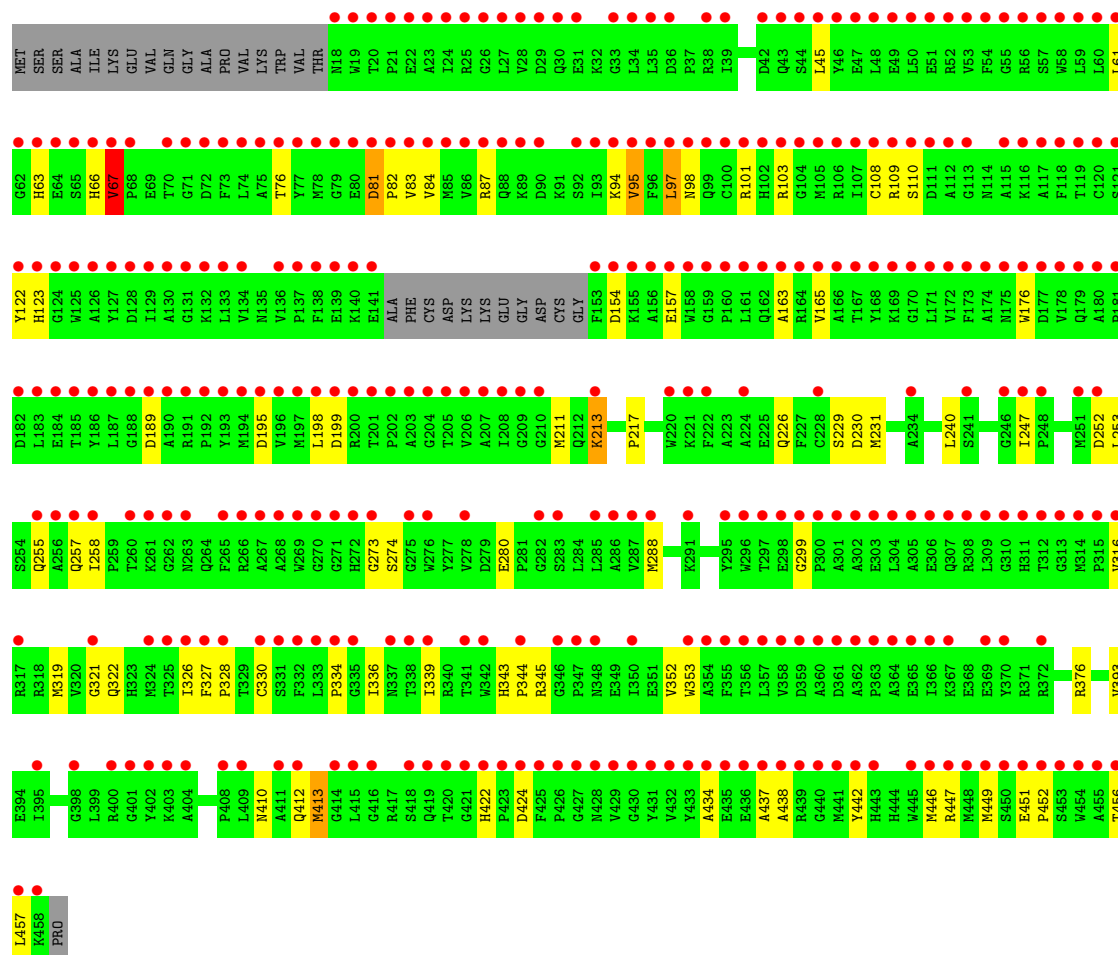
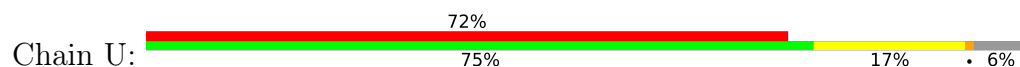


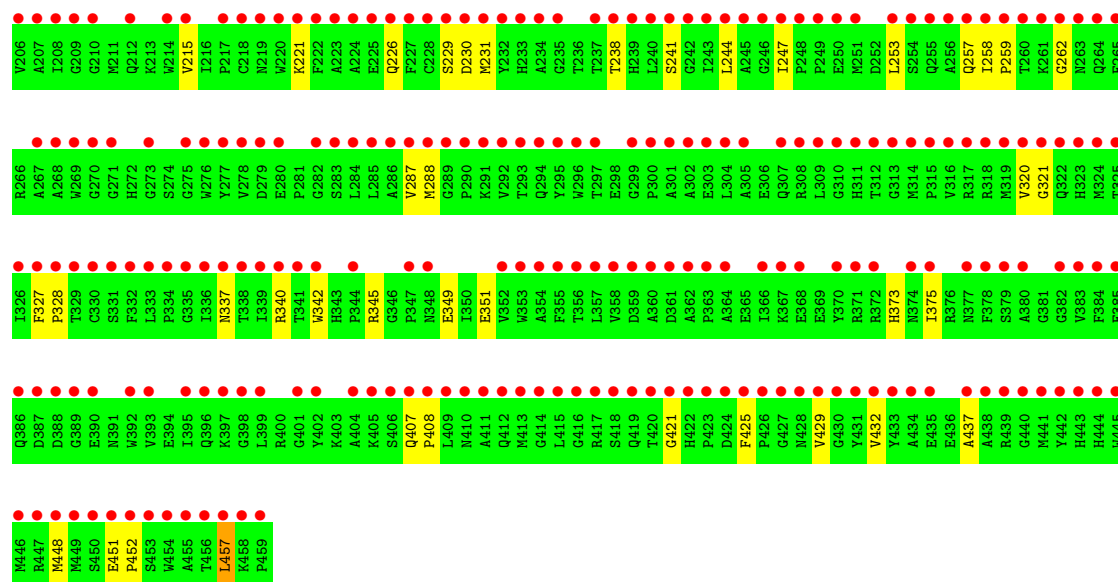
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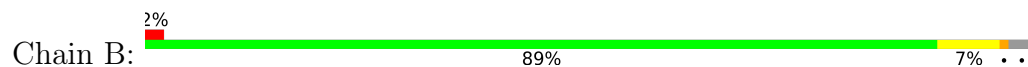


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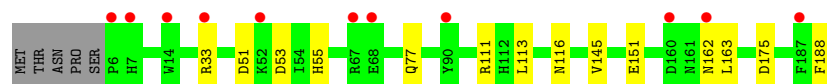
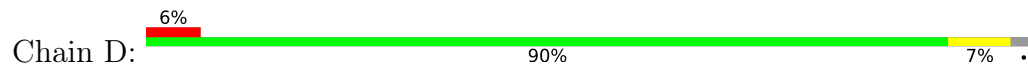




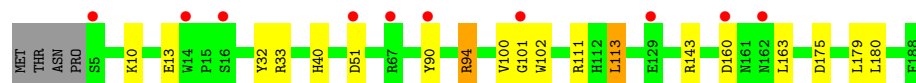
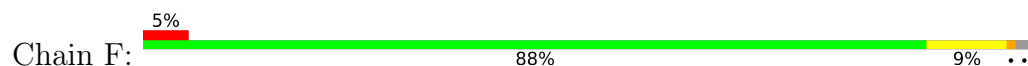
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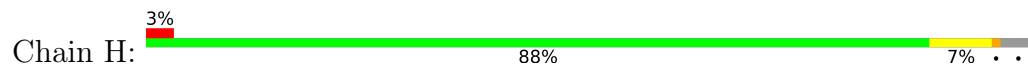
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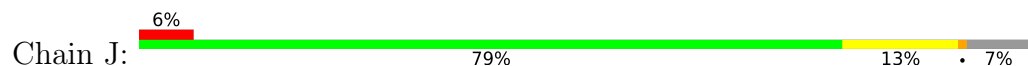
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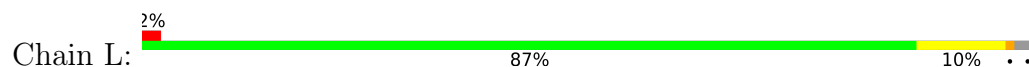


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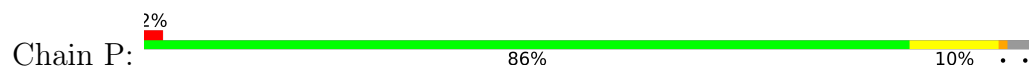
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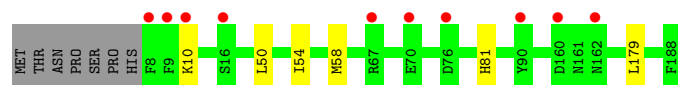
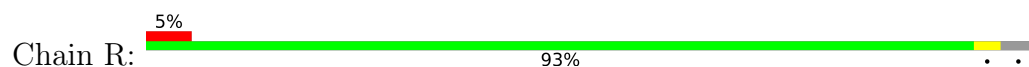
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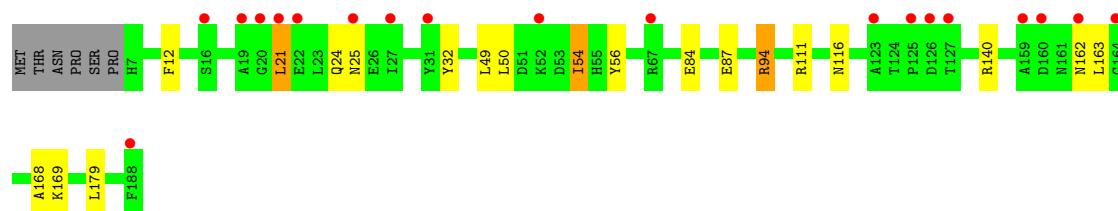
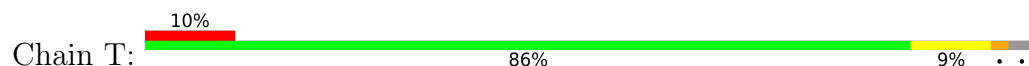
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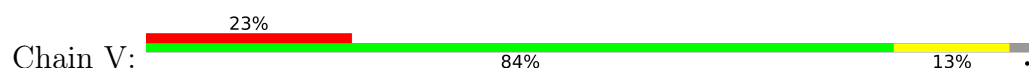
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

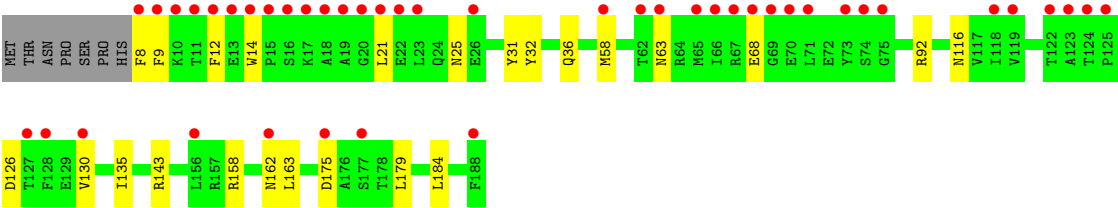


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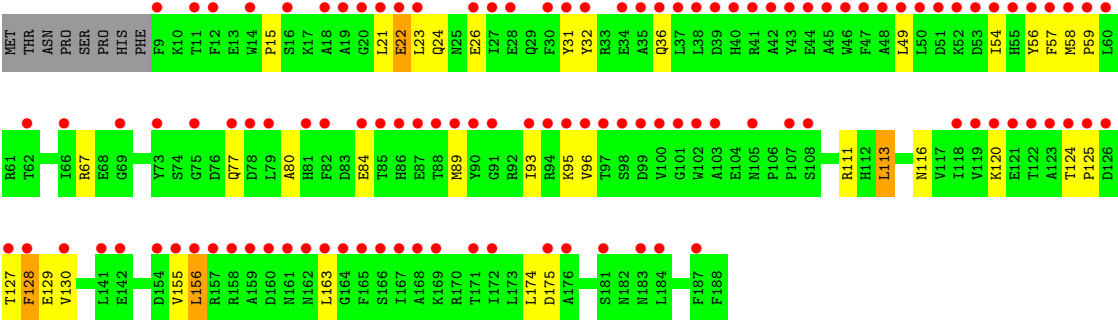
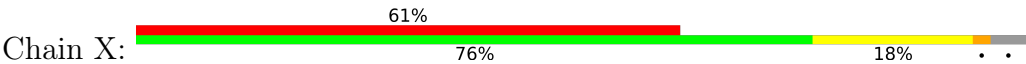


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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	132.77Å 133.19Å 133.97Å 102.31° 102.54° 104.54°	Depositor
Resolution (Å)	23.34 – 1.88 23.34 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.1 (23.34-1.88) 96.3 (23.34-1.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.225 , 0.263 0.225 , 0.263	Depositor DCC
R_{free} test set	32697 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for k,l,h 0.027 for l,h,k 0.013 for -k,-h,-l 0.018 for -l,-k,-h 0.016 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	63519	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, BNL, 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	0.49	0/3547	0.77	2/4814 (0.0%)
1	C	0.49	0/3549	0.78	2/4816 (0.0%)
1	E	0.48	0/3530	0.79	1/4792 (0.0%)
1	G	0.48	0/3530	0.78	0/4792
1	I	0.48	0/3538	0.77	2/4802 (0.0%)
1	K	0.46	0/3530	0.77	2/4792 (0.0%)
1	M	0.47	0/3539	0.76	0/4804
1	O	0.45	0/3538	0.76	0/4802
1	Q	0.45	0/3530	0.80	2/4792 (0.0%)
1	S	0.43	0/3530	0.78	0/4792
1	U	0.44	0/3505	0.82	8/4757 (0.2%)
1	W	0.42	0/3518	0.80	0/4776
2	B	0.48	0/1569	0.69	0/2121
2	D	0.49	0/1578	0.72	0/2133
2	F	0.50	0/1584	0.76	2/2142 (0.1%)
2	H	0.47	0/1550	0.71	0/2095
2	J	0.50	0/1489	0.72	0/2014
2	L	0.47	0/1561	0.71	0/2110
2	N	0.45	0/1561	0.70	0/2110
2	P	0.46	0/1566	0.72	0/2117
2	R	0.45	0/1542	0.71	0/2084
2	T	0.42	0/1553	0.71	0/2099
2	V	0.42	0/1542	0.71	0/2084
2	X	0.40	0/1538	0.74	0/2079
All	All	0.46	0/61017	0.76	21/82719 (0.0%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	343	HIS	CA-C-N	7.28	128.94	119.84
1	U	343	HIS	C-N-CA	7.28	128.94	119.84
1	E	422	HIS	N-CA-C	6.91	118.07	109.57
2	F	102	TRP	N-CA-C	6.56	118.43	111.28
1	U	81	ASP	CA-C-N	6.17	127.55	119.84
1	U	81	ASP	C-N-CA	6.17	127.55	119.84
1	A	299	GLY	CA-C-N	5.56	125.66	119.32
1	A	299	GLY	C-N-CA	5.56	125.66	119.32
1	K	299	GLY	CA-C-N	5.46	124.65	118.97
1	K	299	GLY	C-N-CA	5.46	124.65	118.97
1	U	299	GLY	CA-C-N	5.42	124.61	118.97
1	U	299	GLY	C-N-CA	5.42	124.61	118.97
2	F	100	VAL	N-CA-C	5.38	120.52	109.34
1	Q	299	GLY	CA-C-N	5.30	125.37	119.32
1	Q	299	GLY	C-N-CA	5.30	125.37	119.32
1	C	248	PRO	CA-C-N	5.07	125.36	119.47
1	C	248	PRO	C-N-CA	5.07	125.36	119.47
1	U	258	ILE	N-CA-C	5.07	112.17	107.56
1	U	345	ARG	N-CA-C	5.07	118.59	111.90
1	I	379	SER	N-CA-C	-5.06	101.22	108.60
1	I	230	ASP	N-CA-C	5.03	116.26	109.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	0	3300	21	0
1	C	3444	0	3305	13	0
1	E	3428	0	3284	19	0
1	G	3428	0	3284	19	0
1	I	3433	0	3293	27	0
1	K	3428	0	3284	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3434	0	3292	30	0
1	O	3433	0	3293	13	0
1	Q	3428	0	3284	19	0
1	S	3428	0	3284	26	0
1	U	3405	0	3263	50	0
1	W	3417	0	3275	31	0
2	B	1532	0	1474	15	0
2	D	1541	0	1479	12	0
2	F	1544	0	1484	16	0
2	H	1515	0	1459	17	0
2	J	1454	0	1407	24	0
2	L	1522	0	1467	19	0
2	N	1524	0	1471	15	0
2	P	1522	0	1473	15	0
2	R	1507	0	1456	4	0
2	T	1517	0	1463	20	0
2	V	1507	0	1456	21	0
2	X	1501	0	1451	32	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	3	0
3	I	4	0	0	0	0
3	K	4	0	0	0	0
3	M	4	0	0	1	0
3	O	4	0	0	1	0
3	Q	4	0	0	2	0
3	S	4	0	0	1	0
3	U	4	0	0	1	0
3	W	4	0	0	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
4	S	1	0	0	0	0
4	U	1	0	0	0	0
4	W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	12	0	10	3	0
5	E	12	0	10	1	0
5	I	12	0	10	0	0
5	K	12	0	10	0	0
5	M	12	0	10	1	0
5	O	12	0	10	0	0
5	Q	12	0	10	0	0
5	S	12	0	10	0	0
5	W	12	0	10	0	0
6	A	381	0	0	1	0
6	B	194	0	0	1	0
6	C	376	0	0	5	0
6	D	169	0	0	1	0
6	E	266	0	0	2	0
6	F	177	0	0	1	0
6	G	239	0	0	0	0
6	H	138	0	0	0	0
6	I	241	0	0	3	0
6	J	136	0	0	5	0
6	K	241	0	0	1	0
6	L	130	0	0	1	0
6	M	204	0	0	1	0
6	N	101	0	0	1	0
6	O	205	0	0	0	0
6	P	108	0	0	1	0
6	Q	150	0	0	0	0
6	R	124	0	0	0	0
6	S	95	0	0	4	0
6	T	73	0	0	0	0
6	U	107	0	0	5	0
6	V	54	0	0	0	0
6	W	73	0	0	0	0
6	X	35	0	0	1	0
All	All	63519	0	57071	426	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (426) 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)
1:E:167:THR:HB	6:E:2123:HOH:O	1.39	1.19
1:K:287:VAL:HG12	1:K:288:MET:HE3	1.25	1.17
2:F:94:ARG:HG2	2:F:94:ARG:HH11	1.22	1.03
2:X:128:PHE:O	2:X:155:VAL:O	1.77	1.02
1:K:287:VAL:HG12	1:K:288:MET:CE	1.90	1.00
1:M:339:ILE:HD11	1:M:357:LEU:HG	1.43	1.00
1:C:201:THR:HG22	1:C:203:ALA:H	1.29	0.95
1:G:259:PRO:HB3	1:G:280:GLU:HG2	1.46	0.94
2:B:113:LEU:HD21	2:L:113:LEU:HD22	1.46	0.94
1:A:252:ASP:H	1:A:255:GLN:HE21	0.94	0.94
1:E:287:VAL:HG12	1:E:288:MET:CE	2.01	0.90
1:E:287:VAL:HG12	1:E:288:MET:HE3	1.52	0.90
2:T:25:ASN:HD21	2:X:24:GLN:HG2	1.39	0.87
1:S:270:GLY:HA2	6:S:2059:HOH:O	1.73	0.87
5:E:462:BNL:H15	6:E:2167:HOH:O	1.75	0.85
1:G:120:CYS:SG	3:G:460:FES:FE1	1.69	0.85
1:Q:287:VAL:HG12	1:Q:288:MET:HE3	1.59	0.84
1:S:53:VAL:HG23	6:S:2092:HOH:O	1.80	0.82
2:T:94:ARG:HG3	2:T:94:ARG:HH11	1.43	0.82
1:G:287:VAL:HG12	1:G:288:MET:CE	2.10	0.81
1:K:287:VAL:CG1	1:K:288:MET:HE3	2.06	0.81
1:A:252:ASP:H	1:A:255:GLN:NE2	1.77	0.80
1:M:259:PRO:HB3	1:M:280:GLU:HG2	1.64	0.79
1:G:287:VAL:HG12	1:G:288:MET:HE3	1.65	0.79
1:Q:102:HIS:O	3:Q:460:FES:S1	2.41	0.78
1:U:274:SER:HB2	6:U:2086:HOH:O	1.81	0.78
1:M:339:ILE:CD1	1:M:357:LEU:HG	2.12	0.77
1:U:97:LEU:HD22	1:U:176:TRP:CH2	2.20	0.77
1:S:123:HIS:HB2	3:S:460:FES:S2	2.24	0.76
1:M:52:ARG:CG	1:M:52:ARG:HH11	1.99	0.76
1:A:252:ASP:N	1:A:255:GLN:HE21	1.78	0.76
2:T:12:PHE:H	2:V:36:GLN:HE21	1.33	0.76
1:Q:417:ARG:HG3	1:Q:417:ARG:HH11	1.49	0.75
2:T:94:ARG:HH11	2:T:94:ARG:CG	1.98	0.75
2:J:33:ARG:NE	6:J:2016:HOH:O	2.20	0.75
1:U:195:ASP:HA	6:U:2058:HOH:O	1.87	0.73
2:D:188:PHE:C	6:D:2063:HOH:O	2.32	0.72
2:F:90:TYR:CE2	2:F:94:ARG:HD2	2.23	0.72
1:S:287:VAL:HG12	1:S:288:MET:HE3	1.72	0.72
1:C:422:HIS:HD2	1:C:424:ASP:H	1.38	0.71
2:X:31:TYR:HE2	2:X:130:VAL:HG11	1.55	0.71
1:S:247:ILE:HG13	1:S:248:PRO:HD2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:94:LYS:HA	1:U:165:VAL:HG21	1.74	0.69
2:T:32:TYR:CD1	2:X:116:ASN:HA	2.28	0.69
2:H:58:MET:CE	2:H:174:LEU:HD22	2.21	0.69
6:A:2122:HOH:O	1:O:394:GLU:HG3	1.91	0.69
1:W:226:GLN:HA	1:W:230:ASP:HB3	1.75	0.69
1:U:61:LEU:HB3	1:U:76:THR:HG21	1.75	0.68
2:H:9:PHE:O	2:H:10:LYS:HG2	1.92	0.68
1:M:52:ARG:HH11	1:M:52:ARG:HG3	1.58	0.68
1:G:100:CYS:SG	3:G:460:FES:FE1	1.85	0.68
1:U:67:VAL:HG23	1:U:87:ARG:HB2	1.76	0.68
1:M:107:ILE:HG22	1:M:118:PHE:HB3	1.75	0.68
2:T:25:ASN:ND2	2:X:24:GLN:HG2	2.10	0.67
1:I:287:VAL:HG12	1:I:288[A]:MET:HE3	1.75	0.67
1:W:100:CYS:SG	3:W:460:FES:FE1	1.86	0.67
2:B:36:GLN:HE21	2:L:12:PHE:H	1.41	0.67
2:B:22:GLU:CD	2:B:22:GLU:H	2.01	0.67
2:H:58:MET:HE2	2:H:81:HIS:CD2	2.30	0.66
1:Q:287:VAL:HG12	1:Q:288:MET:CE	2.25	0.66
2:H:58:MET:HE1	2:H:174:LEU:HD22	1.76	0.66
2:J:14:TRP:HB2	2:J:15:PRO:HD3	1.77	0.66
1:A:422:HIS:HD2	1:A:424:ASP:H	1.42	0.66
1:I:309:LEU:HD12	1:I:316:VAL:HG21	1.77	0.66
2:X:56:TYR:HB3	2:X:84:GLU:HB2	1.79	0.65
1:W:345:ARG:HB2	1:W:349:GLU:HG3	1.79	0.65
2:X:84:GLU:HG3	2:X:89:MET:HE3	1.79	0.65
2:V:12:PHE:O	2:V:14:TRP:HE3	1.80	0.64
2:T:24:GLN:HG2	2:V:25:ASN:HD21	1.63	0.64
1:U:82:PRO:HB2	1:U:98:ASN:HB3	1.79	0.64
1:U:123:HIS:HB2	3:U:460:FES:S2	2.37	0.64
1:U:63:HIS:H	1:U:66:HIS:HD2	1.43	0.64
2:R:58:MET:HE2	2:R:81:HIS:CB	2.28	0.63
1:G:123:HIS:HB2	3:G:460:FES:S2	2.38	0.63
1:Q:417:ARG:HH11	1:Q:417:ARG:CG	2.11	0.63
1:I:201:THR:HG22	1:I:203:ALA:H	1.61	0.63
2:L:58:MET:HE2	2:L:81:HIS:CB	2.29	0.62
1:E:247:ILE:HD12	1:E:251:MET:HB3	1.81	0.62
1:O:164:ARG:HD2	1:O:178:VAL:HA	1.81	0.62
2:D:151:GLU:OE1	2:J:40:HIS:HE1	1.80	0.62
1:S:101:ARG:HD3	1:S:159:GLY:O	1.99	0.62
1:E:287:VAL:HG12	1:E:288:MET:HE2	1.79	0.62
1:M:52:ARG:HG3	1:M:52:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:247:ILE:HG13	1:I:248:PRO:HD2	1.82	0.61
1:S:229:SER:HB2	1:S:437:ALA:HB3	1.81	0.61
2:F:94:ARG:HH11	2:F:94:ARG:CG	2.05	0.61
1:S:231:MET:HG2	1:S:323:HIS:CD2	2.36	0.61
2:H:36:GLN:HE21	2:N:12:PHE:H	1.49	0.60
1:M:247:ILE:HG23	1:M:251:MET:HB3	1.83	0.60
1:S:187:LEU:HD22	1:S:194:MET:HE1	1.84	0.60
1:W:287:VAL:HG12	1:W:288:MET:HE3	1.84	0.60
5:C:462:BNL:C15	6:C:2244:HOH:O	2.49	0.60
2:T:12:PHE:H	2:V:36:GLN:NE2	1.99	0.59
2:T:49:LEU:HD21	2:T:163:LEU:HD13	1.83	0.59
1:G:287:VAL:HG12	1:G:288:MET:HE2	1.84	0.59
1:O:123:HIS:HB2	3:O:460:FES:S2	2.42	0.59
2:N:58:MET:HE3	2:N:81:HIS:CB	2.33	0.58
2:N:58:MET:CE	2:N:81:HIS:CB	2.81	0.58
2:B:12:PHE:H	2:P:36:GLN:HE21	1.49	0.58
2:J:33:ARG:CZ	6:J:2016:HOH:O	2.52	0.58
2:H:50:LEU:HD22	2:H:54:ILE:HD12	1.84	0.58
2:L:158:ARG:HD3	6:L:2124:HOH:O	2.04	0.58
1:M:332:PHE:HB3	1:M:339:ILE:HG23	1.84	0.58
2:B:36:GLN:NE2	2:L:12:PHE:H	2.02	0.58
1:W:107:ILE:HG22	1:W:118:PHE:HB3	1.85	0.58
2:X:49:LEU:HD21	2:X:163:LEU:HD13	1.85	0.58
2:D:111:ARG:HB2	2:F:175:ASP:OD2	2.04	0.58
2:D:175:ASP:OD2	2:J:111:ARG:HB2	2.04	0.58
2:N:58:MET:CE	2:N:81:HIS:HB3	2.34	0.57
2:V:8:PHE:HD1	2:V:9:PHE:H	1.50	0.57
1:A:231:MET:HE1	1:A:321:GLY:O	2.04	0.57
2:J:33:ARG:NH1	6:J:2029:HOH:O	2.37	0.57
2:N:58:MET:HE1	2:N:184:LEU:HD13	1.87	0.57
2:X:15:PRO:HG3	2:X:120:LYS:HA	1.85	0.57
2:V:126:ASP:HB3	2:V:158:ARG:HB2	1.86	0.57
2:F:143:ARG:NH2	1:I:349:GLU:OE2	2.38	0.57
2:X:58:MET:HE3	2:X:174:LEU:HD22	1.87	0.57
1:M:259:PRO:HG2	1:M:283:SER:HB3	1.87	0.56
2:X:89:MET:HE2	2:X:89:MET:HA	1.86	0.56
2:D:33:ARG:HD2	2:D:163:LEU:HG	1.86	0.56
2:F:40:HIS:HE1	2:J:151:GLU:OE1	1.88	0.56
2:H:50:LEU:HD22	2:H:54:ILE:CD1	2.35	0.56
6:F:2014:HOH:O	2:N:67:ARG:HD3	2.05	0.56
1:G:107:ILE:HG22	1:G:118:PHE:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:231:MET:HE1	1:U:321:GLY:O	2.06	0.56
6:C:2325:HOH:O	2:D:77:GLN:NE2	2.38	0.56
1:E:287:VAL:CG1	1:E:288:MET:HE3	2.29	0.56
2:T:50:LEU:HD22	2:T:54:ILE:HD12	1.87	0.56
2:H:32:TYR:CD1	2:N:116:ASN:HA	2.41	0.56
1:Q:231:MET:HE1	1:Q:321:GLY:O	2.06	0.56
1:Q:448:MET:HA	1:Q:457:LEU:HD11	1.88	0.56
1:M:185:THR:HG22	1:M:459:PRO:HG2	1.88	0.55
1:U:288:MET:HE3	1:U:336:ILE:HG23	1.87	0.55
1:K:217:PRO:HG2	1:K:393:VAL:HG22	1.87	0.55
1:S:215:VAL:HG21	2:V:143:ARG:HD3	1.88	0.55
1:U:123:HIS:HE2	1:W:230:ASP:CG	2.14	0.55
2:T:32:TYR:CG	2:X:116:ASN:HA	2.41	0.55
1:I:422:HIS:HD2	1:I:424:ASP:H	1.55	0.55
1:O:68:PRO:HD2	1:O:72:ASP:OD2	2.07	0.55
2:P:9:PHE:O	2:P:10:LYS:HG2	2.07	0.55
1:I:287:VAL:HG12	1:I:288[A]:MET:CE	2.37	0.54
1:A:123:HIS:HB2	3:A:460:FES:S2	2.48	0.54
2:F:94:ARG:HG2	2:F:94:ARG:NH1	2.02	0.54
1:E:422:HIS:HD2	1:E:424:ASP:H	1.55	0.54
1:G:231:MET:HE1	1:G:321:GLY:O	2.08	0.53
2:L:143:ARG:NH2	1:O:349:GLU:OE2	2.39	0.53
1:G:422:HIS:HD2	1:G:424:ASP:H	1.56	0.53
1:K:287:VAL:HG12	1:K:288:MET:HE2	1.88	0.53
1:I:422:HIS:CD2	1:I:424:ASP:H	2.27	0.53
1:A:414:GLY:HA2	1:A:417:ARG:HD2	1.90	0.53
1:M:231:MET:HE1	1:M:321:GLY:O	2.09	0.53
1:O:201:THR:HG22	1:O:203:ALA:H	1.73	0.53
1:W:164:ARG:HD2	1:W:178:VAL:HA	1.90	0.53
1:Q:107:ILE:HG22	1:Q:118:PHE:HB3	1.90	0.53
1:Q:123:HIS:HB2	3:Q:460:FES:S2	2.48	0.53
2:T:21:LEU:HB2	2:X:21:LEU:HD21	1.90	0.52
2:F:113:LEU:HD13	2:J:135:ILE:HG13	1.91	0.52
6:I:2205:HOH:O	2:J:77:GLN:NE2	2.43	0.52
2:T:56:TYR:HB3	2:T:84:GLU:HB2	1.90	0.52
2:B:116:ASN:HA	2:P:32:TYR:CD1	2.45	0.52
1:Q:259:PRO:HB3	1:Q:280:GLU:HG2	1.90	0.52
2:R:50:LEU:HD22	2:R:54:ILE:HD13	1.90	0.52
1:E:259:PRO:HB3	1:E:280:GLU:HG2	1.91	0.52
2:T:116:ASN:HA	2:V:32:TYR:CD1	2.45	0.52
1:U:198:LEU:HB2	6:U:2058:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:413:MET:HB3	1:U:434:ALA:HA	1.92	0.51
1:M:287:VAL:HG21	5:M:462:BNL:H5	1.93	0.51
1:U:63:HIS:H	1:U:66:HIS:CD2	2.27	0.51
1:U:61:LEU:HB2	6:U:2023:HOH:O	2.09	0.51
2:V:135:ILE:HG13	2:X:113:LEU:HD13	1.92	0.51
1:C:414:GLY:HA2	1:C:417:ARG:HD2	1.91	0.51
1:W:425:PHE:HB2	1:W:429:VAL:HG21	1.92	0.51
1:O:414:GLY:HA2	1:O:417:ARG:HD2	1.93	0.51
1:S:283:SER:O	1:S:287:VAL:HG23	2.11	0.51
2:V:175:ASP:OD2	2:X:111:ARG:HB2	2.11	0.51
2:D:53[B]:ASP:O	2:D:55:HIS:HD2	1.94	0.51
2:X:130:VAL:HG21	2:X:156:LEU:HD12	1.92	0.51
1:K:232:TYR:CD1	1:K:413:MET:HE1	2.46	0.51
2:H:58:MET:HE3	2:H:174:LEU:HD22	1.92	0.50
1:C:349:GLU:OE2	2:J:143:ARG:NH2	2.40	0.50
1:U:45:LEU:HD22	1:U:449:MET:HE1	1.92	0.50
1:U:322:GLN:HB3	1:U:334:PRO:HG2	1.93	0.50
2:H:22:GLU:H	2:H:22:GLU:CD	2.20	0.50
1:U:252:ASP:H	1:U:255:GLN:HE21	1.59	0.50
2:F:111:ARG:HB2	2:J:175:ASP:OD2	2.12	0.50
1:I:243:ILE:HD13	1:I:384:PHE:HZ	1.77	0.50
2:T:111:ARG:HB2	2:X:175:ASP:OD2	2.12	0.50
1:A:77:TYR:OH	2:P:142:GLU:OE2	2.30	0.50
1:C:240:LEU:O	1:C:253:LEU:HD21	2.12	0.50
1:U:95:VAL:HG12	1:U:165:VAL:HG22	1.94	0.50
1:U:217:PRO:HD2	1:U:393:VAL:HG22	1.93	0.50
1:A:251:MET:HG2	1:A:255:GLN:HG3	1.94	0.50
1:K:164:ARG:HD2	1:K:178:VAL:HA	1.94	0.50
1:S:390:GLU:OE2	2:T:140:ARG:NH2	2.45	0.50
1:G:239:HIS:O	1:G:243:ILE:HG12	2.11	0.49
1:A:349:GLU:OE2	2:P:143:ARG:NH2	2.34	0.49
1:G:287:VAL:CG1	1:G:288:MET:HE3	2.39	0.49
2:H:148:PHE:HB3	2:H:174:LEU:HD11	1.95	0.49
1:S:231:MET:HG2	1:S:323:HIS:HD2	1.76	0.49
1:M:123:HIS:HB2	3:M:460:FES:S2	2.53	0.49
2:B:12:PHE:H	2:P:36:GLN:NE2	2.09	0.49
1:C:123:HIS:HB2	3:C:460:FES:S2	2.53	0.49
1:Q:269:TRP:CG	1:Q:459:PRO:HB3	2.48	0.49
1:G:414:GLY:HA2	1:G:417:ARG:HD2	1.95	0.49
2:B:143:ARG:NH2	1:K:349:GLU:OE2	2.36	0.48
1:M:212:GLN:HG3	1:M:354:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:123:HIS:HB2	3:W:460:FES:S2	2.53	0.48
2:H:111:ARG:HB2	2:N:175:ASP:OD2	2.13	0.48
1:S:191:ARG:HA	1:S:194:MET:HE3	1.95	0.48
1:U:213:LYS:HA	1:U:352:VAL:O	2.13	0.48
2:R:58:MET:HE2	2:R:81:HIS:HB2	1.95	0.48
1:U:154:ASP:HB3	1:U:157:GLU:HB2	1.95	0.48
1:K:107:ILE:HG22	1:K:118:PHE:HB3	1.95	0.48
1:O:288[A]:MET:HE3	1:O:336:ILE:HG23	1.95	0.48
1:U:67:VAL:CG2	1:U:87:ARG:HB2	2.41	0.48
1:I:107:ILE:HG22	1:I:118:PHE:HB3	1.95	0.48
2:J:54:ILE:HA	2:J:168:ALA:O	2.14	0.48
2:L:36:GLN:HE21	2:P:12:PHE:H	1.60	0.48
1:S:326:ILE:HB	1:S:330:CYS:HB3	1.96	0.48
1:W:241:SER:HB2	2:X:95:LYS:HG3	1.94	0.48
2:J:51:ASP:OD2	2:J:166:SER:OG	2.20	0.48
1:Q:417:ARG:CG	1:Q:417:ARG:NH1	2.76	0.48
6:B:2132:HOH:O	2:L:67:ARG:HG2	2.14	0.48
1:M:233:HIS:CE1	6:M:2132:HOH:O	2.56	0.48
1:W:229:SER:HB2	1:W:437:ALA:HB3	1.94	0.48
1:S:449:MET:HG2	6:S:2092:HOH:O	2.12	0.48
2:D:51:ASP:OD2	2:D:53[A]:ASP:OD1	2.32	0.47
2:F:10:LYS:HD2	2:F:13:GLU:OE1	2.14	0.47
1:G:212:GLN:OE1	1:G:379:SER:HA	2.14	0.47
1:M:259:PRO:CB	1:M:280:GLU:HG2	2.41	0.47
2:V:162:ASN:HB3	2:V:163:LEU:HD12	1.96	0.47
1:M:36:ASP:O	1:M:39:ILE:HG12	2.14	0.47
1:S:143:PHE:CZ	1:U:413:MET:HG2	2.49	0.47
1:S:287:VAL:HG12	1:S:288:MET:CE	2.41	0.47
1:M:287:VAL:HG12	1:M:288:MET:HE3	1.95	0.47
2:H:113:LEU:HD21	2:N:113:LEU:HD23	1.97	0.47
1:O:410:ASN:ND2	1:O:412:GLN:H	2.13	0.47
2:V:179:LEU:HD21	2:V:184:LEU:HD11	1.97	0.47
1:A:131:GLY:O	1:A:160:PRO:HD2	2.15	0.47
1:K:105:MET:HB3	1:K:120:CYS:SG	2.54	0.47
1:I:252:ASP:H	1:I:255:GLN:HE21	1.63	0.47
1:S:126:ALA:HB3	1:S:135:ASN:HB3	1.97	0.47
1:G:410:ASN:ND2	1:G:412:GLN:H	2.13	0.46
2:V:58:MET:HE1	2:V:184:LEU:HD13	1.97	0.46
2:T:21:LEU:HD13	2:V:21:LEU:HB2	1.96	0.46
1:W:340:ARG:HD2	1:W:342:TRP:CH2	2.50	0.46
5:C:462:BNL:H15	6:C:2244:HOH:O	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:169:LYS:HE2	1:I:199:ASP:CG	2.39	0.46
2:V:31:TYR:HE2	2:V:130:VAL:HG11	1.81	0.46
2:H:143:ARG:NH2	1:M:349:GLU:OE2	2.42	0.46
1:G:215:VAL:O	2:H:182:ASN:HA	2.16	0.46
1:E:265:PHE:CZ	1:E:267:ALA:HA	2.50	0.46
1:K:244:LEU:HD13	1:K:253:LEU:HG	1.96	0.46
2:N:58:MET:HE2	2:N:81:HIS:CB	2.46	0.46
1:I:105:MET:HB3	1:I:120:CYS:SG	2.56	0.46
1:I:201:THR:HG21	1:I:361:ASP:OD1	2.16	0.46
1:O:422:HIS:HD2	1:O:424:ASP:H	1.64	0.46
2:X:31:TYR:HE2	2:X:130:VAL:CG1	2.27	0.46
1:U:226:GLN:HG3	1:U:230:ASP:HB3	1.97	0.45
2:X:120:LYS:HB3	2:X:129:GLU:O	2.16	0.45
1:I:217:PRO:HG2	1:I:393:VAL:HG22	1.97	0.45
1:K:422:HIS:HD2	1:K:424:ASP:H	1.63	0.45
2:B:175:ASP:OD2	2:P:111:ARG:HB2	2.16	0.45
2:L:49:LEU:HD21	2:L:163:LEU:HD13	1.97	0.45
2:N:58:MET:HE2	2:N:81:HIS:HB3	1.98	0.45
1:W:375:ILE:HG12	2:X:80:ALA:H	1.81	0.45
2:F:143:ARG:HD3	1:I:215:VAL:HG21	1.97	0.45
2:J:50:LEU:HD22	2:J:54:ILE:HD13	1.98	0.45
2:F:32:TYR:CD1	2:J:116:ASN:HA	2.52	0.45
1:W:49:GLU:OE2	1:W:221:LYS:NZ	2.49	0.45
1:W:215:VAL:HG22	1:W:351:GLU:HG2	1.98	0.45
2:B:32:TYR:CD1	2:L:116:ASN:HA	2.52	0.45
2:L:111:ARG:HB2	2:P:175:ASP:OD2	2.17	0.45
1:W:241:SER:HB2	2:X:95:LYS:CG	2.47	0.45
2:J:90:TYR:HE1	2:J:94:ARG:HD2	1.81	0.45
2:L:32:TYR:CD1	2:P:116:ASN:HA	2.51	0.45
1:I:164:ARG:HD2	1:I:178:VAL:HA	1.98	0.45
1:Q:262:GLY:HA2	1:Q:278:VAL:HG23	1.98	0.44
1:E:269:TRP:CZ2	1:E:444:HIS:HE1	2.35	0.44
1:I:372:ARG:HG3	6:I:2207:HOH:O	2.17	0.44
1:S:167:THR:HG23	6:S:2011:HOH:O	2.17	0.44
1:A:192:PRO:HB3	1:A:312:THR:HG21	1.99	0.44
1:W:244:LEU:HD13	1:W:253:LEU:HG	2.00	0.44
1:W:451:GLU:HA	1:W:452:PRO:HD3	1.88	0.44
1:M:226:GLN:HA	1:M:230:ASP:HB3	2.00	0.44
2:B:14:TRP:CD2	2:P:33:ARG:HG2	2.53	0.44
2:T:94:ARG:CG	2:T:94:ARG:NH1	2.66	0.44
1:W:20:THR:O	1:W:24:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:HIS:HB2	3:E:460:FES:S2	2.58	0.44
1:M:422:HIS:HD2	1:M:424:ASP:H	1.64	0.44
2:J:33:ARG:NH2	6:J:2016:HOH:O	2.50	0.44
1:U:252:ASP:H	1:U:255:GLN:NE2	2.16	0.44
2:V:12:PHE:H	2:X:36:GLN:HE21	1.64	0.44
2:X:58:MET:CE	2:X:174:LEU:HD22	2.48	0.44
1:C:217:PRO:HD2	1:C:393:VAL:HG22	1.99	0.44
1:C:382:GLY:O	1:C:386:GLN:HG3	2.18	0.44
1:C:422:HIS:CD2	1:C:424:ASP:H	2.26	0.44
2:X:93:ILE:HA	2:X:96:VAL:HG12	1.99	0.44
1:K:239:HIS:CD2	6:K:2161:HOH:O	2.69	0.43
1:W:288:MET:HE2	1:W:373:HIS:HB3	2.00	0.43
2:P:131:ASN:ND2	6:P:2075:HOH:O	2.50	0.43
1:Q:90:ASP:O	1:Q:91:LYS:HB2	2.18	0.43
2:T:24:GLN:HG2	2:V:25:ASN:ND2	2.31	0.43
2:V:116:ASN:HA	2:X:32:TYR:CD1	2.54	0.43
2:L:126:ASP:OD1	2:L:158:ARG:NH1	2.51	0.43
1:C:201:THR:HG23	1:C:202:PRO:HD2	2.00	0.43
1:I:373:HIS:HD2	1:I:376:ARG:HE	1.65	0.43
1:O:269:TRP:CD2	1:O:459:PRO:HG3	2.54	0.43
2:P:148:PHE:HB3	2:P:174:LEU:HD11	1.99	0.43
2:T:54:ILE:HA	2:T:168:ALA:O	2.18	0.43
1:A:410:ASN:HD21	1:A:412:GLN:HB2	1.84	0.43
2:N:131:ASN:ND2	6:N:2071:HOH:O	2.51	0.43
2:X:124:THR:HA	2:X:125:PRO:HD3	1.90	0.43
1:C:212:GLN:HG3	1:C:354:ALA:HB3	1.99	0.43
1:U:81:ASP:HA	1:U:82:PRO:HD2	1.86	0.43
1:U:95:VAL:HG13	1:U:163:ALA:HB3	2.00	0.43
1:U:273:GLY:HA3	1:U:437:ALA:HB1	2.01	0.43
1:A:410:ASN:ND2	1:A:412:GLN:H	2.16	0.43
1:E:197:MET:HB2	1:E:334:PRO:HB3	2.01	0.43
2:H:32:TYR:CG	2:N:116:ASN:HA	2.54	0.43
1:M:164:ARG:HD2	1:M:178:VAL:HA	2.00	0.43
2:X:22:GLU:HG3	6:X:2005:HOH:O	2.17	0.43
2:D:116:ASN:HA	2:J:32:TYR:CD1	2.53	0.43
1:I:239:HIS:CD2	6:I:2142:HOH:O	2.60	0.43
1:O:107:ILE:HG22	1:O:118:PHE:HB3	2.01	0.43
1:W:197:MET:HG3	1:W:337:ASN:ND2	2.33	0.43
1:U:326:ILE:N	1:U:330:CYS:O	2.48	0.43
2:F:33:ARG:NH2	2:F:163:LEU:O	2.52	0.42
1:G:136:VAL:O	1:G:139:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:105:MET:HB3	1:M:120:CYS:SG	2.58	0.42
1:Q:213:LYS:HA	1:Q:352:VAL:O	2.19	0.42
1:M:225:GLU:OE1	1:M:442:TYR:OH	2.35	0.42
1:M:339:ILE:HD12	1:M:355:PHE:O	2.18	0.42
1:Q:102:HIS:HB2	1:Q:125:TRP:CH2	2.54	0.42
1:E:448:MET:HA	1:E:457:LEU:HD11	2.00	0.42
1:K:390:GLU:O	1:K:394:GLU:HG3	2.19	0.42
2:L:179:LEU:HD21	2:L:184:LEU:HD11	2.02	0.42
2:F:32:TYR:CG	2:J:116:ASN:HA	2.55	0.42
1:G:422:HIS:CD2	1:G:424:ASP:H	2.35	0.42
1:I:61:LEU:CD1	1:I:95:VAL:HG21	2.49	0.42
2:B:111:ARG:HB2	2:L:175:ASP:OD2	2.19	0.42
1:U:213:LYS:HG2	1:U:353:TRP:CE2	2.55	0.42
1:U:327:PHE:CG	1:U:328:PRO:HA	2.55	0.42
1:W:327:PHE:HA	1:W:328:PRO:HA	1.84	0.42
1:A:259:PRO:HB2	1:A:277:TYR:CE1	2.54	0.42
1:A:382:GLY:O	1:A:386:GLN:HG3	2.19	0.42
1:I:390:GLU:O	1:I:394:GLU:HG3	2.20	0.42
1:W:231:MET:HE1	1:W:321:GLY:O	2.19	0.42
1:E:422:HIS:CD2	1:E:424:ASP:H	2.35	0.42
2:L:50:LEU:HD22	2:L:54:ILE:HD13	2.01	0.42
2:N:58:MET:CE	2:N:81:HIS:HB2	2.48	0.42
1:U:446:MET:SD	1:U:446:MET:C	3.03	0.42
1:U:451:GLU:HA	1:U:452:PRO:HD3	1.90	0.42
1:E:212:GLN:HG3	1:E:354:ALA:HB3	2.01	0.42
2:J:143:ARG:HD2	6:J:2113:HOH:O	2.20	0.42
2:L:58:MET:HE2	2:L:81:HIS:HB2	1.99	0.42
1:Q:44:SER:O	1:Q:48:LEU:HD23	2.19	0.42
1:U:199:ASP:HB2	6:U:2058:HOH:O	2.20	0.42
2:X:49:LEU:HD11	2:X:163:LEU:HD22	2.00	0.42
1:C:77:TYR:OH	2:J:142:GLU:OE2	2.35	0.42
1:C:212:GLN:NE2	6:C:2233:HOH:O	2.51	0.42
1:Q:315:PRO:HB2	1:Q:318:ARG:HD3	2.01	0.42
1:U:84:VAL:HG21	1:U:108:CYS:HB3	2.00	0.42
1:W:126:ALA:HB3	1:W:135:ASN:HB3	2.01	0.42
2:J:53:ASP:OD2	2:J:157:ARG:NH2	2.42	0.42
1:O:276:TRP:HB3	1:O:322:GLN:HG3	2.02	0.41
1:S:420:THR:HA	1:S:428:ASN:HA	2.02	0.41
1:U:288:MET:HE3	1:U:336:ILE:HG12	2.02	0.41
1:U:412:GLN:O	1:U:413:MET:C	2.63	0.41
2:X:89:MET:O	2:X:93:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:HIS:O	1:A:243:ILE:HG12	2.20	0.41
1:S:379:SER:O	1:S:385:GLU:HB3	2.20	0.41
1:A:265:PHE:CZ	1:A:267:ALA:HA	2.55	0.41
1:A:193:TYR:CE1	1:A:276:TRP:CH2	3.08	0.41
2:B:50:LEU:HD22	2:B:54:ILE:HD13	2.02	0.41
2:D:113:LEU:HD23	2:J:113:LEU:CD2	2.51	0.41
1:K:258:ILE:HA	1:K:259:PRO:HD3	1.95	0.41
1:U:240:LEU:HB3	1:U:253:LEU:HD11	2.01	0.41
2:D:145:VAL:CG2	2:F:180:LEU:HD11	2.51	0.41
1:S:202:PRO:HD3	1:S:308:ARG:HD2	2.03	0.41
1:U:438:ALA:O	1:U:442:TYR:HD1	2.03	0.41
2:V:12:PHE:O	2:V:14:TRP:CE3	2.67	0.41
2:P:56:TYR:HB3	2:P:84:GLU:HB2	2.02	0.41
1:S:284:LEU:HD23	1:S:293:THR:HG23	2.02	0.41
1:S:404:ALA:HA	1:W:97:LEU:HD21	2.02	0.41
1:U:326:ILE:HB	1:U:330:CYS:HB3	2.02	0.41
1:U:376:ARG:HA	2:V:92:ARG:NH2	2.35	0.41
1:U:229:SER:HB2	1:U:437:ALA:HB3	2.02	0.41
1:W:407:GLN:HA	1:W:408:PRO:HD3	1.96	0.41
2:P:126:ASP:OD1	2:P:158:ARG:HD2	2.20	0.41
1:Q:262:GLY:C	1:Q:432:VAL:HB	2.46	0.41
1:I:213:LYS:HA	1:I:352:VAL:O	2.20	0.41
1:K:327:PHE:CG	1:K:328:PRO:HA	2.56	0.41
1:U:122:TYR:O	1:W:238:THR:OG1	2.39	0.41
1:U:422:HIS:HD2	1:U:424:ASP:H	1.68	0.41
1:W:46:TYR:O	1:W:49:GLU:HB2	2.21	0.41
1:W:69:GLU:O	1:W:87:ARG:HB3	2.20	0.41
1:W:262:GLY:C	1:W:432:VAL:HB	2.45	0.41
1:A:199:ASP:HB3	1:A:309:LEU:HD21	2.03	0.41
1:I:288[A]:MET:HE2	1:I:373:HIS:HB3	2.02	0.41
1:S:123:HIS:HE2	1:U:230:ASP:CG	2.29	0.41
1:U:110:SER:HB2	2:V:63:ASN:O	2.21	0.41
2:B:32:TYR:CG	2:L:116:ASN:HA	2.56	0.40
5:C:462:BNL:H1	6:C:2244:HOH:O	2.21	0.40
1:E:116:LYS:HA	1:E:116:LYS:HD3	1.78	0.40
1:E:213:LYS:HA	1:E:352:VAL:O	2.22	0.40
1:I:37:PRO:HG2	1:I:405:LYS:HA	2.02	0.40
1:I:410:ASN:ND2	1:I:412:GLN:H	2.19	0.40
1:U:447:ARG:NH2	1:U:456:THR:O	2.53	0.40
1:W:448:MET:HA	1:W:457:LEU:HD11	2.02	0.40
2:X:57:PHE:CZ	2:X:59:PRO:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:ASP:O	1:I:91:LYS:HB2	2.20	0.40
1:M:103:ARG:HA	1:M:103:ARG:HD3	1.94	0.40
1:M:287:VAL:HG12	1:M:288:MET:CE	2.51	0.40
1:E:241:SER:HB3	2:F:101:GLY:N	2.36	0.40
1:E:262:GLY:C	1:E:432:VAL:HB	2.46	0.40
2:L:58:MET:HE2	2:L:81:HIS:CG	2.57	0.40
2:X:23:LEU:HA	2:X:26:GLU:HG2	2.03	0.40
1:A:326:ILE:HB	1:A:330:CYS:HB3	2.04	0.40
2:J:151:GLU:HG2	2:J:173:LEU:HB2	2.03	0.40
2:R:50:LEU:HD22	2:R:54:ILE:CD1	2.51	0.40
2:B:162:ASN:OD1	2:D:53[B]:ASP:OD2	2.40	0.40
1:G:413:MET:HG3	1:M:143:PHE:CZ	2.55	0.40
2:H:113:LEU:CD2	2:N:113:LEU:HD23	2.52	0.40
1:M:389:GLY:O	1:M:393:VAL:HG23	2.21	0.40
1:U:316:VAL:HA	1:U:319:MET:SD	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/459 (94%)	419 (97%)	12 (3%)	0	100	100
1	C	431/459 (94%)	418 (97%)	13 (3%)	0	100	100
1	E	429/459 (94%)	419 (98%)	10 (2%)	0	100	100
1	G	429/459 (94%)	416 (97%)	13 (3%)	0	100	100
1	I	430/459 (94%)	415 (96%)	15 (4%)	0	100	100
1	K	429/459 (94%)	413 (96%)	16 (4%)	0	100	100
1	M	430/459 (94%)	413 (96%)	17 (4%)	0	100	100
1	O	430/459 (94%)	413 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	429/459 (94%)	415 (97%)	13 (3%)	1 (0%)	43	34
1	S	429/459 (94%)	411 (96%)	17 (4%)	1 (0%)	43	34
1	U	426/459 (93%)	400 (94%)	22 (5%)	4 (1%)	14	4
1	W	428/459 (93%)	406 (95%)	19 (4%)	3 (1%)	18	7
2	B	182/188 (97%)	177 (97%)	5 (3%)	0	100	100
2	D	183/188 (97%)	176 (96%)	7 (4%)	0	100	100
2	F	184/188 (98%)	179 (97%)	5 (3%)	0	100	100
2	H	180/188 (96%)	174 (97%)	6 (3%)	0	100	100
2	J	174/188 (93%)	167 (96%)	6 (3%)	1 (1%)	21	10
2	L	181/188 (96%)	176 (97%)	5 (3%)	0	100	100
2	N	181/188 (96%)	177 (98%)	4 (2%)	0	100	100
2	P	182/188 (97%)	172 (94%)	9 (5%)	1 (0%)	24	13
2	R	179/188 (95%)	173 (97%)	5 (3%)	1 (1%)	21	10
2	T	180/188 (96%)	175 (97%)	5 (3%)	0	100	100
2	V	179/188 (95%)	170 (95%)	8 (4%)	1 (1%)	21	10
2	X	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	21	10
All	All	7315/7764 (94%)	7043 (96%)	258 (4%)	14 (0%)	43	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	67	VAL
1	U	83	VAL
2	V	68	GLU
1	W	257	GLN
1	W	259	PRO
1	U	413	MET
2	P	10	LYS
1	Q	103	ARG
2	X	156	LEU
2	J	15	PRO
2	R	10	LYS
1	S	68	PRO
1	W	421	GLY
1	U	344	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/372 (95%)	348 (99%)	5 (1%)	59	48
1	C	353/372 (95%)	347 (98%)	6 (2%)	53	40
1	E	351/372 (94%)	344 (98%)	7 (2%)	48	33
1	G	351/372 (94%)	346 (99%)	5 (1%)	59	48
1	I	352/372 (95%)	343 (97%)	9 (3%)	40	24
1	K	351/372 (94%)	342 (97%)	9 (3%)	40	24
1	M	352/372 (95%)	341 (97%)	11 (3%)	35	18
1	O	352/372 (95%)	345 (98%)	7 (2%)	48	33
1	Q	351/372 (94%)	341 (97%)	10 (3%)	38	22
1	S	351/372 (94%)	345 (98%)	6 (2%)	53	40
1	U	349/372 (94%)	334 (96%)	15 (4%)	26	10
1	W	350/372 (94%)	345 (99%)	5 (1%)	59	48
2	B	163/167 (98%)	160 (98%)	3 (2%)	51	38
2	D	164/167 (98%)	163 (99%)	1 (1%)	78	72
2	F	165/167 (99%)	160 (97%)	5 (3%)	36	19
2	H	161/167 (96%)	160 (99%)	1 (1%)	78	72
2	J	155/167 (93%)	151 (97%)	4 (3%)	40	24
2	L	162/167 (97%)	161 (99%)	1 (1%)	78	72
2	N	162/167 (97%)	160 (99%)	2 (1%)	63	53
2	P	163/167 (98%)	161 (99%)	2 (1%)	63	53
2	R	160/167 (96%)	159 (99%)	1 (1%)	78	72
2	T	161/167 (96%)	154 (96%)	7 (4%)	26	10
2	V	160/167 (96%)	160 (100%)	0	100	100
2	X	160/167 (96%)	153 (96%)	7 (4%)	25	9
All	All	6152/6468 (95%)	6023 (98%)	129 (2%)	47	32

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	103	ARG
1	A	255	GLN
1	A	410	ASN
1	A	457	LEU
2	B	10	LYS
2	B	22	GLU
2	B	179	LEU
1	C	86	VAL
1	C	103	ARG
1	C	280	GLU
1	C	309	LEU
1	C	385	GLU
1	C	457	LEU
2	D	162	ASN
1	E	31	GLU
1	E	86	VAL
1	E	103	ARG
1	E	251	MET
1	E	280	GLU
1	E	307	GLN
1	E	410	ASN
2	F	51	ASP
2	F	94	ARG
2	F	113	LEU
2	F	160	ASP
2	F	179	LEU
1	G	48	LEU
1	G	100	CYS
1	G	103	ARG
1	G	410	ASN
1	G	457	LEU
2	H	22	GLU
1	I	48	LEU
1	I	86	VAL
1	I	247	ILE
1	I	283	SER
1	I	309	LEU
1	I	320	VAL
1	I	385	GLU
1	I	410	ASN
1	I	457	LEU
2	J	51	ASP

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Mol	Chain	Res	Type
2	J	160	ASP
2	J	162	ASN
2	J	179	LEU
1	K	48	LEU
1	K	86	VAL
1	K	103	ARG
1	K	250	GLU
1	K	309	LEU
1	K	316	VAL
1	K	320	VAL
1	K	385	GLU
1	K	457	LEU
2	L	179	LEU
1	M	48	LEU
1	M	52	ARG
1	M	103	ARG
1	M	167	THR
1	M	247	ILE
1	M	253	LEU
1	M	257	GLN
1	M	280	GLU
1	M	339	ILE
1	M	385	GLU
1	M	457	LEU
2	N	169	LYS
2	N	179	LEU
1	O	86	VAL
1	O	103	ARG
1	O	247	ILE
1	O	257	GLN
1	O	320	VAL
1	O	385	GLU
1	O	410	ASN
2	P	113	LEU
2	P	179	LEU
1	Q	86	VAL
1	Q	103	ARG
1	Q	247	ILE
1	Q	258	ILE
1	Q	280	GLU
1	Q	294	GLN
1	Q	385	GLU

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Mol	Chain	Res	Type
1	Q	413	MET
1	Q	417	ARG
1	Q	457	LEU
2	R	179	LEU
1	S	167	THR
1	S	221	LYS
1	S	247	ILE
1	S	258	ILE
1	S	320	VAL
1	S	339	ILE
2	T	21	LEU
2	T	54	ILE
2	T	87	GLU
2	T	94	ARG
2	T	162	ASN
2	T	169	LYS
2	T	179	LEU
1	U	67	VAL
1	U	95	VAL
1	U	97	LEU
1	U	101	ARG
1	U	103	ARG
1	U	109	ARG
1	U	189	ASP
1	U	211	MET
1	U	213	LYS
1	U	247	ILE
1	U	257	GLN
1	U	280	GLU
1	U	339	ILE
1	U	410	ASN
1	U	457	LEU
1	W	103	ARG
1	W	247	ILE
1	W	258	ILE
1	W	320	VAL
1	W	457	LEU
2	X	22	GLU
2	X	54	ILE
2	X	67	ARG
2	X	77	GLN
2	X	113	LEU

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Mol	Chain	Res	Type
2	X	127	THR
2	X	128	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	135	ASN
1	A	255	GLN
1	A	257	GLN
1	A	386	GLN
1	A	391	ASN
1	A	410	ASN
1	A	412	GLN
1	A	422	HIS
2	B	36	GLN
2	B	131	ASN
2	B	144	GLN
2	B	162	ASN
1	C	99	GLN
1	C	135	ASN
1	C	386	GLN
1	C	391	ASN
1	C	407	GLN
1	C	410	ASN
1	C	412	GLN
1	C	422	HIS
1	C	444	HIS
2	D	7	HIS
2	D	25	ASN
2	D	55	HIS
2	D	77	GLN
2	D	162	ASN
1	E	18	ASN
1	E	99	GLN
1	E	114	ASN
1	E	135	ASN
1	E	255	GLN
1	E	311	HIS
1	E	386	GLN
1	E	391	ASN
1	E	407	GLN

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Mol	Chain	Res	Type
1	E	410	ASN
1	E	412	GLN
1	E	422	HIS
2	F	25	ASN
2	F	40	HIS
2	F	55	HIS
2	F	144	GLN
1	G	88	GLN
1	G	99	GLN
1	G	386	GLN
1	G	391	ASN
1	G	410	ASN
1	G	412	GLN
1	G	422	HIS
2	H	25	ASN
2	H	36	GLN
2	H	131	ASN
2	H	162	ASN
1	I	18	ASN
1	I	226	GLN
1	I	255	GLN
1	I	294	GLN
1	I	307	GLN
1	I	311	HIS
1	I	373	HIS
1	I	386	GLN
1	I	391	ASN
1	I	407	GLN
1	I	410	ASN
1	I	412	GLN
1	I	422	HIS
1	I	443	HIS
1	I	444	HIS
2	J	25	ASN
2	J	36	GLN
2	J	40	HIS
2	J	55	HIS
2	J	77	GLN
1	K	18	ASN
1	K	99	GLN
1	K	135	ASN
1	K	226	GLN

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Mol	Chain	Res	Type
1	K	311	HIS
1	K	386	GLN
1	K	391	ASN
1	K	410	ASN
1	K	412	GLN
1	K	419	GLN
1	K	444	HIS
2	L	25	ASN
2	L	29	GLN
2	L	36	GLN
2	L	131	ASN
2	L	162	ASN
1	M	135	ASN
1	M	255	GLN
1	M	257	GLN
1	M	377	ASN
1	M	391	ASN
1	M	410	ASN
1	M	412	GLN
1	M	422	HIS
2	N	131	ASN
2	N	162	ASN
1	O	88	GLN
1	O	226	GLN
1	O	257	GLN
1	O	264	GLN
1	O	386	GLN
1	O	391	ASN
1	O	410	ASN
1	O	412	GLN
1	O	422	HIS
1	O	444	HIS
2	P	25	ASN
2	P	36	GLN
2	P	131	ASN
2	P	162	ASN
1	Q	43	GLN
1	Q	135	ASN
1	Q	257	GLN
1	Q	263	ASN
1	Q	294	GLN
1	Q	386	GLN

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Mol	Chain	Res	Type
1	Q	391	ASN
1	Q	412	GLN
1	Q	419	GLN
1	Q	422	HIS
2	R	77	GLN
1	S	43	GLN
1	S	88	GLN
1	S	226	GLN
1	S	257	GLN
1	S	294	GLN
1	S	343	HIS
1	S	377	ASN
1	S	410	ASN
1	S	412	GLN
1	S	419	GLN
1	S	422	HIS
2	T	25	ASN
2	T	77	GLN
2	T	162	ASN
1	U	18	ASN
1	U	30	GLN
1	U	43	GLN
1	U	66	HIS
1	U	99	GLN
1	U	255	GLN
1	U	257	GLN
1	U	343	HIS
1	U	386	GLN
1	U	410	ASN
1	U	412	GLN
1	U	422	HIS
2	V	25	ASN
2	V	36	GLN
2	V	77	GLN
1	W	255	GLN
1	W	257	GLN
1	W	264	GLN
1	W	311	HIS
1	W	322	GLN
1	W	343	HIS
1	W	391	ASN
1	W	410	ASN

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Mol	Chain	Res	Type
1	W	412	GLN
1	W	428	ASN
1	W	443	HIS
2	X	24	GLN
2	X	25	ASN
2	X	77	GLN
2	X	162	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 33 ligands modelled in this entry, 12 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FES	C	460	1	0,4,4	-	-	-		
5	BNL	K	462	-	13,13,13	1.22	1 (7%)	16,16,16	0.49	0
3	FES	W	460	1	0,4,4	-	-	-		
3	FES	S	460	1,6	0,4,4	-	-	-		
3	FES	E	460	1	0,4,4	-	-	-		
3	FES	O	460	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BNL	O	462	-	13,13,13	1.25	1 (7%)	16,16,16	0.64	0
3	FES	U	460	1	0,4,4	-	-	-		
3	FES	A	460	1	0,4,4	-	-	-		
3	FES	Q	460	1	0,4,4	-	-	-		
3	FES	K	460	1	0,4,4	-	-	-		
5	BNL	M	462	-	13,13,13	1.19	1 (7%)	16,16,16	0.44	0
5	BNL	Q	462	-	13,13,13	1.24	1 (7%)	16,16,16	0.50	0
5	BNL	S	462	-	13,13,13	1.16	1 (7%)	16,16,16	0.64	0
3	FES	I	460	1	0,4,4	-	-	-		
5	BNL	C	462	-	13,13,13	1.16	1 (7%)	16,16,16	0.46	0
5	BNL	E	462	-	13,13,13	1.19	1 (7%)	16,16,16	0.73	0
5	BNL	I	462	-	13,13,13	1.22	1 (7%)	16,16,16	0.44	0
3	FES	G	460	1	0,4,4	-	-	-		
5	BNL	W	462	-	13,13,13	1.20	1 (7%)	16,16,16	0.52	0
3	FES	M	460	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	C	460	1	-	-	0/1/1/1
5	BNL	K	462	-	-	0/4/4/4	0/2/2/2
3	FES	W	460	1	-	-	0/1/1/1
3	FES	S	460	1,6	-	-	0/1/1/1
3	FES	E	460	1	-	-	0/1/1/1
5	BNL	O	462	-	-	0/4/4/4	0/2/2/2
3	FES	O	460	1	-	-	0/1/1/1
3	FES	U	460	1	-	-	0/1/1/1
3	FES	A	460	1	-	-	0/1/1/1
3	FES	Q	460	1	-	-	0/1/1/1
3	FES	K	460	1	-	-	0/1/1/1
5	BNL	M	462	-	-	0/4/4/4	0/2/2/2
5	BNL	Q	462	-	-	4/4/4/4	0/2/2/2
5	BNL	S	462	-	-	0/4/4/4	0/2/2/2
3	FES	I	460	1	-	-	0/1/1/1
5	BNL	C	462	-	-	4/4/4/4	0/2/2/2
5	BNL	E	462	-	-	4/4/4/4	0/2/2/2
5	BNL	I	462	-	-	0/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	G	460	1	-	-	0/1/1/1
5	BNL	W	462	-	-	4/4/4/4	0/2/2/2
3	FES	M	460	1	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	462	BNL	C16-C2	-4.00	1.39	1.49
5	O	462	BNL	C16-C2	-3.81	1.40	1.49
5	W	462	BNL	C16-C2	-3.77	1.40	1.49
5	Q	462	BNL	C16-C2	-3.76	1.40	1.49
5	K	462	BNL	C16-C2	-3.73	1.40	1.49
5	E	462	BNL	C16-C2	-3.69	1.40	1.49
5	M	462	BNL	C16-C2	-3.63	1.40	1.49
5	I	462	BNL	C16-C2	-3.43	1.40	1.49
5	C	462	BNL	C16-C2	-3.37	1.41	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	462	BNL	C15-C16-C2-C1
5	Q	462	BNL	C17-C16-C2-C3
5	Q	462	BNL	C17-C16-C2-C1
5	Q	462	BNL	C15-C16-C2-C3
5	E	462	BNL	C15-C16-C2-C3
5	E	462	BNL	C17-C16-C2-C3
5	E	462	BNL	C15-C16-C2-C1
5	E	462	BNL	C17-C16-C2-C1
5	W	462	BNL	C15-C16-C2-C1
5	W	462	BNL	C17-C16-C2-C3
5	W	462	BNL	C15-C16-C2-C3
5	W	462	BNL	C17-C16-C2-C1
5	C	462	BNL	C15-C16-C2-C1
5	C	462	BNL	C17-C16-C2-C3
5	C	462	BNL	C17-C16-C2-C1
5	C	462	BNL	C15-C16-C2-C3

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	460	FES	1	0
3	W	460	FES	2	0
3	S	460	FES	1	0
3	E	460	FES	1	0
3	O	460	FES	1	0
3	U	460	FES	1	0
3	A	460	FES	1	0
3	Q	460	FES	2	0
5	M	462	BNL	1	0
5	C	462	BNL	3	0
5	E	462	BNL	1	0
3	G	460	FES	3	0
3	M	460	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	433/459 (94%)	0.40	18 (4%)	40	44	13, 26, 40, 53	13 (3%)
1	C	433/459 (94%)	0.56	30 (6%)	23	25	12, 26, 40, 87	17 (3%)
1	E	433/459 (94%)	0.57	30 (6%)	23	25	20, 29, 47, 96	12 (2%)
1	G	433/459 (94%)	0.50	20 (4%)	37	40	17, 29, 46, 63	16 (3%)
1	I	433/459 (94%)	0.49	22 (5%)	33	35	18, 30, 45, 61	17 (3%)
1	K	433/459 (94%)	0.65	30 (6%)	23	25	21, 33, 51, 64	15 (3%)
1	M	433/459 (94%)	0.69	35 (8%)	18	20	19, 32, 54, 65	17 (3%)
1	O	433/459 (94%)	0.67	24 (5%)	30	33	20, 35, 54, 68	21 (4%)
1	Q	433/459 (94%)	0.90	48 (11%)	10	12	20, 39, 63, 85	12 (2%)
1	S	433/459 (94%)	2.34	239 (55%)	0	0	36, 74, 111, 129	48 (11%)
1	U	430/459 (93%)	3.12	331 (76%)	0	0	32, 78, 105, 122	53 (12%)
1	W	432/459 (94%)	3.06	341 (78%)	0	0	34, 67, 96, 112	71 (16%)
2	B	183/188 (97%)	0.51	4 (2%)	62	68	13, 25, 31, 50	4 (2%)
2	D	183/188 (97%)	0.67	11 (6%)	27	30	13, 25, 33, 43	9 (4%)
2	F	184/188 (97%)	0.60	10 (5%)	31	33	14, 26, 33, 40	6 (3%)
2	H	181/188 (96%)	0.39	5 (2%)	55	59	13, 26, 37, 47	4 (2%)
2	J	175/188 (93%)	0.68	12 (6%)	23	25	16, 26, 33, 67	9 (5%)
2	L	182/188 (96%)	0.37	4 (2%)	62	68	20, 27, 35, 58	5 (2%)
2	N	183/188 (97%)	0.39	5 (2%)	56	61	20, 26, 37, 58	6 (3%)
2	P	181/188 (96%)	0.39	4 (2%)	62	68	16, 26, 38, 53	6 (3%)
2	R	181/188 (96%)	0.47	10 (5%)	30	33	20, 30, 40, 48	3 (1%)
2	T	182/188 (96%)	0.99	19 (10%)	11	14	28, 41, 61, 68	3 (1%)
2	V	181/188 (96%)	1.37	44 (24%)	2	1	23, 43, 86, 97	11 (6%)
2	X	180/188 (95%)	2.86	114 (63%)	0	0	37, 69, 99, 111	22 (12%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7368/7764 (94%)	1.06	1410 (19%) 3 3	12, 32, 86, 129	400 (5%)

All (1410) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	122	THR	9.2
2	X	127	THR	9.2
1	U	269	TRP	9.1
1	S	455	ALA	9.1
1	U	93	ILE	8.7
1	W	432	VAL	8.7
1	U	100	CYS	8.6
2	X	125	PRO	8.3
1	S	258	ILE	8.2
1	U	67	VAL	8.1
2	X	159	ALA	7.9
2	X	123	ALA	7.9
2	X	102	TRP	7.8
2	X	124	THR	7.7
1	U	95	VAL	7.7
1	S	178	VAL	7.7
1	U	82	PRO	7.6
1	E	256	ALA	7.5
1	W	230	ASP	7.5
2	X	155	VAL	7.4
1	U	102	HIS	7.3
1	U	33	GLY	7.1
1	U	186	TYR	6.9
1	U	79	GLY	6.9
1	U	92	SER	6.8
1	S	159	GLY	6.7
1	W	292	VAL	6.7
1	W	430	GLY	6.6
1	W	20	THR	6.5
2	V	69	GLY	6.5
1	U	128	ASP	6.5
1	W	224	ALA	6.4
1	W	270	GLY	6.4
2	X	47	PHE	6.4
1	W	258	ILE	6.4
1	Q	256	ALA	6.3
1	U	158	TRP	6.2

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Mol	Chain	Res	Type	RSRZ
1	W	276	TRP	6.2
1	U	156	ALA	6.1
1	W	305	ALA	6.1
1	U	457	LEU	6.1
1	W	265	PHE	6.0
1	W	23	ALA	6.0
1	U	206	VAL	6.0
1	U	181	PRO	6.0
1	U	180	ALA	6.0
1	U	449	MET	6.0
1	U	188	GLY	6.0
1	U	23	ALA	6.0
1	W	418	SER	6.0
1	W	442	TYR	6.0
1	W	455	ALA	5.9
1	U	165	VAL	5.9
1	W	284	LEU	5.9
1	W	285	LEU	5.9
1	U	153	PHE	5.9
1	W	256	ALA	5.8
1	W	295	TYR	5.8
1	U	424	ASP	5.8
2	X	18	ALA	5.8
1	U	452	PRO	5.8
1	U	83	VAL	5.8
1	W	388	ASP	5.7
1	U	127	TYR	5.7
1	U	310	GLY	5.7
1	U	454	TRP	5.7
2	J	14	TRP	5.7
1	W	370	TYR	5.6
2	X	45	ALA	5.6
1	U	355	PHE	5.6
2	V	9	PHE	5.6
1	U	20	THR	5.6
1	S	175	ASN	5.6
2	V	19	ALA	5.6
2	X	42	ALA	5.6
1	W	24	ILE	5.5
1	W	310	GLY	5.5
1	U	304	LEU	5.5
1	K	416	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	S	454	TRP	5.4
2	X	20	GLY	5.4
1	W	21	PRO	5.4
2	X	168	ALA	5.4
1	U	131	GLY	5.4
1	W	190	ALA	5.4
1	S	421	GLY	5.3
1	U	166	ALA	5.3
2	X	161	ASN	5.3
1	S	156	ALA	5.3
1	S	256	ALA	5.3
1	U	94	LYS	5.3
1	S	19	TRP	5.2
2	X	85	THR	5.2
1	U	313	GLY	5.2
1	Q	249	PRO	5.2
1	U	192	PRO	5.2
2	V	8	PHE	5.2
1	S	206	VAL	5.2
1	U	196	VAL	5.2
1	W	413	MET	5.2
1	W	420	THR	5.2
1	U	195	ASP	5.1
2	V	18	ALA	5.1
1	Q	281	PRO	5.1
2	X	100	VAL	5.1
2	X	54	ILE	5.1
1	C	246	GLY	5.1
1	W	362	ALA	5.1
1	U	159	GLY	5.1
2	X	43	TYR	5.1
1	U	456	THR	5.1
1	S	297	THR	5.0
1	W	325	THR	5.0
1	U	301	ALA	5.0
1	U	409	LEU	5.0
1	U	443	HIS	5.0
1	U	110	SER	5.0
1	U	442	TYR	5.0
1	W	196	VAL	5.0
1	S	188	GLY	5.0
2	X	48	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
2	V	14	TRP	4.9
1	W	402	TYR	4.9
1	W	259	PRO	4.9
1	U	122	TYR	4.9
1	S	420	THR	4.9
1	W	312	THR	4.9
1	W	332	PHE	4.9
1	U	123	HIS	4.9
1	U	129	ILE	4.9
2	X	35	ALA	4.9
1	U	58	TRP	4.8
1	U	358	VAL	4.8
2	X	130	VAL	4.8
1	M	255	GLN	4.8
1	U	139	GLU	4.8
1	S	406	SER	4.8
1	U	344	PRO	4.8
1	G	100	CYS	4.8
2	X	21	LEU	4.8
2	X	50	LEU	4.8
2	X	156	LEU	4.8
1	S	401	GLY	4.8
1	W	188	GLY	4.8
1	W	227	PHE	4.8
2	T	160	ASP	4.8
1	W	19	TRP	4.8
1	U	81	ASP	4.7
1	U	138	PHE	4.7
2	R	8	PHE	4.7
1	U	125	TRP	4.7
1	W	287	VAL	4.7
1	E	258	ILE	4.7
1	W	271	GLY	4.7
1	W	309	LEU	4.7
1	W	186	TYR	4.7
1	S	23	ALA	4.7
1	S	26	GLY	4.7
1	E	252	ASP	4.7
1	U	154	ASP	4.7
2	X	128	PHE	4.7
1	W	249	PRO	4.7
1	U	117	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	U	286	ALA	4.7
1	W	411	ALA	4.6
1	E	247	ILE	4.6
1	U	415	LEU	4.6
1	W	207	ALA	4.6
1	U	325	THR	4.6
1	U	134	VAL	4.6
1	W	316	VAL	4.6
1	U	453	SER	4.6
1	W	39	ILE	4.6
1	W	283	SER	4.6
1	U	55	GLY	4.6
1	S	143	PHE	4.6
1	U	75	ALA	4.6
1	U	364	ALA	4.6
1	W	378	PHE	4.6
1	S	255	GLN	4.6
1	S	316	VAL	4.6
1	Q	258	ILE	4.6
1	U	71	GLY	4.6
1	S	265	PHE	4.5
1	U	48	LEU	4.5
2	D	6	PRO	4.5
1	S	269	TRP	4.5
1	U	190	ALA	4.5
2	P	8	PHE	4.5
1	U	133	LEU	4.5
1	U	446	MET	4.5
2	V	70	GLU	4.5
1	W	34	LEU	4.5
1	W	233	HIS	4.5
1	W	457	LEU	4.5
2	X	23	LEU	4.5
1	S	423	PRO	4.5
1	W	192	PRO	4.5
1	U	411	ALA	4.5
1	U	438	ALA	4.5
1	W	142	ALA	4.5
1	W	425	PHE	4.4
1	S	402	TYR	4.4
2	X	163	LEU	4.4
1	E	251	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	U	76	THR	4.4
1	W	294	GLN	4.4
1	W	26	GLY	4.4
1	W	59	LEU	4.4
1	U	208	ILE	4.4
1	U	339	ILE	4.4
1	U	366	ILE	4.4
1	U	137	PRO	4.4
1	S	364	ALA	4.4
1	W	410	ASN	4.4
2	X	30	PHE	4.4
1	S	304	LEU	4.4
1	U	28	VAL	4.4
1	E	249	PRO	4.4
1	U	168	TYR	4.4
1	W	100	CYS	4.4
1	W	247	ILE	4.4
1	W	315	PRO	4.4
1	W	431	TYR	4.4
2	X	94	ARG	4.4
1	Q	416	GLY	4.3
1	U	99	GLN	4.3
1	U	198	LEU	4.3
1	U	455	ALA	4.3
1	U	136	VAL	4.3
1	U	178	VAL	4.3
2	X	40	HIS	4.3
1	U	175	ASN	4.3
1	M	261	LYS	4.3
2	X	120	LYS	4.3
1	U	416	GLY	4.3
1	W	167	THR	4.3
1	W	243	ILE	4.3
1	U	434	ALA	4.3
1	W	180	ALA	4.3
1	U	270	GLY	4.3
1	W	242	GLY	4.3
1	W	269	TRP	4.3
1	W	359	ASP	4.3
1	U	106	ARG	4.2
1	W	228	CYS	4.2
1	W	208	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
2	X	167	ILE	4.2
1	Q	283	SER	4.2
1	S	450	SER	4.2
1	W	204	GLY	4.2
1	U	66	HIS	4.2
1	S	58	TRP	4.2
1	U	103	ARG	4.2
1	U	140	LYS	4.2
1	O	457	LEU	4.2
1	U	429	VAL	4.2
1	W	273	GLY	4.2
2	X	19	ALA	4.2
1	U	109	ARG	4.2
1	W	447	ARG	4.2
1	E	260	THR	4.2
1	U	161	LEU	4.2
1	S	283	SER	4.2
1	W	375	ILE	4.2
1	S	335	GLY	4.2
1	U	273	GLY	4.2
1	U	193	TYR	4.2
1	S	362	ALA	4.2
1	U	167	THR	4.2
1	W	296	TRP	4.2
1	W	33	GLY	4.1
1	U	295	TYR	4.1
1	S	259	PRO	4.1
2	N	7	HIS	4.1
2	X	141	LEU	4.1
1	W	62	GLY	4.1
1	W	392	TRP	4.1
1	U	118	PHE	4.1
1	U	327	PHE	4.1
1	W	429	VAL	4.1
2	X	27	ILE	4.1
1	W	293	THR	4.1
1	W	257	GLN	4.1
2	X	86	HIS	4.1
1	U	61	LEU	4.1
1	U	104	GLY	4.1
1	W	409	LEU	4.1
2	T	21	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	S	446	MET	4.1
1	U	73	PHE	4.1
1	U	425	PHE	4.1
2	D	14	TRP	4.1
1	U	107	ILE	4.1
1	S	268	ALA	4.1
2	V	127	THR	4.1
1	S	440	GLY	4.1
1	U	210	GLY	4.1
1	U	84	VAL	4.0
1	W	445	TRP	4.0
2	N	123	ALA	4.0
1	W	307	GLN	4.0
1	W	29	ASP	4.0
1	W	338	THR	4.0
1	S	418	SER	4.0
1	M	421	GLY	4.0
1	U	271	GLY	4.0
1	W	55	GLY	4.0
1	S	419	GLN	4.0
1	U	115	ALA	4.0
1	W	178	VAL	4.0
1	U	21	PRO	4.0
1	U	300	PRO	4.0
2	V	125	PRO	4.0
1	W	220	TRP	4.0
2	X	98	SER	4.0
1	S	313	GLY	4.0
1	U	62	GLY	4.0
1	U	285	LEU	4.0
1	C	252	ASP	4.0
2	X	51	ASP	4.0
1	U	163	ALA	4.0
1	W	438	ALA	4.0
2	L	8	PHE	4.0
1	S	44	SER	4.0
1	C	255	GLN	4.0
1	W	27	LEU	4.0
2	X	53	ASP	4.0
1	U	448	MET	4.0
1	W	334	PRO	4.0
1	W	366	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	W	406	SER	4.0
1	U	172	VAL	4.0
1	W	238	THR	3.9
1	S	193	TYR	3.9
2	V	71	LEU	3.9
1	C	256	ALA	3.9
1	W	217	PRO	3.9
1	W	426	PRO	3.9
1	Q	260	THR	3.9
2	X	88	THR	3.9
2	B	8	PHE	3.9
1	O	310	GLY	3.9
2	F	14	TRP	3.9
1	C	253	LEU	3.9
1	W	241	SER	3.9
1	Q	257	GLN	3.9
2	B	6	PRO	3.9
1	U	120	CYS	3.9
1	U	265	PHE	3.9
1	W	422	HIS	3.9
2	F	160	ASP	3.9
1	M	18	ASN	3.9
1	W	407	GLN	3.9
1	W	229	SER	3.9
2	F	5	SER	3.9
1	U	176	TRP	3.9
1	U	183	LEU	3.9
1	U	305	ALA	3.9
1	I	389	GLY	3.9
1	I	421	GLY	3.9
1	S	204	GLY	3.9
2	T	20	GLY	3.9
1	S	432	VAL	3.9
1	W	254	SER	3.8
1	C	421	GLY	3.8
1	S	142	ALA	3.8
1	S	275	GLY	3.8
1	S	404	ALA	3.8
1	W	360	ALA	3.8
2	X	101	GLY	3.8
1	I	252	ASP	3.8
1	U	194	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	U	251	MET	3.8
2	V	67	ARG	3.8
2	X	79	LEU	3.8
1	S	21	PRO	3.8
1	U	70	THR	3.8
2	V	20	GLY	3.8
1	C	251	MET	3.8
1	I	256	ALA	3.8
1	U	267	ALA	3.8
2	X	176	ALA	3.8
1	M	257	GLN	3.8
1	W	384	PHE	3.8
2	V	16	SER	3.8
1	W	168	TYR	3.8
2	N	6	PRO	3.8
1	S	311	HIS	3.7
1	W	361	ASP	3.7
1	W	446	MET	3.7
1	S	31	GLU	3.7
1	U	59	LEU	3.7
1	U	97	LEU	3.7
1	W	45	LEU	3.7
1	W	277	TYR	3.7
1	W	433	TYR	3.7
2	V	68	GLU	3.7
1	S	203	ALA	3.7
2	X	96	VAL	3.7
1	U	173	PHE	3.7
1	E	255	GLN	3.7
1	W	226	GLN	3.7
1	W	202	PRO	3.7
1	W	328	PRO	3.7
2	V	73	TYR	3.7
1	W	434	ALA	3.7
1	S	39	ILE	3.7
1	W	58	TRP	3.7
1	U	18	ASN	3.7
1	U	426	PRO	3.7
2	V	15	PRO	3.7
1	S	201	THR	3.7
1	U	201	THR	3.7
1	W	221	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	S	45	LEU	3.7
1	U	171	LEU	3.7
1	U	77	TYR	3.7
1	S	254	SER	3.7
1	W	358	VAL	3.7
1	U	89	LYS	3.7
1	W	327	PHE	3.7
1	M	259	PRO	3.7
1	S	20	THR	3.7
1	W	248	PRO	3.7
1	S	296	TRP	3.7
1	W	297	THR	3.7
1	W	35	LEU	3.6
1	W	253	LEU	3.6
1	E	257	GLN	3.6
1	U	90	ASP	3.6
1	W	219	ASN	3.6
1	W	408	PRO	3.6
1	C	283	SER	3.6
1	W	187	LEU	3.6
2	V	21	LEU	3.6
1	S	42	ASP	3.6
1	S	189	ASP	3.6
1	S	424	ASP	3.6
1	U	29	ASP	3.6
1	U	112	ALA	3.6
1	W	354	ALA	3.6
1	W	437	ALA	3.6
2	V	162	ASN	3.6
1	W	330	CYS	3.6
1	S	271	GLY	3.6
1	S	282	GLY	3.6
1	W	427	GLY	3.6
1	S	366	ILE	3.6
1	U	160	PRO	3.6
2	V	11	THR	3.6
1	A	311	HIS	3.6
2	V	12	PHE	3.6
2	X	165	PHE	3.6
1	W	183	LEU	3.6
1	W	198	LEU	3.6
1	U	126	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	U	308	ARG	3.6
1	U	353	TRP	3.6
1	W	421	GLY	3.6
1	W	339	ILE	3.6
1	U	363	PRO	3.6
1	W	67	VAL	3.6
2	X	157	ARG	3.6
1	S	224	ALA	3.5
1	U	187	LEU	3.6
1	W	267	ALA	3.5
1	W	380	ALA	3.5
2	V	123	ALA	3.5
1	W	43	GLN	3.5
1	W	414	GLY	3.5
2	X	75	GLY	3.5
1	U	108	CYS	3.5
1	W	314	MET	3.5
1	K	252	ASP	3.5
1	S	90	ASP	3.5
1	U	42	ASP	3.5
1	U	297	THR	3.5
1	U	432	VAL	3.5
1	M	256	ALA	3.5
1	U	141	GLU	3.5
1	W	240	LEU	3.5
1	G	416	GLY	3.5
1	U	65	SER	3.5
1	U	439	ARG	3.5
1	S	312	THR	3.5
1	Q	247	ILE	3.5
1	W	320	VAL	3.5
2	X	162	ASN	3.5
1	I	255	GLN	3.5
1	Q	364	ALA	3.5
1	S	301	ALA	3.5
1	W	48	LEU	3.5
1	W	302	ALA	3.5
1	W	275	GLY	3.5
1	W	448	MET	3.5
2	V	75	GLY	3.5
1	U	68	PRO	3.5
1	U	408	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	W	237	THR	3.5
1	S	176	TRP	3.5
1	U	220	TRP	3.5
2	X	22	GLU	3.5
1	W	395	ILE	3.5
1	W	419	GLN	3.5
1	U	86	VAL	3.5
1	S	267	ALA	3.5
1	U	302	ALA	3.5
1	S	33	GLY	3.5
1	S	310	GLY	3.5
1	S	430	GLY	3.5
1	S	261	LYS	3.5
1	U	189	ASP	3.5
1	W	189	ASP	3.5
1	U	331	SER	3.4
2	X	166	SER	3.4
1	W	385	GLU	3.4
1	U	423	PRO	3.4
1	S	431	TYR	3.4
1	W	214	TRP	3.4
1	O	316	VAL	3.4
1	U	447	ARG	3.4
1	W	231	MET	3.4
2	D	7	HIS	3.4
1	W	209	GLY	3.4
1	W	235	GLY	3.4
1	E	142	ALA	3.4
1	K	256	ALA	3.4
1	W	41	ALA	3.4
1	W	304	LEU	3.4
1	W	415	LEU	3.4
1	U	338	THR	3.4
1	W	363	PRO	3.4
2	X	90	TYR	3.4
1	M	311	HIS	3.4
1	U	182	ASP	3.4
1	U	414	GLY	3.4
1	W	313	GLY	3.4
1	U	256	ALA	3.4
1	U	121	SER	3.4
1	S	459	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	U	185	THR	3.4
1	S	447	ARG	3.4
1	S	422	HIS	3.4
1	W	239	HIS	3.4
1	K	258	ILE	3.4
1	Q	389	GLY	3.4
1	U	179	GLN	3.4
1	S	34	LEU	3.4
1	U	54	PHE	3.4
1	W	97	LEU	3.4
2	F	162	ASN	3.4
2	H	8	PHE	3.4
1	U	105	MET	3.4
1	W	288	MET	3.4
2	X	87	GLU	3.3
1	U	361	ASP	3.3
2	X	126	ASP	3.3
1	U	209	GLY	3.3
1	U	440	GLY	3.3
1	C	258	ILE	3.3
1	U	326	ILE	3.3
1	W	326	ILE	3.3
2	V	66	ILE	3.3
1	S	18	ASN	3.3
1	U	98	ASN	3.3
2	J	162	ASN	3.3
1	W	54	PHE	3.3
1	S	260	THR	3.3
1	S	300	PRO	3.3
1	U	169	LYS	3.3
1	U	420	THR	3.3
1	W	205	THR	3.3
2	X	26	GLU	3.3
2	X	121	GLU	3.3
1	W	120	CYS	3.3
1	U	427	GLY	3.3
1	W	44	SER	3.3
2	R	90	TYR	3.3
2	X	32	TYR	3.3
1	C	18	ASN	3.3
1	S	24	ILE	3.3
1	S	245	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	U	268	ALA	3.3
1	W	245	ALA	3.3
1	W	244	LEU	3.3
1	U	96	PHE	3.3
1	U	119	THR	3.3
1	C	249	PRO	3.3
1	S	416	GLY	3.3
1	W	159	GLY	3.3
1	M	258	ILE	3.3
1	K	420	THR	3.3
1	S	205	THR	3.3
1	U	34	LEU	3.3
1	S	426	PRO	3.3
1	S	138	PHE	3.3
1	W	454	TRP	3.3
1	M	282	GLY	3.3
1	C	247	ILE	3.2
1	I	258	ILE	3.2
1	W	193	TYR	3.2
1	M	252	ASP	3.2
1	W	53	VAL	3.2
2	X	119	VAL	3.2
1	E	244	LEU	3.2
1	K	260	THR	3.2
1	W	201	THR	3.2
1	C	254	SER	3.2
1	G	310	GLY	3.2
1	W	51	GLU	3.2
1	W	289	GLY	3.2
1	W	303	GLU	3.2
1	U	44	SER	3.2
1	W	440	GLY	3.2
1	K	255	GLN	3.2
1	Q	102	HIS	3.2
1	S	52	ARG	3.2
1	U	52	ARG	3.2
1	U	203	ALA	3.2
1	U	360	ALA	3.2
1	W	115	ALA	3.2
1	W	223	ALA	3.2
1	W	268	ALA	3.2
1	S	202	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	U	283	SER	3.2
1	U	450	SER	3.2
1	W	153	PHE	3.2
1	W	379	SER	3.2
2	X	91	GLY	3.2
1	W	255	GLN	3.2
1	U	228	CYS	3.2
1	W	177	ASP	3.2
1	U	24	ILE	3.2
1	S	185	THR	3.2
1	U	31	GLU	3.2
1	U	47	GLU	3.2
1	U	362	ALA	3.2
1	W	203	ALA	3.2
1	W	286	ALA	3.2
1	S	285	LEU	3.2
1	S	457	LEU	3.2
1	U	45	LEU	3.2
1	W	311	HIS	3.2
1	I	29	ASP	3.2
1	W	218	CYS	3.2
2	V	26	GLU	3.2
1	U	130	ALA	3.1
1	W	261	LYS	3.1
1	C	248	PRO	3.1
1	Q	423	PRO	3.1
1	U	328	PRO	3.1
2	V	65	MET	3.1
1	M	285	LEU	3.1
1	S	409	LEU	3.1
1	W	28	VAL	3.1
2	X	69	GLY	3.1
1	U	252	ASP	3.1
1	C	250	GLU	3.1
1	E	250	GLU	3.1
1	W	64	GLU	3.1
1	O	307	GLN	3.1
1	W	344	PRO	3.1
1	W	423	PRO	3.1
1	E	246	GLY	3.1
1	W	232	TYR	3.1
1	W	416	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	S	429	VAL	3.1
1	S	81	ASP	3.1
1	S	195	ASP	3.1
1	W	22	GLU	3.1
1	Q	18	ASN	3.1
1	W	441	MET	3.1
1	U	260	THR	3.1
1	E	248	PRO	3.1
1	W	331	SER	3.1
1	W	459	PRO	3.1
1	U	346	GLY	3.1
1	Q	285	LEU	3.1
1	Q	320	VAL	3.1
1	S	276	TRP	3.1
1	U	309	LEU	3.1
2	X	14	TRP	3.1
2	X	52	LYS	3.1
1	Q	419	GLN	3.1
2	N	8	PHE	3.1
1	S	56	ARG	3.1
1	S	272	HIS	3.1
1	W	185	THR	3.1
2	T	16	SER	3.1
2	X	11	THR	3.1
1	Q	282	GLY	3.1
1	S	190	ALA	3.1
1	W	234	ALA	3.1
1	W	389	GLY	3.1
1	U	72	ASP	3.0
2	R	76	ASP	3.0
2	R	160	ASP	3.0
2	X	93	ILE	3.0
1	G	457	LEU	3.0
1	I	18	ASN	3.0
1	S	25	ARG	3.0
1	W	18	ASN	3.0
1	S	153	PHE	3.0
1	S	425	PHE	3.0
1	U	22	GLU	3.0
1	W	368	GLU	3.0
2	X	55	HIS	3.0
1	W	70	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	Q	310	GLY	3.0
1	Q	421	GLY	3.0
1	W	210	GLY	3.0
1	C	142	ALA	3.0
1	C	245	ALA	3.0
1	U	177	ASP	3.0
1	U	85	MET	3.0
1	U	433	TYR	3.0
1	W	250	GLU	3.0
1	U	296	TRP	3.0
1	S	229	SER	3.0
1	W	329	THR	3.0
1	G	313	GLY	3.0
1	M	310	GLY	3.0
1	S	55	GLY	3.0
1	S	228	CYS	3.0
1	S	281	PRO	3.0
1	S	289	GLY	3.0
1	W	42	ASP	3.0
1	S	305	ALA	3.0
1	S	434	ALA	3.0
1	W	364	ALA	3.0
2	N	162	ASN	3.0
1	E	253	LEU	3.0
1	S	232	TYR	3.0
1	U	422	HIS	3.0
1	U	431	TYR	3.0
1	W	40	TYR	3.0
2	J	16	SER	3.0
1	W	458	LYS	3.0
2	X	46	TRP	3.0
1	W	246	GLY	3.0
1	U	202	PRO	3.0
2	J	15	PRO	3.0
1	W	251	MET	3.0
1	S	69	GLU	3.0
1	U	350	ILE	3.0
1	C	244	LEU	2.9
1	M	253	LEU	2.9
2	V	119	VAL	2.9
1	Q	252	ASP	2.9
2	H	126	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	420	THR	2.9
1	K	421	GLY	2.9
1	S	299	GLY	2.9
1	W	176	TRP	2.9
2	T	162	ASN	2.9
1	W	174	ALA	2.9
1	U	258	ILE	2.9
1	K	89	LYS	2.9
1	W	453	SER	2.9
1	S	29	ASP	2.9
1	S	317	ARG	2.9
1	W	52	ARG	2.9
1	W	128	ASP	2.9
1	W	172	VAL	2.9
1	U	46	TYR	2.9
2	J	90	TYR	2.9
1	U	314	MET	2.9
1	W	398	GLY	2.9
2	T	127	THR	2.9
2	V	122	THR	2.9
2	X	58	MET	2.9
1	S	436	GLU	2.9
1	U	306	GLU	2.9
1	U	342	TRP	2.9
1	M	247	ILE	2.9
1	S	247	ILE	2.9
1	K	48	LEU	2.9
1	S	35	LEU	2.9
1	W	435	GLU	2.9
1	S	71	GLY	2.9
1	U	53	VAL	2.9
1	W	262	GLY	2.9
1	W	278	VAL	2.9
1	U	312	THR	2.9
1	W	46	TYR	2.9
2	V	124	THR	2.9
2	X	97	THR	2.9
1	U	263	ASN	2.9
1	W	428	ASN	2.9
1	M	281	PRO	2.9
1	S	444	HIS	2.9
1	U	332	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	307	GLN	2.9
1	U	162	GLN	2.9
1	U	224	ALA	2.9
1	U	403	LYS	2.9
1	A	424	ASP	2.9
1	S	92	SER	2.9
1	W	158	TRP	2.9
1	W	353	TRP	2.9
1	U	247	ILE	2.9
1	M	416	GLY	2.9
1	Q	414	GLY	2.9
2	X	105	ASN	2.8
1	U	402	TYR	2.8
1	W	347	PRO	2.8
2	V	10	LYS	2.8
1	S	302	ALA	2.8
1	W	199	ASP	2.8
1	W	57	SER	2.8
2	F	16	SER	2.8
1	U	324	MET	2.8
1	Q	253	LEU	2.8
1	W	50	LEU	2.8
1	W	171	LEU	2.8
1	W	399	LEU	2.8
1	O	313	GLY	2.8
1	W	282	GLY	2.8
1	M	260	THR	2.8
1	Q	259	PRO	2.8
1	S	192	PRO	2.8
2	X	107	PRO	2.8
2	X	31	TYR	2.8
2	V	13	GLU	2.8
1	U	57	SER	2.8
1	W	449	MET	2.8
2	X	57	PHE	2.8
1	U	330	CYS	2.8
1	W	175	ASN	2.8
1	A	421	GLY	2.8
1	U	321	GLY	2.8
1	S	161	LEU	2.8
1	W	161	LEU	2.8
2	V	23	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	W	342	TRP	2.8
1	W	456	THR	2.8
2	T	52	LYS	2.8
1	I	31	GLU	2.8
1	W	225	GLU	2.8
1	W	290	PRO	2.8
1	U	316	VAL	2.8
1	K	182	ASP	2.8
1	S	370	TYR	2.8
1	M	283	SER	2.8
1	Q	142	ALA	2.8
1	U	207	ALA	2.8
1	W	404	ALA	2.8
2	H	9	PHE	2.8
2	X	9	PHE	2.8
1	U	337	ASN	2.8
1	W	337	ASN	2.8
1	W	348	ASN	2.8
1	Q	321	GLY	2.8
1	S	102	HIS	2.8
1	W	323	HIS	2.8
1	U	60	LEU	2.8
1	U	356	THR	2.8
1	S	315	PRO	2.8
1	Q	19	TRP	2.8
2	X	78	ASP	2.8
1	S	287	VAL	2.8
1	Q	286	ALA	2.7
1	S	428	ASN	2.7
1	U	101	ARG	2.7
1	W	318	ARG	2.7
2	X	103	ALA	2.7
1	W	291	LYS	2.7
2	R	9	PHE	2.7
1	U	272	HIS	2.7
1	W	390	GLU	2.7
2	X	84	GLU	2.7
1	A	312	THR	2.7
1	W	260	THR	2.7
1	W	356	THR	2.7
1	C	388	ASP	2.7
1	U	395	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	W	336	ILE	2.7
2	X	99[A]	ASP	2.7
1	W	452	PRO	2.7
1	A	255	GLN	2.7
1	U	25	ARG	2.7
1	W	165	VAL	2.7
1	S	410	ASN	2.7
1	G	156	ALA	2.7
1	U	64	GLU	2.7
1	U	132	LYS	2.7
1	U	63	HIS	2.7
1	G	120	CYS	2.7
1	W	357	LEU	2.7
1	S	363	PRO	2.7
1	S	400	ARG	2.7
1	U	56	ARG	2.7
1	U	87	ARG	2.7
1	W	212	GLN	2.7
1	E	18	ASN	2.7
2	D	162	ASN	2.7
1	U	451	GLU	2.7
2	V	22	GLU	2.7
1	W	443	HIS	2.7
1	S	180	ALA	2.7
1	U	19	TRP	2.7
1	W	301	ALA	2.7
1	O	421	GLY	2.7
1	S	277	TYR	2.7
1	S	73	PHE	2.7
1	U	36	ASP	2.7
1	Q	312	THR	2.7
1	E	307	GLN	2.7
1	S	48	LEU	2.7
1	U	315	PRO	2.7
1	U	357	LEU	2.7
1	U	418	SER	2.7
1	W	181	PRO	2.7
1	W	333	LEU	2.7
2	V	74	SER	2.7
2	V	177	SER	2.7
1	S	306	GLU	2.7
1	S	136	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	W	352	VAL	2.7
1	W	383	VAL	2.7
1	E	245	ALA	2.6
1	S	321	GLY	2.6
1	U	174	ALA	2.6
1	U	204	GLY	2.6
1	W	131	GLY	2.6
1	W	197	MET	2.6
1	W	195	ASP	2.6
2	X	39	ASP	2.6
2	X	56	TYR	2.6
2	X	41	ARG	2.6
2	X	82	PHE	2.6
1	M	459	PRO	2.6
1	U	116	LYS	2.6
1	W	92	SER	2.6
2	J	17	LYS	2.6
2	X	108	SER	2.6
1	S	183	LEU	2.6
2	X	184	LEU	2.6
1	U	39	ILE	2.6
2	X	66	ILE	2.6
1	E	421	GLY	2.6
1	S	427	GLY	2.6
1	S	411	ALA	2.6
1	U	111	ASP	2.6
2	T	126	ASP	2.6
2	T	159	ALA	2.6
1	U	435	GLU	2.6
1	S	186	TYR	2.6
2	X	73	TYR	2.6
1	S	167	THR	2.6
1	W	341	THR	2.6
1	S	100	CYS	2.6
1	A	283	SER	2.6
1	S	443	HIS	2.6
2	B	7	HIS	2.6
1	S	93	ILE	2.6
2	T	27	ILE	2.6
2	X	118	ILE	2.6
2	T	67	ARG	2.6
1	U	30	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	U	170	GLY	2.6
1	U	412	GLN	2.6
2	F	101	GLY	2.6
1	Q	278	VAL	2.6
1	S	358	VAL	2.6
1	U	213	LYS	2.6
1	S	238	THR	2.6
2	V	63	ASN	2.6
2	X	181	SER	2.6
1	C	259	PRO	2.6
1	O	423	PRO	2.6
1	S	334	PRO	2.6
1	S	222	PHE	2.6
1	U	276	TRP	2.6
1	K	457	LEU	2.6
1	S	399	LEU	2.6
1	U	50	LEU	2.6
1	W	105	MET	2.6
1	W	439	ARG	2.6
2	P	77	GLN	2.6
1	I	298	GLU	2.6
2	D	68	GLU	2.6
1	E	26	GLY	2.6
1	S	209	GLY	2.6
1	A	142	ALA	2.6
2	V	62	THR	2.6
1	K	259	PRO	2.5
1	S	417	ARG	2.5
1	W	191	ARG	2.5
1	K	143	PHE	2.5
1	K	251	MET	2.5
1	A	22	GLU	2.5
1	W	49	GLU	2.5
1	I	48	LEU	2.5
1	W	154	ASP	2.5
2	D	160	ASP	2.5
2	X	49	LEU	2.5
1	S	89	LYS	2.5
1	S	243	ILE	2.5
1	U	282	GLY	2.5
1	U	299	GLY	2.5
1	U	234	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	W	377	ASN	2.5
1	U	241	SER	2.5
1	W	450	SER	2.5
1	W	206	VAL	2.5
1	W	393	VAL	2.5
1	M	420	THR	2.5
1	W	38	ARG	2.5
1	W	371	ARG	2.5
1	S	137	PRO	2.5
1	S	157	GLU	2.5
1	U	49	GLU	2.5
1	U	248	PRO	2.5
1	U	334	PRO	2.5
2	R	70	GLU	2.5
1	S	46	TYR	2.5
1	S	433	TYR	2.5
1	W	77	TYR	2.5
2	F	51	ASP	2.5
2	X	154	ASP	2.5
1	M	389	GLY	2.5
1	U	124	GLY	2.5
1	U	246	GLY	2.5
2	J	161	ASN	2.5
1	K	180	ALA	2.5
1	U	354	ALA	2.5
2	J	123	ALA	2.5
2	T	123	ALA	2.5
1	G	312	THR	2.5
1	I	257	GLN	2.5
1	M	303	GLU	2.5
1	S	86	VAL	2.5
1	S	105	MET	2.5
1	S	278	VAL	2.5
1	U	205	THR	2.5
1	U	255	GLN	2.5
1	U	78	MET	2.5
1	U	278	VAL	2.5
1	W	396	GLN	2.5
2	X	171	THR	2.5
1	W	324	MET	2.5
2	V	58	MET	2.5
1	S	199	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	U	359	ASP	2.5
1	A	397	LYS	2.5
1	K	26	GLY	2.5
1	U	398	GLY	2.5
1	W	73	PHE	2.5
2	X	164	GLY	2.5
1	W	374	ASN	2.5
2	H	162	ASN	2.5
2	B	16	SER	2.5
1	G	419	GLN	2.5
1	U	365	GLU	2.5
1	U	369	GLU	2.5
1	U	436	GLU	2.5
2	J	87	GLU	2.5
1	S	286	ALA	2.5
2	X	89	MET	2.5
1	Q	189	ASP	2.5
1	S	177	ASP	2.5
1	S	196	VAL	2.5
2	X	95	LYS	2.5
1	W	308	ARG	2.4
2	D	67	ARG	2.4
1	A	18	ASN	2.4
1	U	348	ASN	2.4
1	E	457	LEU	2.4
1	S	327	PHE	2.4
1	W	355	PHE	2.4
1	W	444	HIS	2.4
2	X	60	LEU	2.4
1	S	280	GLU	2.4
1	S	303	GLU	2.4
1	S	451	GLU	2.4
1	G	129	ILE	2.4
1	S	375	ILE	2.4
1	O	261	LYS	2.4
1	S	293	THR	2.4
1	S	360	ALA	2.4
1	S	405	LYS	2.4
2	V	175	ASP	2.4
1	S	158	TRP	2.4
1	A	423	PRO	2.4
1	M	316	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	U	347	PRO	2.4
1	W	136	VAL	2.4
1	G	204	GLY	2.4
2	X	183	ASN	2.4
1	K	257	GLN	2.4
1	K	309	LEU	2.4
1	M	453	SER	2.4
1	Q	254	SER	2.4
1	S	168	TYR	2.4
1	S	309	LEU	2.4
1	S	442	TYR	2.4
1	U	74	LEU	2.4
2	T	31	TYR	2.4
1	W	173	PHE	2.4
2	V	128	PHE	2.4
1	C	261	LYS	2.4
1	S	94	LYS	2.4
2	R	10	LYS	2.4
2	V	118	ILE	2.4
2	X	175	ASP	2.4
1	S	166	ALA	2.4
1	U	404	ALA	2.4
1	W	317	ARG	2.4
1	G	294	GLN	2.4
1	M	294	GLN	2.4
1	S	263	ASN	2.4
2	R	162	ASN	2.4
1	U	26	GLY	2.4
1	U	262	GLY	2.4
1	U	401	GLY	2.4
1	W	335	GLY	2.4
1	A	48	LEU	2.4
1	I	253	LEU	2.4
1	S	50	LEU	2.4
1	U	35	LEU	2.4
1	W	367	LYS	2.4
2	X	169	LYS	2.4
1	O	143	PHE	2.4
1	S	332	PHE	2.4
1	A	417	ARG	2.4
2	J	66	ILE	2.4
1	U	437	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	S	298	GLU	2.4
1	U	184	GLU	2.4
2	X	44	GLU	2.4
1	O	259	PRO	2.4
1	W	137	PRO	2.4
1	W	264	GLN	2.4
2	T	125	PRO	2.4
1	W	263	ASN	2.4
1	S	28	VAL	2.4
1	S	134	VAL	2.4
1	W	382	GLY	2.4
1	W	182	ASP	2.3
2	T	22	GLU	2.3
2	X	142	GLU	2.3
1	K	419	GLN	2.3
1	O	255	GLN	2.3
1	O	257	GLN	2.3
1	E	302	ALA	2.3
1	S	68	PRO	2.3
1	A	310	GLY	2.3
1	U	113	GLY	2.3
1	S	403	LYS	2.3
1	U	261	LYS	2.3
2	P	10	LYS	2.3
1	O	320	VAL	2.3
1	C	182	ASP	2.3
2	X	28	GLU	2.3
1	K	285	LEU	2.3
2	X	37	LEU	2.3
1	W	119	THR	2.3
2	P	9	PHE	2.3
1	K	389	GLY	2.3
1	W	397	LYS	2.3
2	V	17	LYS	2.3
2	X	16	SER	2.3
1	S	439	ARG	2.3
2	F	67	ARG	2.3
1	S	141	GLU	2.3
1	S	368	GLU	2.3
1	W	47	GLU	2.3
1	W	280	GLU	2.3
1	C	257	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	W	30	GLN	2.3
1	S	125	TRP	2.3
1	Q	311	HIS	2.3
1	S	114	ASN	2.3
2	T	25	ASN	2.3
1	I	143	PHE	2.3
2	D	90	TYR	2.3
1	M	234	ALA	2.3
1	G	246	GLY	2.3
1	S	318	ARG	2.3
1	S	395	ILE	2.3
1	W	93	ILE	2.3
1	W	321	GLY	2.3
1	W	372	ARG	2.3
1	E	283	SER	2.3
1	M	418	SER	2.3
2	R	16	SER	2.3
1	E	303	GLU	2.3
1	S	36	ASP	2.3
1	S	139	GLU	2.3
1	S	388	ASP	2.3
1	U	80	GLU	2.3
1	S	88	GLN	2.3
1	S	95	VAL	2.3
1	E	167	THR	2.3
1	S	187	LEU	2.3
1	W	61	LEU	2.3
2	X	62	THR	2.3
1	U	38	ARG	2.2
1	A	157	GLU	2.2
1	C	455	ALA	2.2
1	I	414	GLY	2.2
1	K	31	GLU	2.2
1	Q	335	GLY	2.2
1	S	22	GLU	2.2
1	S	438	ALA	2.2
1	U	275	GLY	2.2
1	U	298	GLU	2.2
1	W	184	GLU	2.2
2	F	129	GLU	2.2
1	Q	388	ASP	2.2
1	W	279	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	160	ASP	2.2
1	M	307	GLN	2.2
1	U	257	GLN	2.2
1	W	134	VAL	2.2
1	S	251	MET	2.2
1	O	260	THR	2.2
1	Q	20	THR	2.2
1	U	266	ARG	2.2
1	W	25	ARG	2.2
1	W	417	ARG	2.2
1	G	306	GLU	2.2
1	M	365	GLU	2.2
2	X	34	GLU	2.2
1	I	379	SER	2.2
1	Q	255	GLN	2.2
1	U	419	GLN	2.2
1	O	142	ALA	2.2
2	X	160	ASP	2.2
1	S	122	TYR	2.2
1	K	428	ASN	2.2
1	O	311	HIS	2.2
1	S	132	LYS	2.2
1	U	441	MET	2.2
1	K	429	VAL	2.2
1	S	320	VAL	2.2
1	I	420	THR	2.2
1	O	294	GLN	2.2
1	S	179	GLN	2.2
1	S	412	GLN	2.2
1	W	424	ASP	2.2
1	O	256	ALA	2.2
1	Q	203	ALA	2.2
1	W	112	ALA	2.2
1	W	130	ALA	2.2
2	L	159	ALA	2.2
2	F	90	TYR	2.2
1	E	311	HIS	2.2
1	G	19	TRP	2.2
1	S	445	TRP	2.2
1	K	417	ARG	2.2
1	U	197	MET	2.2
1	S	53	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	257	GLN	2.2
1	U	88	GLN	2.2
2	L	160	ASP	2.2
1	C	389	GLY	2.2
1	K	321	GLY	2.2
1	S	170	GLY	2.2
1	S	253	LEU	2.2
1	U	430	GLY	2.2
1	W	401	GLY	2.2
1	Q	301	ALA	2.2
1	Q	438	ALA	2.2
1	S	174	ALA	2.2
1	S	32	LYS	2.2
1	U	164	ARG	2.2
1	W	169	LYS	2.2
2	R	67	ARG	2.2
1	U	288	MET	2.1
2	X	81	HIS	2.1
1	G	143	PHE	2.1
1	S	40	TYR	2.1
1	S	49	GLU	2.1
1	U	51	GLU	2.1
1	W	138	PHE	2.1
1	W	222	PHE	2.1
1	W	451	GLU	2.1
1	U	307	GLN	2.1
2	X	36	GLN	2.1
1	A	456	THR	2.1
1	K	278	VAL	2.1
1	S	236	THR	2.1
1	U	287	VAL	2.1
1	U	341	THR	2.1
1	C	313	GLY	2.1
1	E	389	GLY	2.1
1	I	321	GLY	2.1
1	U	421	GLY	2.1
1	E	417	ARG	2.1
1	M	309	LEU	2.1
1	O	285	LEU	2.1
1	S	248	PRO	2.1
1	S	333	LEU	2.1
1	U	155	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	U	317	ARG	2.1
1	U	400	ARG	2.1
1	W	155	LYS	2.1
1	W	300	PRO	2.1
1	W	340	ARG	2.1
1	W	405	LYS	2.1
2	D	52	LYS	2.1
1	U	157	GLU	2.1
1	U	303	GLU	2.1
1	U	311	HIS	2.1
2	J	18	ALA	2.1
1	K	294	GLN	2.1
1	S	129	ILE	2.1
1	U	370	TYR	2.1
1	I	20	THR	2.1
1	A	372	ARG	2.1
1	C	417	ARG	2.1
1	M	432	VAL	2.1
1	Q	313	GLY	2.1
1	U	200	ARG	2.1
1	U	372	ARG	2.1
1	W	200	ARG	2.1
1	W	215	VAL	2.1
1	U	221	LYS	2.1
1	U	367	LYS	2.1
1	W	94	LYS	2.1
1	S	64	GLU	2.1
1	G	423	PRO	2.1
1	S	290	PRO	2.1
1	W	102	HIS	2.1
2	L	7	HIS	2.1
1	U	333	LEU	2.1
1	U	428	ASN	2.1
2	X	38	LEU	2.1
1	O	267	ALA	2.1
1	W	322	GLN	2.1
1	S	227	PHE	2.1
1	U	222	PHE	2.1
2	D	187	PHE	2.1
2	X	12	PHE	2.1
2	X	187	PHE	2.1
1	I	247	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	U	199	ASP	2.1
1	Q	418	SER	2.1
1	S	331	SER	2.1
2	D	33	ARG	2.1
2	X	158	ARG	2.1
1	C	280	GLU	2.1
1	U	291	LYS	2.1
1	W	31	GLU	2.1
1	S	113	GLY	2.1
2	T	164	GLY	2.1
1	C	19	TRP	2.1
1	Q	316	VAL	2.1
1	S	82	PRO	2.1
1	W	179	GLN	2.1
1	W	412	GLN	2.1
2	X	59	PRO	2.1
2	X	77	GLN	2.1
1	Q	228	CYS	2.1
1	S	357	LEU	2.1
1	U	27	LEU	2.1
1	Q	23	ALA	2.1
1	Q	302	ALA	2.1
1	S	437	ALA	2.1
1	W	166	ALA	2.1
1	O	128	ASP	2.1
1	W	387	ASP	2.1
1	I	250	GLU	2.0
1	Q	365	GLU	2.0
2	T	188	PHE	2.0
1	I	453	SER	2.0
1	M	251	MET	2.0
1	O	420	THR	2.0
1	W	76	THR	2.0
1	A	55	GLY	2.0
1	G	421	GLY	2.0
1	S	389	GLY	2.0
1	U	335	GLY	2.0
1	E	294	GLN	2.0
1	G	307	GLN	2.0
1	S	391	ASN	2.0
1	U	43	GLN	2.0
1	M	248	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	249	PRO	2.0
1	S	249	PRO	2.0
1	W	68	PRO	2.0
1	U	445	TRP	2.0
2	V	156	LEU	2.0
1	S	279	ASP	2.0
1	U	191	ARG	2.0
1	W	156	ALA	2.0
2	H	123	ALA	2.0
2	T	19	ALA	2.0
1	W	36	ASP	2.0
1	W	80	GLU	2.0
1	U	458	LYS	2.0
1	E	254	SER	2.0
1	S	413	MET	2.0
1	W	319	MET	2.0
1	S	326	ILE	2.0
1	C	419	GLN	2.0
1	S	373	HIS	2.0
2	V	188	PHE	2.0
2	X	172	ILE	2.0
1	O	185	THR	2.0
1	O	381	GLY	2.0
1	Q	294	GLN	2.0
1	W	299	GLY	2.0
1	W	386	GLN	2.0
1	S	135	ASN	2.0
1	S	160	PRO	2.0
2	V	130	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BNL	S	462	12/12	0.76	0.19	56,57,58,58	12
5	BNL	W	462	12/12	0.77	0.15	80,81,83,83	0
5	BNL	C	462	12/12	0.79	0.11	33,34,35,35	0
5	BNL	E	462	12/12	0.80	0.13	47,50,52,52	0
5	BNL	Q	462	12/12	0.80	0.15	56,58,60,60	0
3	FES	U	460	4/4	0.82	0.17	65,66,67,67	4
5	BNL	M	462	12/12	0.85	0.11	49,50,52,52	0
5	BNL	O	462	12/12	0.86	0.09	38,38,40,40	0
3	FES	S	460	4/4	0.86	0.24	82,83,84,86	0
5	BNL	K	462	12/12	0.88	0.09	42,43,44,44	0
5	BNL	I	462	12/12	0.89	0.08	32,32,33,33	0
4	FE2	W	461	1/1	0.91	0.10	75,75,75,75	0
4	FE2	Q	461	1/1	0.95	0.05	50,50,50,50	0
4	FE2	S	461	1/1	0.95	0.08	68,68,68,68	0
3	FES	W	460	4/4	0.95	0.09	55,56,57,57	0
3	FES	G	460	4/4	0.96	0.08	33,34,35,35	0
3	FES	O	460	4/4	0.97	0.06	33,34,34,34	0
4	FE2	U	461	1/1	0.97	0.11	62,62,62,62	0
4	FE2	O	461	1/1	0.98	0.05	26,26,26,26	0
3	FES	Q	460	4/4	0.98	0.05	29,30,30,31	0
3	FES	A	460	4/4	0.98	0.05	26,26,26,26	0
3	FES	I	460	4/4	0.98	0.05	28,28,28,28	0
3	FES	C	460	4/4	0.98	0.06	26,26,26,26	0
4	FE2	C	461	1/1	0.98	0.03	25,25,25,25	0
4	FE2	E	461	1/1	0.98	0.03	31,31,31,31	0
3	FES	K	460	4/4	0.99	0.08	23,24,24,24	0
3	FES	M	460	4/4	0.99	0.04	24,24,24,24	0
3	FES	E	460	4/4	0.99	0.05	24,24,24,25	0
4	FE2	G	461	1/1	0.99	0.02	23,23,23,23	0
4	FE2	I	461	1/1	0.99	0.03	25,25,25,25	0
4	FE2	K	461	1/1	0.99	0.03	30,30,30,30	0
4	FE2	M	461	1/1	0.99	0.03	29,29,29,29	0
4	FE2	A	461	1/1	1.00	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.