



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2016 – 03:38 PM EDT

PDB ID : 5AEW
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

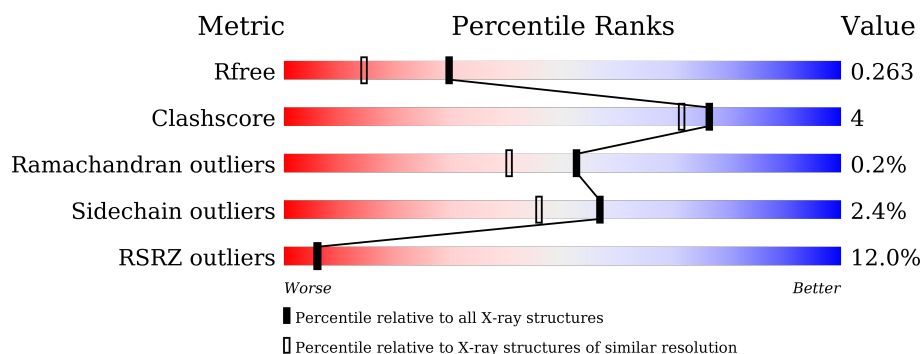
1 Overall quality at a glance

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}	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	459	<div> <div></div> <div>87% 7% 6%</div> </div>
1	C	459	<div> <div>4%</div> <div>89% 5% 6%</div> </div>
1	E	459	<div> <div>5%</div> <div>88% 6% 6%</div> </div>
1	G	459	<div> <div>4%</div> <div>88% 5% 6%</div> </div>
1	I	459	<div> <div>3%</div> <div>83% 10% 6%</div> </div>
1	K	459	<div> <div>6%</div> <div>87% 7% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
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	Q	460	-	-	X	-
3	FES	W	460	-	-	X	-
5	BNL	E	462	-	-	-	X
5	BNL	Q	462	-	-	-	X
5	BNL	S	462	-	-	-	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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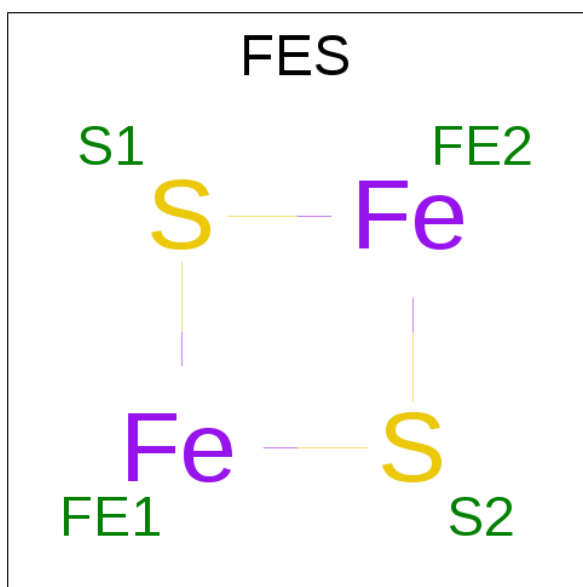
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Chain	Residue	Modelled	Actual	Comment	Reference
W	341	THR	ILE	ENGINEERED MUTATION	UNP P37333

- 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 (three-letter code: FES) (formula: Fe₂S₂).

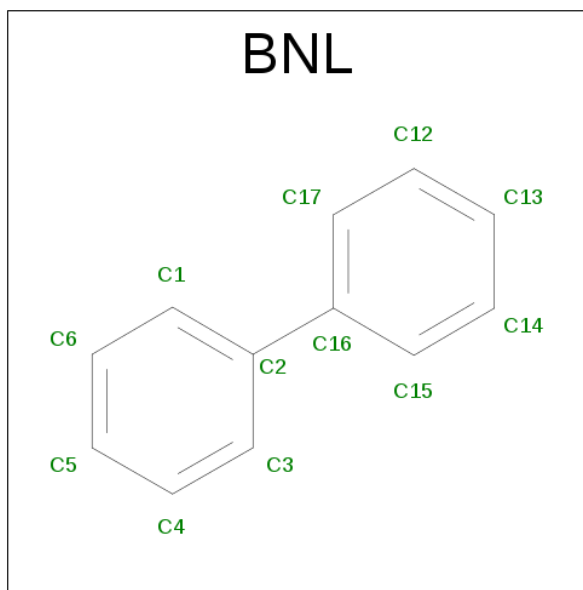


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		
3	M	1	Total	Fe	S	0	0
			4	2	2		
3	O	1	Total	Fe	S	0	0
			4	2	2		
3	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 (three-letter code: FE2) (formula: Fe).

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

- Molecule 5 is BIPHENYL (three-letter code: BNL) (formula: C₁₂H₁₀).



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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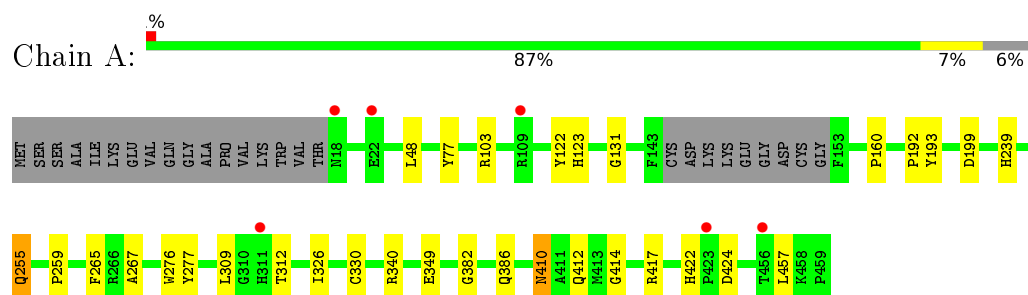
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	130	Total 130	O 130	0	0
6	M	204	Total 204	O 204	0	0
6	N	101	Total 101	O 101	0	0
6	O	205	Total 205	O 205	0	0
6	P	108	Total 108	O 108	0	0
6	Q	150	Total 150	O 150	0	0
6	R	124	Total 124	O 124	0	0
6	S	95	Total 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

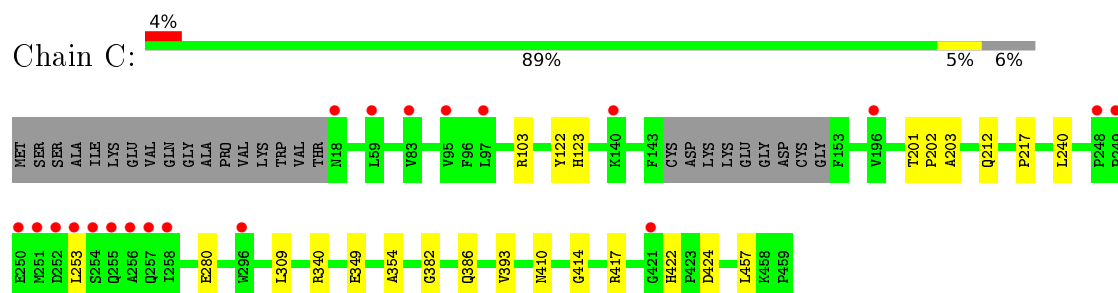
3 Residue-property plots

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

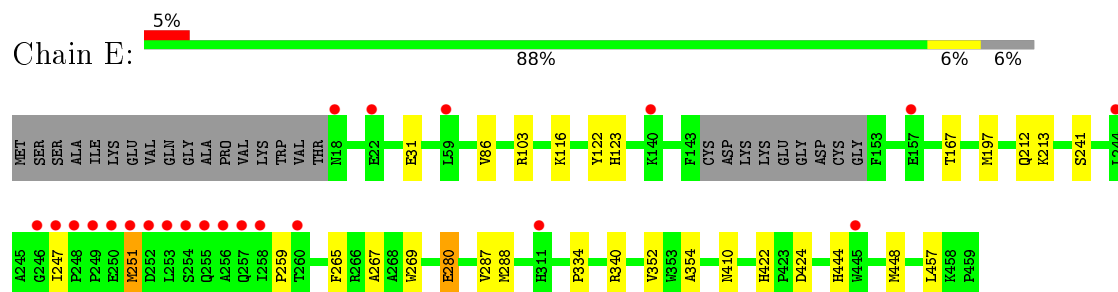
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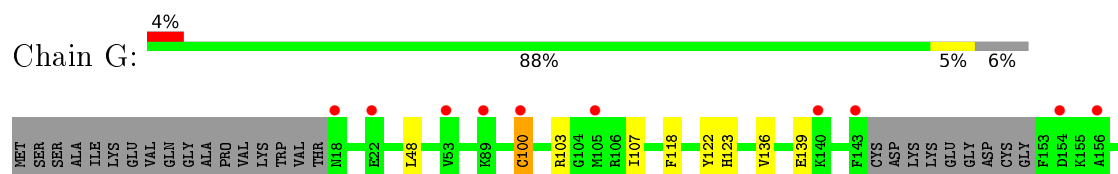
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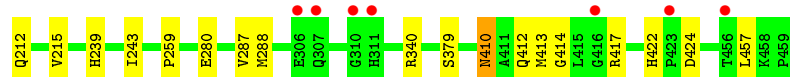


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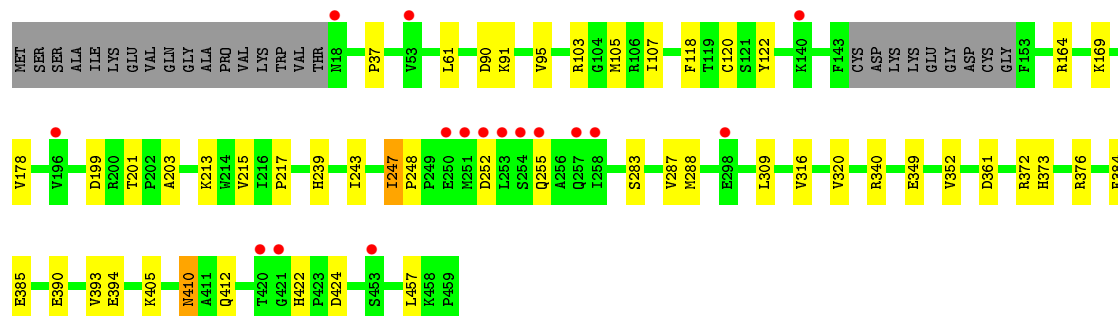
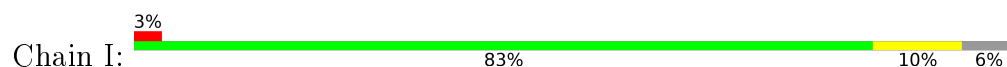


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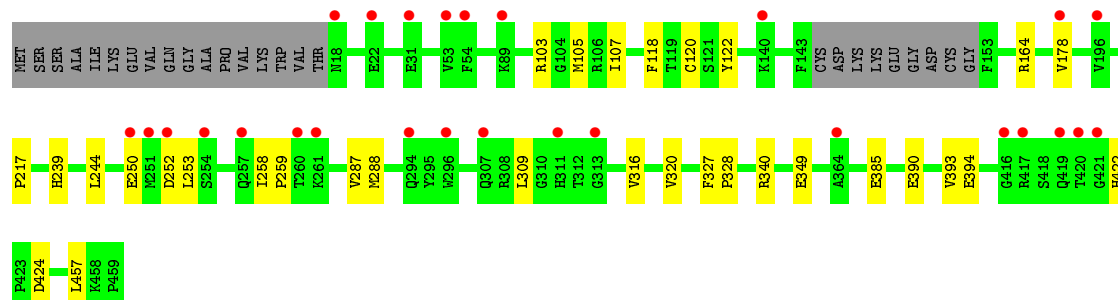
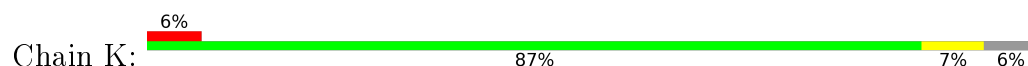




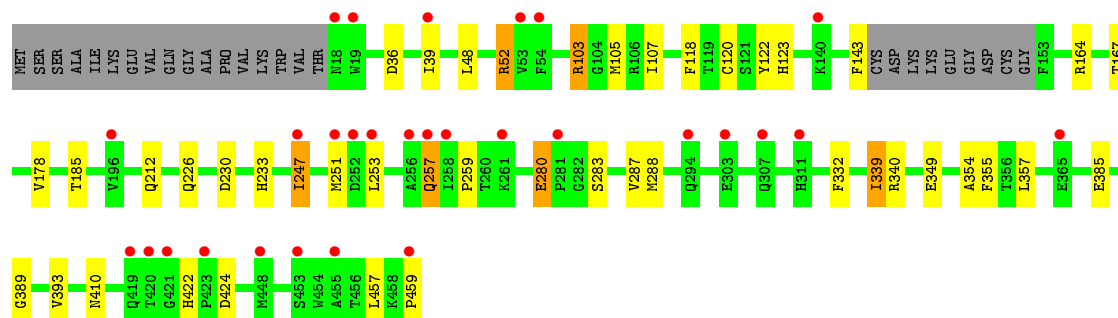
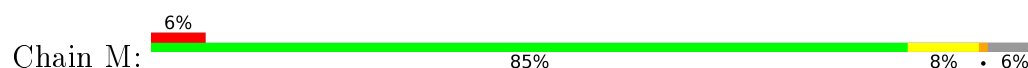
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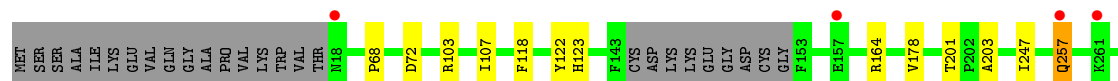
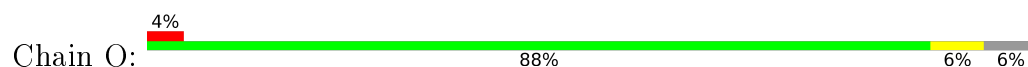
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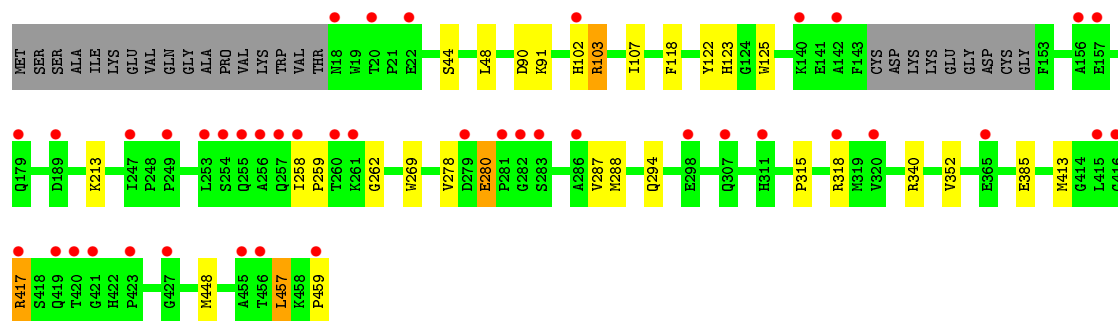
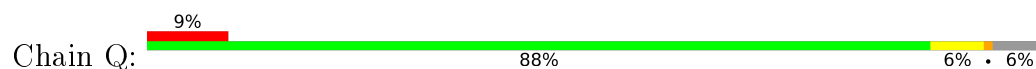


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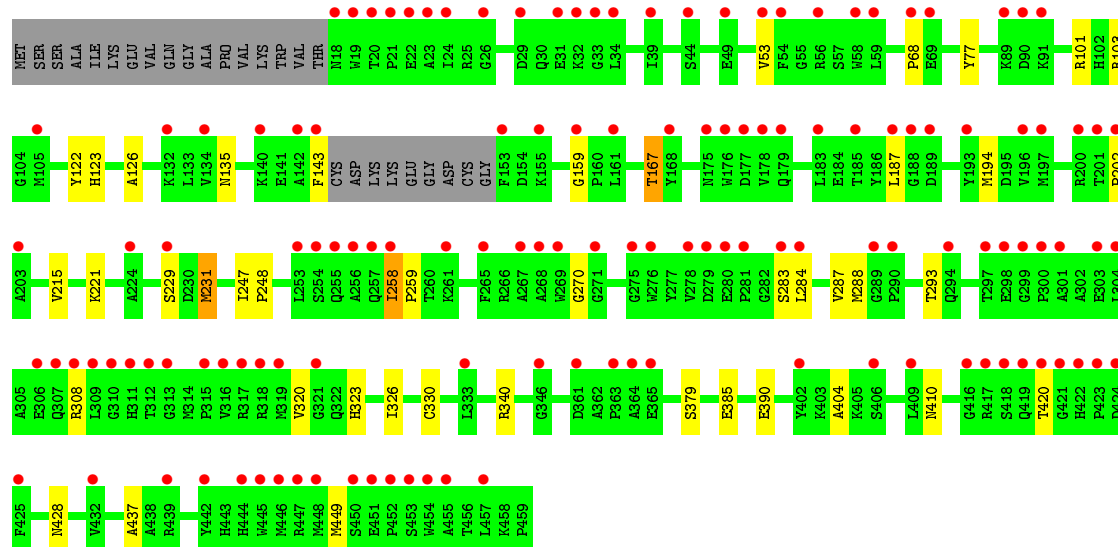
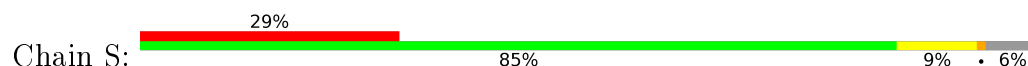




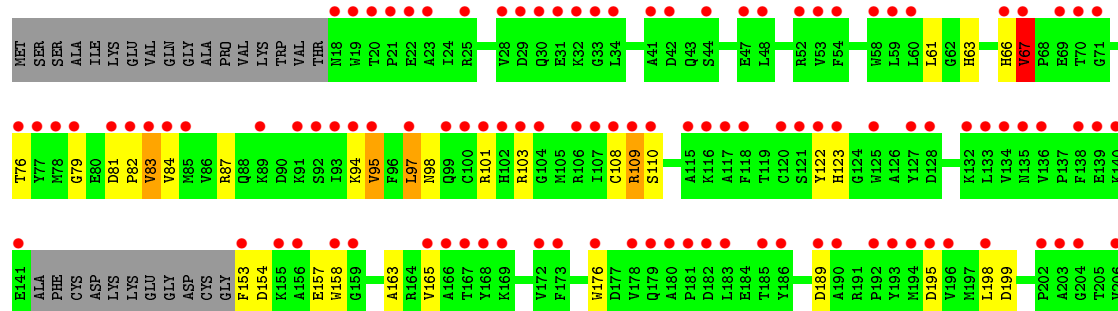
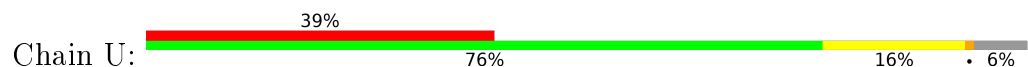
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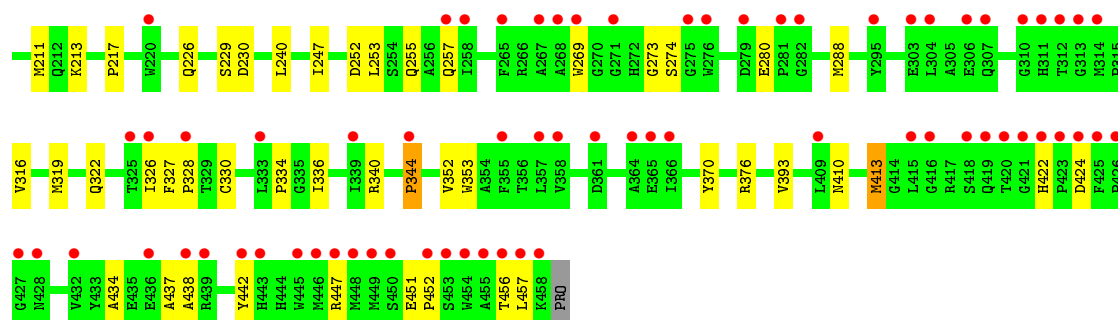


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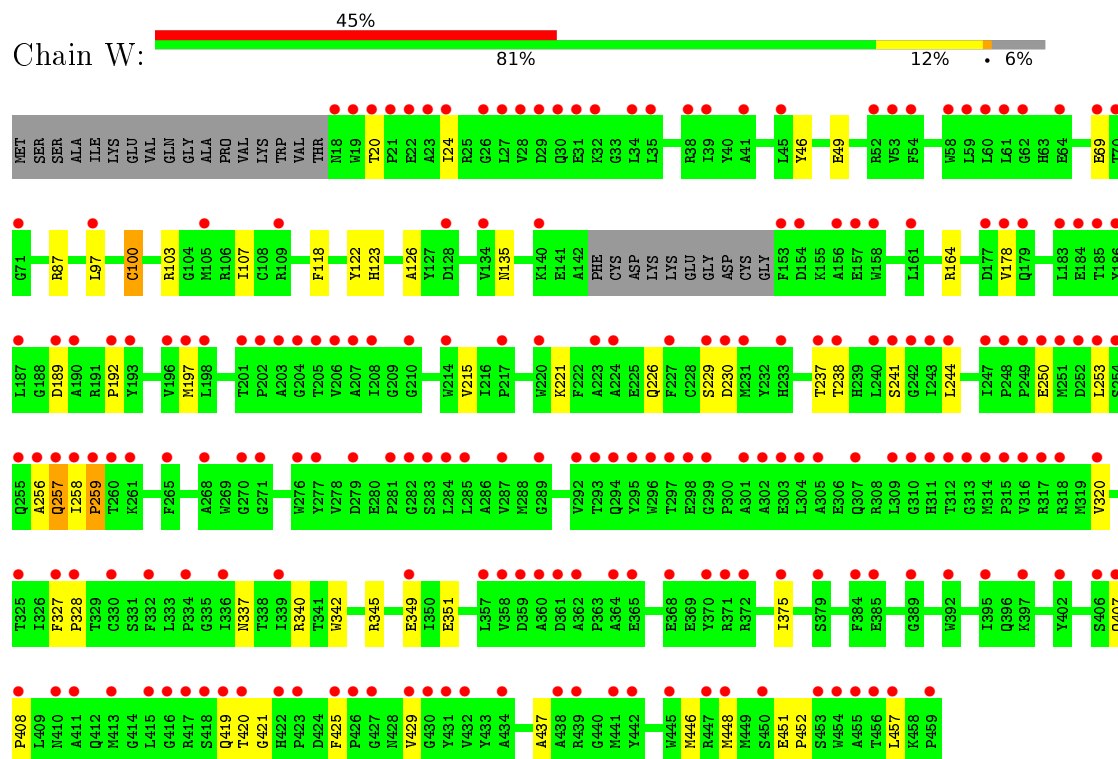


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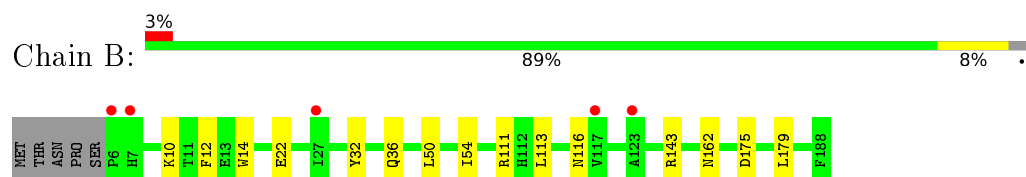




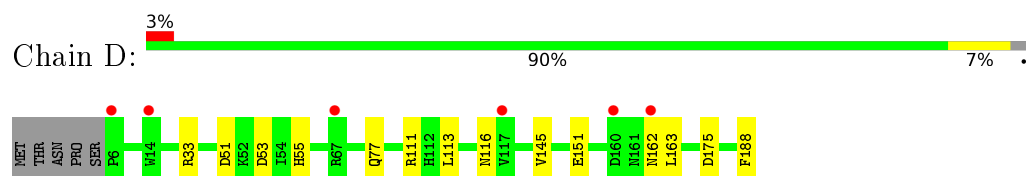
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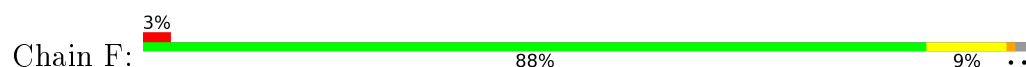
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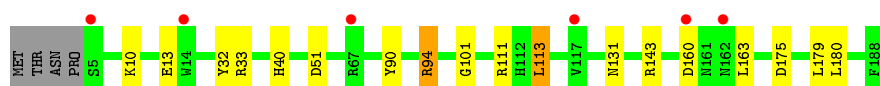


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

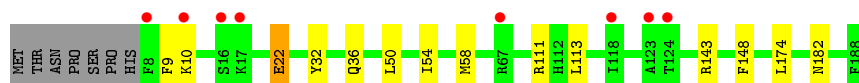
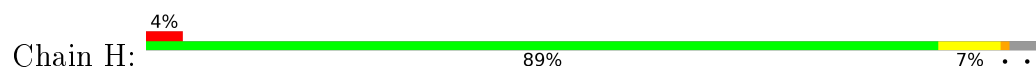


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

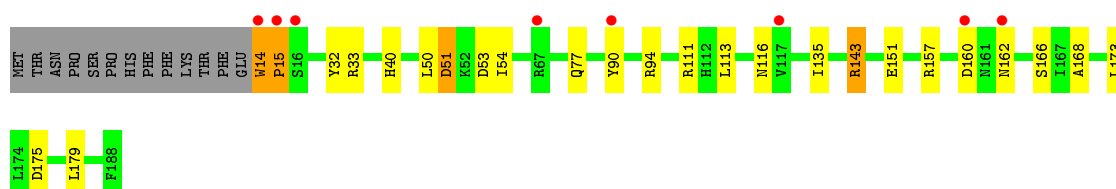
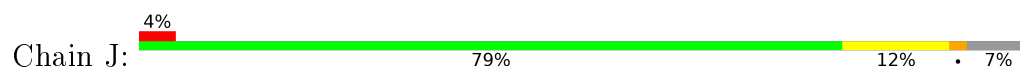




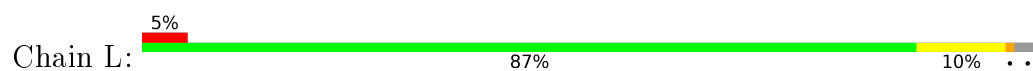
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



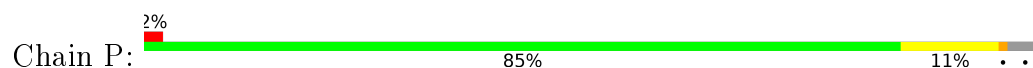
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



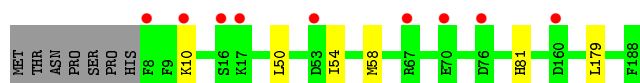
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



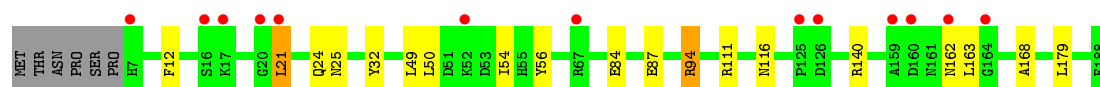
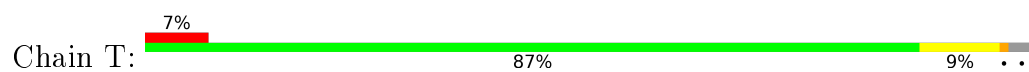
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



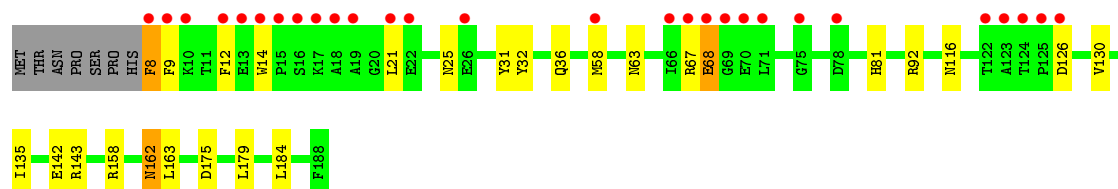
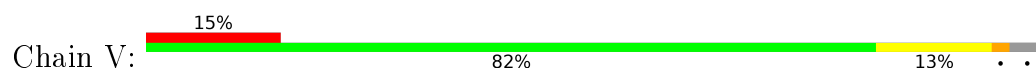
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



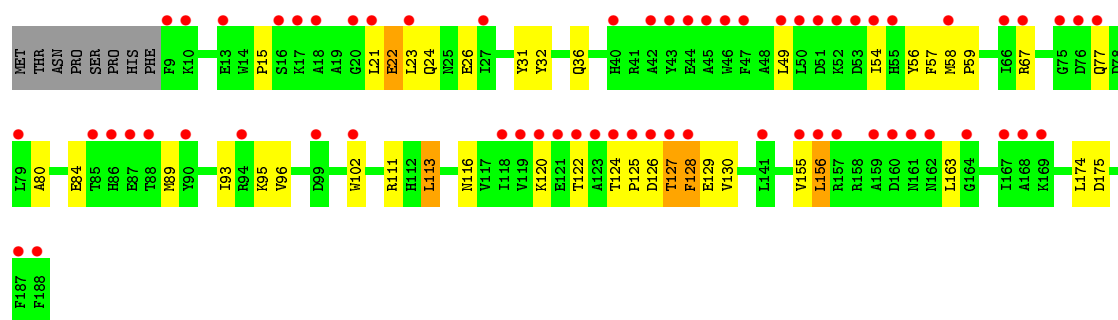
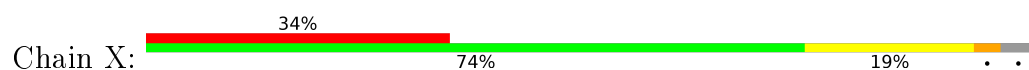
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	132.77Å 133.19Å 133.97Å 102.31° 102.54° 104.54°	Depositor
Resolution (Å)	23.34 – 1.88 23.33 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.1 (23.34-1.88) 87.2 (23.33-1.88)	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 (5.28%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.4	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, FES, BNL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/3547	0.55	0/4814
1	C	0.38	0/3549	0.56	0/4816
1	E	0.37	0/3530	0.56	0/4792
1	G	0.36	0/3530	0.56	1/4792 (0.0%)
1	I	0.36	0/3538	0.55	0/4802
1	K	0.35	0/3530	0.53	0/4792
1	M	0.35	0/3539	0.53	0/4804
1	O	0.33	0/3538	0.52	0/4802
1	Q	0.34	0/3530	0.53	0/4792
1	S	0.31	0/3530	0.49	0/4792
1	U	0.31	0/3505	0.50	0/4757
1	W	0.30	0/3518	0.48	0/4776
2	B	0.39	0/1569	0.59	0/2121
2	D	0.40	0/1578	0.62	0/2133
2	F	0.40	0/1584	0.63	0/2142
2	H	0.38	0/1550	0.58	0/2095
2	J	0.40	0/1489	0.60	1/2014 (0.0%)
2	L	0.38	0/1561	0.56	0/2110
2	N	0.38	0/1561	0.57	0/2110
2	P	0.39	0/1566	0.58	0/2117
2	R	0.37	0/1542	0.55	0/2084
2	T	0.35	0/1553	0.53	0/2099
2	V	0.34	0/1542	0.53	0/2084
2	X	0.31	0/1538	0.51	0/2079
All	All	0.35	0/61017	0.54	2/82719 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	143	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	G	100	CYS	CA-CB-SG	5.08	123.14	114.00

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	20	0
1	C	3444	0	3305	12	0
1	E	3428	0	3284	17	0
1	G	3428	0	3284	16	0
1	I	3433	0	3293	26	0
1	K	3428	0	3284	15	0
1	M	3434	0	3292	29	0
1	O	3433	0	3293	15	0
1	Q	3428	0	3284	17	0
1	S	3428	0	3284	26	0
1	U	3405	0	3263	61	0
1	W	3417	0	3275	39	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	15	0
2	J	1454	0	1407	23	0
2	L	1522	0	1467	17	0
2	N	1524	0	1471	16	0
2	P	1522	0	1473	15	0
2	R	1507	0	1456	3	0
2	T	1517	0	1463	20	0
2	V	1507	0	1456	32	0
2	X	1501	0	1451	35	0
3	A	4	0	0	1	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	443	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 (443) 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:V:67:ARG:O	2:V:68:GLU:HG3	1.21	1.28
1:E:167:THR:HB	6:E:2123:HOH:O	1.39	1.19
2:H:58:MET:HE3	2:H:174:LEU:HD22	1.28	1.14
1:U:109:ARG:HG3	1:U:109:ARG:HH11	1.01	1.12
2:V:67:ARG:O	2:V:68:GLU:CG	2.01	1.08
1:U:67:VAL:HG22	1:U:67:VAL:O	1.51	1.07
1:K:287:VAL:HG12	1:K:288:MET:HE3	1.40	1.04
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	1.01
1:U:109:ARG:HH11	1:U:109:ARG:CG	1.71	1.01
1:M:339:ILE:HD11	1:M:357:LEU:HG	1.43	1.00
1:U:67:VAL:CG2	1:U:67:VAL:O	2.10	0.99
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:W:237:THR:O	2:X:102:TRP:HZ3	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:U:109:ARG:HG3	1:U:109:ARG:NH1	1.81	0.86
5:E:462:BNL:H15	6:E:2167:HOH:O	1.75	0.85
1:S:53:VAL:HG23	6:S:2092:HOH:O	1.80	0.82
2:T:94:ARG:HH11	2:T:94:ARG:HG3	1.43	0.82
1:E:287:VAL:HG12	1:E:288:MET:HE2	1.59	0.82
1:G:287:VAL:HG12	1:G:288:MET:CE	2.10	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: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:W:256:ALA:O	1:W:257:GLN:O	2.03	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:W:237:THR:O	2:X:102:TRP:CZ3	2.38	0.76
1:W:189:ASP:O	1:W:192:PRO:HD2	1.85	0.75
1:Q:417:ARG:HH11	1:Q:417:ARG:HG3	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:153:PHE:CE1	1:U:158:TRP:CD1	2.75	0.74
2:H:58:MET:HE3	2:H:174:LEU:CD2	2.15	0.73
1:U:195:ASP:HA	6:U:2058:HOH:O	1.87	0.73
1:U:82:PRO:O	1:U:83:VAL:O	2.07	0.73
1:Q:287:VAL:HG12	1:Q:288:MET:HE3	1.71	0.72
2:F:90:TYR:CE2	2:F:94:ARG:HD2	2.23	0.72
1:W:420:THR:HG23	1:W:420:THR:O	1.90	0.72
1:E:287:VAL:HG12	1:E:288:MET:HE3	1.71	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:G:287:VAL:HG12	1:G:288:MET:HE3	1.73	0.70
1:S:247:ILE:HG13	1:S:248:PRO:HD2	1.72	0.70
1:W:258:ILE:O	1:W:259:PRO:O	2.08	0.70
1:U:94:LYS:HA	1:U:165:VAL:HG21	1.74	0.69
1:K:287:VAL:HG12	1:K:288:MET:HE2	1.72	0.69
1:U:79:GLY:HA2	1:U:344:PRO:HG2	1.73	0.69
1:K:287:VAL:CG1	1:K:288:MET:HE3	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:32:TYR:CD1	2:X:116:ASN:HA	2.28	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:HG3	1:M:52:ARG:HH11	1.58	0.68
2:V:58:MET:HE3	2:V:81:HIS:HB2	1.76	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: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:D:188:PHE:C	6:D:2063:HOH:O	2.32	0.67
1:Q:287:VAL:HG12	1:Q:288:MET:CE	2.25	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
1:W:250:GLU:CD	1:W:250:GLU:H	1.99	0.66
1:G:287:VAL:HG12	1:G:288:MET:HE2	1.76	0.66
1:U:153:PHE:HE1	1:U:158:TRP:CD1	2.14	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:125:PRO:O	2:X:126:ASP:HB2	1.97	0.65
2:V:12:PHE:O	2:V:14:TRP:HE3	1.80	0.64
1:I:287:VAL:HG12	1:I:288[A]:MET:HE3	1.78	0.64
1:U:82:PRO:HB2	1:U:98:ASN:HB3	1.79	0.64
2:T:24:GLN:HG2	2:V:25:ASN:HD21	1.63	0.64
1:U:123:HIS:HB2	3:U:460:FES:S2	2.37	0.64
2:V:58:MET:CE	2:V:81:HIS:CB	2.76	0.64
1:S:287:VAL:HG12	1:S:288:MET:HE3	1.79	0.64
1:U:63:HIS:H	1:U:66:HIS:HD2	1.43	0.64
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
1:S:258:ILE:HG12	1:S:259:PRO:O	1.99	0.63
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:V:58:MET:HE3	2:V:81:HIS:CB	2.30	0.62
2:D:151:GLU:OE1	2:J:40:HIS:HE1	1.80	0.62
2:V:67:ARG:O	2:V:68:GLU:CB	2.47	0.62
2:B:22:GLU:H	2:B:22:GLU:CD	2.01	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:101:ARG:HD3	1:S:159:GLY:O	1.99	0.62
1:M:52:ARG:HG3	1:M:52:ARG:NH1	2.14	0.62
1:I:247:ILE:HG13	1:I:248:PRO:HD2	1.82	0.61
1:U:79:GLY:HA2	1:U:344:PRO:CG	2.30	0.61
1:S:229:SER:HB2	1:S:437:ALA:HB3	1.81	0.61
2:F:94:ARG:CG	2:F:94:ARG:HH11	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
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
1:W:258:ILE:O	1:W:259:PRO:C	2.41	0.59
2:T:49:LEU:HD21	2:T:163:LEU:HD13	1.83	0.59
1:O:123:HIS:HB2	3:O:460:FES:S2	2.42	0.59
2:N:58:MET:HE1	2:N:184:LEU:HD13	1.86	0.58
2:N:58:MET:CE	2:N:81:HIS:CB	2.81	0.58
2:J:33:ARG:CZ	6:J:2016:HOH:O	2.52	0.58
2:B:12:PHE:H	2:P:36:GLN:HE21	1.49	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:58:MET:CE	2:V:81:HIS:HB2	2.34	0.57
2:V:8:PHE:HD1	2:V:9:PHE:H	1.50	0.57
2:J:33:ARG:NH1	6:J:2029:HOH:O	2.37	0.57
2:X:15:PRO:HG3	2:X:120:LYS:HA	1.85	0.57
2:N:58:MET:HE2	2:N:81:HIS:CB	2.35	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
1:S:187:LEU:HD22	1:S:194:MET:HE1	1.86	0.57
1:M:259:PRO:HG2	1:M:283:SER:HB3	1.87	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
1:G:107:ILE:HG22	1:G:118:PHE:HB3	1.87	0.56
6:F:2014:HOH:O	2:N:67:ARG:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2325:HOH:O	2:D:77:GLN:NE2	2.38	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: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: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:W:419:GLN:OE1	1:W:419:GLN:HA	2.07	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:W:256:ALA:O	1:W:257:GLN:C	2.43	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
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:I:422:HIS:CD2	1:I:424:ASP:H	2.27	0.53
1:U:109:ARG:CB	1:U:109:ARG:HH11	2.21	0.53
1:A:414:GLY:HA2	1:A:417:ARG:HD2	1.90	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:R:58:MET:HE2	2:R:81:HIS:CB	2.39	0.52
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
2:X:122:THR:OG1	2:X:127:THR:HG22	2.09	0.52
6:I:2205:HOH:O	2:J:77:GLN:NE2	2.43	0.52
1:O:257:GLN:HA	1:O:257:GLN:HE21	1.74	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
2:N:58:MET:HE2	2:N:81:HIS:HB3	1.92	0.51
1:U:198:LEU:HB2	6:U:2058:HOH:O	2.09	0.51
1:U:413:MET:HB3	1:U:434:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:58:MET:HE2	2:L:81:HIS:CB	2.40	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
1:U:109:ARG:CG	1:U:109:ARG:NH1	2.42	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:U:123:HIS:HE2	1:W:230:ASP:CG	2.14	0.51
1:S:287:VAL:HG12	1:S:288:MET:CE	2.41	0.50
1:C:349:GLU:OE2	2:J:143:ARG:NH2	2.40	0.50
1:U:322:GLN:HB3	1:U:334:PRO:HG2	1.93	0.50
1:U:252:ASP:H	1:U:255:GLN:HE21	1.59	0.50
1:I:243:ILE:HD13	1:I:384:PHE:HZ	1.77	0.50
2:F:111:ARG:HB2	2:J:175:ASP:OD2	2.12	0.50
2:T:111:ARG:HB2	2:X:175:ASP:OD2	2.12	0.50
1:C:240:LEU:O	1:C:253:LEU:HD21	2.12	0.50
1:A:77:TYR:OH	2:P:142:GLU:OE2	2.30	0.50
1:U:217:PRO:HD2	1:U:393:VAL:HG22	1.93	0.50
1:U:95:VAL:HG12	1:U:165:VAL:HG22	1.94	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
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
1:M:257:GLN:HE21	1:M:257:GLN:CA	2.24	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
1:W:123:HIS:HB2	3:W:460:FES:S2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:111:ARG:HB2	2:N:175:ASP:OD2	2.13	0.48
1:U:213:LYS:HA	1:U:352:VAL:O	2.13	0.48
2:V:58:MET:HE2	2:V:81:HIS:HB3	1.93	0.48
2:N:58:MET:HE3	2:N:81:HIS:CB	2.43	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:U:67:VAL:CG2	1:U:87:ARG:HB2	2.41	0.48
2:X:125:PRO:O	2:X:126:ASP:CB	2.60	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
1:M:287:VAL:HG12	1:M:288:MET:HE3	1.94	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:NH1	1:Q:417:ARG:CG	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
2:N:58:MET:HE2	2:N:81:HIS:HB2	1.96	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
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:U:109:ARG:CB	1:U:109:ARG:NH1	2.78	0.47
2:V:67:ARG:C	2:V:68:GLU:HG3	2.21	0.47
1:G:410:ASN:ND2	1:G:412:GLN:H	2.13	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)
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
1:U:288:MET:HE3	1:U:336:ILE:HG12	1.98	0.46
2:V:58:MET:CE	2:V:81:HIS:HB3	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:O:288[A]:MET:HE3	1:O:336:ILE:HG23	1.98	0.45
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
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:215:VAL:HG22	1:W:351:GLU:HG2	1.98	0.45
1:W:49:GLU:OE2	1:W:221:LYS:NZ	2.49	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
2:H:22:GLU:H	2:H:22:GLU:CD	2.20	0.44
1:U:153:PHE:CD1	1:U:158:TRP:CD1	3.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:382:GLY:O	1:C:386:GLN:HG3	2.18	0.44
1:C:217:PRO:HD2	1:C:393:VAL:HG22	1.99	0.44
1:C:422:HIS:CD2	1:C:424:ASP:H	2.26	0.44
1:S:77:TYR:OH	2:V:142:GLU:OE2	2.27	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
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:273:GLY:HA3	1:U:437:ALA:HB1	2.01	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: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
1:M:164:ARG:HD2	1:M:178:VAL:HA	2.00	0.43
2:H:32:TYR:CG	2:N:116:ASN:HA	2.54	0.43
2:X:22:GLU:HG3	6:X:2005:HOH:O	2.17	0.43
1:I:239:HIS:CD2	6:I:2142:HOH:O	2.60	0.43
2:D:116:ASN:HA	2:J:32:TYR:CD1	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:U:269:TRP:O	1:U:269:TRP:CE3	2.71	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:X:58:MET:HE1	2:X:174:LEU:HD22	2.01	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:F:32:TYR:CG	2:J:116:ASN:HA	2.55	0.42
1:U:79:GLY:CA	1:U:344:PRO:HG2	2.47	0.42
1:W:256:ALA:C	1:W:257:GLN:O	2.57	0.42
2:B:111:ARG:HB2	2:L:175:ASP:OD2	2.19	0.42
1:U:327:PHE:CG	1:U:328:PRO:HA	2.55	0.42
1:U:213:LYS:HG2	1:U:353:TRP:CE2	2.55	0.42
2:V:58:MET:HE2	2:V:81:HIS:CB	2.44	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:250:GLU:CD	1:W:250:GLU:N	2.70	0.42
1:E:422:HIS:CD2	1:E:424:ASP:H	2.35	0.42
1:G:287:VAL:CG1	1:G:288:MET:HE3	2.46	0.42
2:L:50:LEU:HD22	2:L:54:ILE:HD13	2.01	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
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: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
2:N:58:MET:CE	2:N:81:HIS:HB2	2.48	0.42
1:O:276:TRP:HB3	1:O:322:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:420:THR:HA	1:S:428:ASN:HA	2.02	0.41
2:X:89:MET:O	2:X:93:ILE:HG12	2.20	0.41
1:A:239:HIS:O	1:A:243:ILE:HG12	2.20	0.41
1:I:169:LYS:HE2	1:I:199:ASP:CG	2.39	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:I:213:LYS:HA	1:I:352:VAL:O	2.20	0.41
1:W:69:GLU:O	1:W:87:ARG:HB3	2.20	0.41
1:K:327:PHE:CG	1:K:328:PRO:HA	2.56	0.41
1:O:257:GLN:HE21	1:O:257:GLN:CA	2.31	0.41
1:U:269:TRP:O	1:U:269:TRP:HE3	2.04	0.41
1:U:422:HIS:HD2	1:U:424:ASP:H	1.68	0.41
1:U:122:TYR:O	1:W:238:THR:OG1	2.39	0.41
1:W:46:TYR:O	1:W:49:GLU:HB2	2.21	0.41
1:A:199:ASP:HB3	1:A:309:LEU:HD21	2.03	0.41
1:U:110:SER:HB2	2:V:63:ASN:O	2.21	0.41
5:C:462:BNL:H1	6:C:2244:HOH:O	2.21	0.40
1:E:116:LYS:HD3	1:E:116:LYS:HA	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
2:B:32:TYR:CG	2:L:116:ASN:HA	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:57:PHE:CZ	2:X:59:PRO:HB3	2.56	0.40
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
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
1	Q	429/459 (94%)	415 (97%)	13 (3%)	1 (0%)	52	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	429/459 (94%)	411 (96%)	17 (4%)	1 (0%)	52	40
1	U	426/459 (93%)	400 (94%)	22 (5%)	4 (1%)	21	8
1	W	428/459 (93%)	406 (95%)	19 (4%)	3 (1%)	26	13
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%)	30	16
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%)	34	20
2	R	179/188 (95%)	173 (97%)	5 (3%)	1 (1%)	30	16
2	T	180/188 (96%)	175 (97%)	5 (3%)	0	100	100
2	V	179/188 (95%)	170 (95%)	8 (4%)	1 (1%)	30	16
2	X	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	30	16
All	All	7315/7764 (94%)	7043 (96%)	258 (4%)	14 (0%)	52	40

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%)	346 (98%)	7 (2%)	63	54
1	C	353/372 (95%)	346 (98%)	7 (2%)	63	54
1	E	351/372 (94%)	343 (98%)	8 (2%)	58	48
1	G	351/372 (94%)	344 (98%)	7 (2%)	63	54
1	I	352/372 (95%)	343 (97%)	9 (3%)	54	42
1	K	351/372 (94%)	341 (97%)	10 (3%)	51	39
1	M	352/372 (95%)	338 (96%)	14 (4%)	38	24
1	O	352/372 (95%)	345 (98%)	7 (2%)	63	54
1	Q	351/372 (94%)	341 (97%)	10 (3%)	51	39
1	S	351/372 (94%)	342 (97%)	9 (3%)	54	42
1	U	349/372 (94%)	334 (96%)	15 (4%)	35	21
1	W	350/372 (94%)	345 (99%)	5 (1%)	74	69
2	B	163/167 (98%)	161 (99%)	2 (1%)	78	74
2	D	164/167 (98%)	163 (99%)	1 (1%)	90	89
2	F	165/167 (99%)	159 (96%)	6 (4%)	42	28
2	H	161/167 (96%)	160 (99%)	1 (1%)	90	89
2	J	155/167 (93%)	150 (97%)	5 (3%)	46	33
2	L	162/167 (97%)	161 (99%)	1 (1%)	90	89
2	N	162/167 (97%)	159 (98%)	3 (2%)	65	56
2	P	163/167 (98%)	160 (98%)	3 (2%)	66	59
2	R	160/167 (96%)	159 (99%)	1 (1%)	90	89
2	T	161/167 (96%)	156 (97%)	5 (3%)	47	34
2	V	160/167 (96%)	158 (99%)	2 (1%)	76	71
2	X	160/167 (96%)	153 (96%)	7 (4%)	35	20
All	All	6152/6468 (95%)	6007 (98%)	145 (2%)	57	46

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	103	ARG
1	A	122	TYR
1	A	255	GLN
1	A	340	ARG
1	A	410	ASN
1	A	457	LEU
2	B	10	LYS
2	B	179	LEU
1	C	103	ARG
1	C	122	TYR
1	C	280	GLU
1	C	309	LEU
1	C	340	ARG
1	C	410	ASN
1	C	457	LEU
2	D	162	ASN
1	E	31	GLU
1	E	86	VAL
1	E	103	ARG
1	E	122	TYR
1	E	251	MET
1	E	280	GLU
1	E	340	ARG
1	E	410	ASN
2	F	51	ASP
2	F	94	ARG
2	F	113	LEU
2	F	131	ASN
2	F	160	ASP
2	F	179	LEU
1	G	48	LEU
1	G	100	CYS
1	G	103	ARG
1	G	122	TYR
1	G	340	ARG
1	G	410	ASN
1	G	457	LEU
2	H	22	GLU
1	I	103	ARG
1	I	122	TYR
1	I	247	ILE
1	I	283	SER

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Mol	Chain	Res	Type
1	I	320	VAL
1	I	340	ARG
1	I	385	GLU
1	I	410	ASN
1	I	457	LEU
2	J	14	TRP
2	J	51	ASP
2	J	160	ASP
2	J	162	ASN
2	J	179	LEU
1	K	103	ARG
1	K	122	TYR
1	K	250	GLU
1	K	252	ASP
1	K	309	LEU
1	K	316	VAL
1	K	320	VAL
1	K	340	ARG
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	122	TYR
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	340	ARG
1	M	385	GLU
1	M	410	ASN
1	M	457	LEU
2	N	162	ASN
2	N	169	LYS
2	N	179	LEU
1	O	103	ARG
1	O	122	TYR
1	O	247	ILE
1	O	257	GLN

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Mol	Chain	Res	Type
1	O	340	ARG
1	O	385	GLU
1	O	410	ASN
2	P	52	LYS
2	P	113	LEU
2	P	179	LEU
1	Q	103	ARG
1	Q	122	TYR
1	Q	258	ILE
1	Q	280	GLU
1	Q	294	GLN
1	Q	340	ARG
1	Q	385	GLU
1	Q	413	MET
1	Q	417	ARG
1	Q	457	LEU
2	R	179	LEU
1	S	103	ARG
1	S	122	TYR
1	S	167	THR
1	S	221	LYS
1	S	231	MET
1	S	258	ILE
1	S	320	VAL
1	S	340	ARG
1	S	410	ASN
2	T	21	LEU
2	T	87	GLU
2	T	94	ARG
2	T	162	ASN
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	247	ILE
1	U	257	GLN
1	U	280	GLU

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Mol	Chain	Res	Type
1	U	340	ARG
1	U	370	TYR
1	U	410	ASN
1	U	457	LEU
2	V	8	PHE
2	V	162	ASN
1	W	100	CYS
1	W	103	ARG
1	W	122	TYR
1	W	320	VAL
1	W	446	MET
2	X	22	GLU
2	X	54	ILE
2	X	67	ARG
2	X	77	GLN
2	X	113	LEU
2	X	127	THR
2	X	128	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN
1	A	257	GLN
1	A	391	ASN
1	A	410	ASN
1	A	412	GLN
1	A	422	HIS
2	B	25	ASN
2	B	36	GLN
2	B	131	ASN
2	B	162	ASN
1	C	391	ASN
1	C	410	ASN
1	C	412	GLN
1	C	422	HIS
1	C	444	HIS
2	D	25	ASN
2	D	55	HIS
2	D	77	GLN
2	D	131	ASN
2	D	162	ASN

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Mol	Chain	Res	Type
1	E	18	ASN
1	E	410	ASN
1	E	412	GLN
1	E	422	HIS
2	F	25	ASN
2	F	40	HIS
2	F	77	GLN
2	F	131	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	255	GLN
1	I	294	GLN
1	I	307	GLN
1	I	373	HIS
1	I	391	ASN
1	I	410	ASN
1	I	412	GLN
1	I	422	HIS
1	I	444	HIS
2	J	25	ASN
2	J	40	HIS
2	J	55	HIS
2	J	77	GLN
1	K	18	ASN
1	K	391	ASN
1	K	410	ASN
1	K	412	GLN
1	K	422	HIS
1	K	444	HIS
2	L	25	ASN
2	L	36	GLN
2	L	131	ASN
2	L	162	ASN
1	M	255	GLN
1	M	257	GLN
1	M	391	ASN

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Mol	Chain	Res	Type
1	M	410	ASN
1	M	412	GLN
1	M	422	HIS
2	N	25	ASN
2	N	131	ASN
2	N	162	ASN
1	O	255	GLN
1	O	257	GLN
1	O	391	ASN
1	O	410	ASN
1	O	412	GLN
1	O	422	HIS
2	P	25	ASN
2	P	36	GLN
2	P	131	ASN
2	P	162	ASN
1	Q	135	ASN
1	Q	257	GLN
1	Q	294	GLN
1	Q	391	ASN
1	Q	412	GLN
1	Q	422	HIS
2	R	25	ASN
2	R	77	GLN
2	R	131	ASN
1	S	257	GLN
1	S	343	HIS
1	S	391	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	131	ASN
1	U	30	GLN
1	U	66	HIS
1	U	99	GLN
1	U	102	HIS
1	U	255	GLN
1	U	257	GLN
1	U	410	ASN

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Mol	Chain	Res	Type
1	U	412	GLN
1	U	422	HIS
1	U	444	HIS
2	V	25	ASN
2	V	36	GLN
2	V	81	HIS
2	V	131	ASN
1	W	257	GLN
1	W	311	HIS
1	W	343	HIS
1	W	410	ASN
1	W	412	GLN
1	W	444	HIS
2	X	24	GLN
2	X	25	ASN
2	X	36	GLN
2	X	77	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	A	460	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	C	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	C	462	-	13,13,13	1.07	1 (7%)	16,16,16	0.45	0
3	FES	E	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	E	462	-	13,13,13	1.10	1 (7%)	16,16,16	0.70	0
3	FES	G	460	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	I	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	I	462	-	13,13,13	1.13	1 (7%)	16,16,16	0.47	0
3	FES	K	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	K	462	-	13,13,13	1.12	1 (7%)	16,16,16	0.51	0
3	FES	M	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	M	462	-	13,13,13	1.10	1 (7%)	16,16,16	0.46	0
3	FES	O	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	O	462	-	13,13,13	1.15	1 (7%)	16,16,16	0.65	0
3	FES	Q	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	Q	462	-	13,13,13	1.14	1 (7%)	16,16,16	0.52	0
3	FES	S	460	1,6	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	S	462	-	13,13,13	1.07	1 (7%)	16,16,16	0.65	0
3	FES	U	460	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	W	460	1	0,4,4	0.00	-	0,4,4	0.00	-
5	BNL	W	462	-	13,13,13	1.11	1 (7%)	16,16,16	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	A	460	1	-	0/0/4/4	0/1/1/1
3	FES	C	460	1	-	0/0/4/4	0/1/1/1
5	BNL	C	462	-	-	0/4/4/4	0/2/2/2
3	FES	E	460	1	-	0/0/4/4	0/1/1/1
5	BNL	E	462	-	-	0/4/4/4	0/2/2/2
3	FES	G	460	1	-	0/0/4/4	0/1/1/1
3	FES	I	460	1	-	0/0/4/4	0/1/1/1
5	BNL	I	462	-	-	0/4/4/4	0/2/2/2
3	FES	K	460	1	-	0/0/4/4	0/1/1/1
5	BNL	K	462	-	-	0/4/4/4	0/2/2/2
3	FES	M	460	1	-	0/0/4/4	0/1/1/1
5	BNL	M	462	-	-	0/4/4/4	0/2/2/2
3	FES	O	460	1	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BNL	O	462	-	-	0/4/4/4	0/2/2/2
3	FES	Q	460	1	-	0/0/4/4	0/1/1/1
5	BNL	Q	462	-	-	0/4/4/4	0/2/2/2
3	FES	S	460	1,6	-	0/0/4/4	0/1/1/1
5	BNL	S	462	-	-	0/4/4/4	0/2/2/2
3	FES	U	460	1	-	0/0/4/4	0/1/1/1
3	FES	W	460	1	-	0/0/4/4	0/1/1/1
5	BNL	W	462	-	-	0/4/4/4	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	462	BNL	C16-C2	-3.63	1.39	1.49
5	O	462	BNL	C16-C2	-3.46	1.40	1.49
5	W	462	BNL	C16-C2	-3.42	1.40	1.49
5	Q	462	BNL	C16-C2	-3.42	1.40	1.49
5	K	462	BNL	C16-C2	-3.39	1.40	1.49
5	E	462	BNL	C16-C2	-3.35	1.40	1.49
5	M	462	BNL	C16-C2	-3.30	1.40	1.49
5	I	462	BNL	C16-C2	-3.12	1.40	1.49
5	C	462	BNL	C16-C2	-3.06	1.41	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	460	FES	1	0
3	C	460	FES	1	0
5	C	462	BNL	3	0
3	E	460	FES	1	0
5	E	462	BNL	1	0
3	G	460	FES	1	0
3	M	460	FES	1	0
5	M	462	BNL	1	0
3	O	460	FES	1	0
3	Q	460	FES	2	0
3	S	460	FES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	460	FES	1	0
3	W	460	FES	2	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%)	0.08	6 (1%) 78 80	23, 26, 40, 53	11 (2%)
1	C	433/459 (94%)	0.24	20 (4%) 36 38	23, 26, 41, 87	15 (3%)
1	E	433/459 (94%)	0.14	22 (5%) 32 33	22, 29, 47, 96	12 (2%)
1	G	433/459 (94%)	0.08	17 (3%) 43 45	23, 29, 46, 63	16 (3%)
1	I	433/459 (94%)	0.05	16 (3%) 45 47	22, 30, 45, 61	16 (3%)
1	K	433/459 (94%)	0.19	27 (6%) 24 26	22, 33, 51, 64	15 (3%)
1	M	433/459 (94%)	0.22	29 (6%) 21 22	22, 33, 54, 65	16 (3%)
1	O	433/459 (94%)	0.12	20 (4%) 36 38	22, 36, 54, 68	20 (4%)
1	Q	433/459 (94%)	0.43	42 (9%) 10 10	25, 39, 65, 85	12 (2%)
1	S	433/459 (94%)	1.67	134 (30%) 1 0	43, 77, 113, 129	48 (11%)
1	U	430/459 (93%)	2.10	179 (41%) 0 0	42, 81, 106, 122	53 (12%)
1	W	432/459 (94%)	2.29	205 (47%) 0 0	46, 72, 97, 112	71 (16%)
2	B	183/188 (97%)	0.22	5 (2%) 58 60	24, 25, 31, 50	3 (1%)
2	D	183/188 (97%)	0.26	6 (3%) 50 52	24, 25, 33, 43	7 (3%)
2	F	184/188 (97%)	0.14	6 (3%) 50 52	24, 26, 33, 40	4 (2%)
2	H	181/188 (96%)	-0.00	8 (4%) 38 40	24, 26, 37, 47	3 (1%)
2	J	175/188 (93%)	0.19	8 (4%) 36 38	24, 26, 33, 67	8 (4%)
2	L	182/188 (96%)	0.03	9 (4%) 33 35	23, 27, 35, 58	4 (2%)
2	N	183/188 (97%)	0.04	8 (4%) 38 40	24, 27, 37, 58	6 (3%)
2	P	181/188 (96%)	-0.00	4 (2%) 65 67	23, 27, 38, 53	3 (1%)
2	R	181/188 (96%)	-0.02	9 (4%) 32 34	23, 30, 40, 48	3 (1%)
2	T	182/188 (96%)	0.40	13 (7%) 19 20	28, 41, 61, 68	3 (1%)
2	V	181/188 (96%)	0.68	28 (15%) 3 3	25, 44, 87, 107	11 (6%)
2	X	180/188 (95%)	1.77	64 (35%) 0 0	45, 72, 101, 111	21 (11%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7368/7764 (94%)	0.54	885 (12%) 6 6	22, 32, 89, 129	381 (5%)

All (885) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	418	SER	22.0
1	U	409	LEU	13.5
1	W	284	LEU	12.0
1	W	230	ASP	11.6
1	U	100	CYS	11.6
1	S	258	ILE	11.3
1	U	99	GLN	10.1
1	W	258	ILE	9.9
1	S	364	ALA	9.8
2	X	122	THR	9.7
1	U	269	TRP	9.7
1	W	442	TYR	9.5
2	X	125	PRO	9.4
1	U	355	PHE	9.3
1	U	153	PHE	9.1
1	U	67	VAL	9.1
1	U	109	ARG	9.1
1	S	321	GLY	9.0
1	W	364	ALA	8.5
1	U	158	TRP	8.4
1	S	455	ALA	8.4
1	E	251	MET	8.3
1	W	257	GLN	8.3
1	W	26	GLY	7.9
2	V	8	PHE	7.9
1	W	249	PRO	7.7
1	U	82	PRO	7.7
1	S	313	GLY	7.6
1	E	256	ALA	7.6
1	U	95	VAL	7.6
1	S	202	PRO	7.5
1	W	312	THR	7.4
2	X	102	TRP	7.3
1	U	449	MET	7.3
2	V	123	ALA	7.3
2	V	67	ARG	7.2
1	W	224	ALA	7.1

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Mol	Chain	Res	Type	RSRZ
1	S	420	THR	7.1
1	U	442	TYR	7.1
1	Q	421	GLY	7.0
2	X	168	ALA	7.0
1	Q	257	GLN	6.9
1	S	416	GLY	6.9
1	U	79	GLY	6.9
1	S	18	ASN	6.7
1	W	419	GLN	6.7
1	W	19	TRP	6.7
1	U	457	LEU	6.7
1	U	103	ARG	6.7
1	E	254	SER	6.6
1	U	455	ALA	6.6
1	U	140	LYS	6.5
1	W	34	LEU	6.5
1	W	294	GLN	6.4
1	U	178	VAL	6.4
1	E	250	GLU	6.3
1	W	22	GLU	6.3
1	W	260	THR	6.2
1	Q	258	ILE	6.2
1	S	419	GLN	6.1
1	C	255	GLN	6.1
1	W	256	ALA	6.1
1	U	313	GLY	6.1
1	S	159	GLY	6.1
1	W	422	HIS	6.0
1	W	316	VAL	6.0
2	X	54	ILE	6.0
1	S	311	HIS	6.0
1	S	178	VAL	5.9
1	U	156	ALA	5.9
1	U	93	ILE	5.9
1	U	21	PRO	5.8
1	U	132	LYS	5.8
1	W	202	PRO	5.8
1	S	153	PHE	5.7
1	W	203	ALA	5.7
2	X	20	GLY	5.7
1	S	261	LYS	5.7
2	X	90	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
1	W	20	THR	5.7
1	U	166	ALA	5.7
1	W	455	ALA	5.7
2	P	8	PHE	5.7
1	C	251	MET	5.6
1	E	258	ILE	5.6
1	S	424	ASP	5.6
2	X	127	THR	5.6
1	U	186	TYR	5.6
1	C	254	SER	5.6
2	R	8	PHE	5.6
1	U	83	VAL	5.6
1	S	19	TRP	5.5
2	V	18	ALA	5.5
2	V	125	PRO	5.5
1	W	420	THR	5.5
1	S	418	SER	5.4
1	U	179	GLN	5.4
1	W	432	VAL	5.4
1	U	419	GLN	5.4
1	W	292	VAL	5.4
1	U	127	TYR	5.4
1	W	265	PHE	5.3
1	W	413	MET	5.3
1	C	250	GLU	5.3
1	S	316	VAL	5.3
1	W	423	PRO	5.3
1	S	421	GLY	5.2
1	S	143	PHE	5.2
2	T	160	ASP	5.2
1	S	188	GLY	5.2
1	U	453	SER	5.2
1	S	58	TRP	5.1
1	S	179	GLN	5.1
1	U	18	ASN	5.1
2	X	155	VAL	5.1
1	U	94	LYS	5.0
1	W	28	VAL	5.0
1	W	328	PRO	5.0
1	S	183	LEU	5.0
1	E	255	GLN	5.0
1	U	311	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
2	X	16	SER	5.0
1	Q	281	PRO	5.0
1	U	134	VAL	5.0
2	V	69	GLY	5.0
1	W	189	ASP	4.9
2	R	160	ASP	4.9
2	X	161	ASN	4.9
1	M	253	LEU	4.9
1	U	106	ARG	4.9
1	E	18	ASN	4.9
1	U	138	PHE	4.8
1	S	189	ASP	4.8
2	X	87	GLU	4.8
1	S	417	ARG	4.8
1	U	91	LYS	4.8
1	S	423	PRO	4.8
1	U	202	PRO	4.8
1	S	310	GLY	4.8
1	U	204	GLY	4.8
1	U	420	THR	4.8
1	U	28	VAL	4.8
1	E	257	GLN	4.8
2	X	120	LYS	4.8
1	U	165	VAL	4.8
2	T	159	ALA	4.7
1	U	307	GLN	4.7
1	A	18	ASN	4.7
1	S	255	GLN	4.7
2	X	17	LYS	4.7
1	U	181	PRO	4.7
1	U	454	TRP	4.6
1	W	276	TRP	4.6
1	U	89	LYS	4.6
1	I	255	GLN	4.6
1	W	456	THR	4.6
1	U	421	GLY	4.6
2	N	6	PRO	4.6
2	X	27	ILE	4.6
1	E	252	ASP	4.6
2	V	75	GLY	4.6
1	W	361	ASP	4.6
2	X	162	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	S	268	ALA	4.6
1	Q	256	ALA	4.5
2	X	124	THR	4.5
2	J	14	TRP	4.5
1	Q	423	PRO	4.5
1	W	285	LEU	4.5
1	W	430	GLY	4.5
1	U	115	ALA	4.5
1	C	252	ASP	4.5
1	S	90	ASP	4.4
1	I	254	SER	4.4
1	Q	254	SER	4.4
1	Q	419	GLN	4.4
1	U	425	PHE	4.4
1	W	295	TYR	4.4
1	W	157	GLU	4.4
1	W	415	LEU	4.4
2	X	156	LEU	4.4
1	M	18	ASN	4.4
1	I	250	GLU	4.4
1	W	303	GLU	4.4
1	S	307	GLN	4.4
2	T	126	ASP	4.4
2	V	9	PHE	4.4
2	X	21	LEU	4.4
2	X	55	HIS	4.4
2	X	160	ASP	4.4
1	E	248	PRO	4.3
2	T	21	LEU	4.3
1	U	92	SER	4.3
2	X	77	GLN	4.3
1	W	359	ASP	4.3
2	L	160	ASP	4.3
1	M	421	GLY	4.3
1	S	265	PHE	4.3
1	U	33	GLY	4.3
1	U	54	PHE	4.3
1	U	66	HIS	4.3
1	W	425	PHE	4.2
1	W	207	ALA	4.2
1	W	18	ASN	4.2
1	W	402	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	I	252	ASP	4.2
1	U	415	LEU	4.2
2	X	47	PHE	4.2
1	S	256	ALA	4.2
1	W	279	ASP	4.2
1	W	140	LYS	4.2
1	W	227	PHE	4.2
2	V	17	LYS	4.2
2	X	94	ARG	4.1
2	X	51	ASP	4.1
1	W	411	ALA	4.1
2	B	6	PRO	4.1
1	W	183	LEU	4.1
1	W	410	ASN	4.1
2	F	160	ASP	4.1
2	P	160[A]	ASP	4.1
2	X	121	GLU	4.1
1	M	258	ILE	4.1
1	U	122	TYR	4.1
2	L	8	PHE	4.1
1	S	454	TRP	4.1
1	S	278	VAL	4.1
2	X	23	LEU	4.0
1	W	370	TYR	4.0
1	U	268	ALA	4.0
2	N	7	HIS	4.0
1	U	416	GLY	4.0
1	W	307	GLN	4.0
1	W	298	GLU	4.0
1	W	408	PRO	4.0
1	C	248	PRO	4.0
1	W	259	PRO	3.9
1	K	252	ASP	3.9
2	V	16	SER	3.9
1	S	306	GLU	3.9
2	N	123	ALA	3.9
1	W	261	LYS	3.9
1	W	217	PRO	3.9
1	S	193	TYR	3.9
1	S	89	LYS	3.9
2	X	187	PHE	3.9
1	U	52	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	U	344	PRO	3.9
1	W	255	GLN	3.9
1	W	375	ILE	3.9
1	K	419	GLN	3.9
1	S	140	LYS	3.9
1	M	311	HIS	3.9
1	W	271	GLY	3.8
1	S	402	TYR	3.8
1	U	20	THR	3.8
1	U	116	LYS	3.8
1	S	298	GLU	3.8
1	U	365	GLU	3.8
1	W	156	ALA	3.8
1	W	186	TYR	3.8
1	Q	416	GLY	3.8
1	C	253	LEU	3.8
1	E	253	LEU	3.8
1	K	420	THR	3.8
1	W	268	ALA	3.8
2	X	123	ALA	3.8
1	W	204	GLY	3.8
1	C	18	ASN	3.8
1	W	431	TYR	3.8
1	W	248	PRO	3.8
1	W	327	PHE	3.8
2	V	71	LEU	3.8
1	Q	156	ALA	3.7
1	W	282	GLY	3.7
1	W	270	GLY	3.7
1	U	314	MET	3.7
1	U	424	ASP	3.7
1	W	313	GLY	3.7
1	W	304	LEU	3.7
1	Q	247	ILE	3.7
1	U	312	THR	3.7
1	W	251	MET	3.7
1	W	314	MET	3.7
1	U	267	ALA	3.7
1	U	426	PRO	3.7
1	W	192	PRO	3.7
1	E	247	ILE	3.7
1	U	203	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	W	360	ALA	3.7
1	U	48	LEU	3.7
1	W	417	ARG	3.7
2	X	10	LYS	3.7
2	T	162	ASN	3.6
1	W	45	LEU	3.6
2	V	14	TRP	3.6
1	W	178	VAL	3.6
2	H	8	PHE	3.6
2	X	58	MET	3.6
1	S	69	GLU	3.6
1	S	257	GLN	3.6
2	X	159	ALA	3.6
1	S	134	VAL	3.6
1	S	155	LYS	3.6
1	W	459	PRO	3.6
2	R	76	ASP	3.6
1	M	261	LYS	3.6
1	W	24	ILE	3.6
1	W	254	SER	3.6
2	J	162	ASN	3.6
1	S	425	PHE	3.6
1	S	33	GLY	3.6
1	U	128	ASP	3.6
1	W	365	GLU	3.6
1	M	420	THR	3.5
1	S	267	ALA	3.5
1	W	301	ALA	3.5
1	W	208	ILE	3.5
1	U	304	LEU	3.5
1	U	69	GLU	3.5
1	S	290	PRO	3.5
1	W	416	GLY	3.5
1	W	21	PRO	3.5
1	S	317	ARG	3.5
1	U	326	ILE	3.5
1	I	140	LYS	3.5
1	S	196	VAL	3.5
2	X	126	ASP	3.5
1	W	64	GLU	3.5
1	Q	420	THR	3.5
2	V	122	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	18	ASN	3.4
1	S	361	ASP	3.4
1	U	258	ILE	3.4
1	W	32	LYS	3.4
1	U	53	VAL	3.4
1	W	447	ARG	3.4
2	V	70	GLU	3.4
1	S	300	PRO	3.4
1	U	133	LEU	3.4
2	X	50	LEU	3.4
2	X	85	THR	3.4
1	W	427	GLY	3.4
1	S	187	LEU	3.4
1	U	136	VAL	3.4
1	K	254	SER	3.4
1	W	229	SER	3.4
1	M	455	ALA	3.4
1	S	299	GLY	3.4
1	S	457	LEU	3.4
1	W	35	LEU	3.4
1	O	18	ASN	3.4
1	K	364	ALA	3.4
1	U	23	ALA	3.4
1	U	31	GLU	3.4
1	U	139	GLU	3.4
1	U	102	HIS	3.4
1	K	251	MET	3.4
1	W	29	ASP	3.4
1	G	423	PRO	3.3
2	F	14	TRP	3.3
1	A	311	HIS	3.3
1	U	310	GLY	3.3
1	W	205	THR	3.3
1	S	22	GLU	3.3
1	W	406	SER	3.3
1	C	249	PRO	3.3
2	V	15	PRO	3.3
1	W	190	ALA	3.3
2	H	123	ALA	3.3
2	F	5	SER	3.3
1	W	448	MET	3.3
2	B	123	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	R	67	ARG	3.3
2	V	68	GLU	3.3
1	W	247	ILE	3.3
2	V	22	GLU	3.3
1	S	91	LYS	3.2
1	W	392	TRP	3.2
2	D	6	PRO	3.2
2	X	169	LYS	3.2
1	S	29	ASP	3.2
1	U	265	PHE	3.2
2	N	160	ASP	3.2
1	W	320	VAL	3.2
1	U	125	TRP	3.2
1	Q	283	SER	3.2
1	S	450	SER	3.2
2	V	13	GLU	3.2
1	K	18	ASN	3.2
1	S	301	ALA	3.2
1	S	34	LEU	3.2
2	V	21	LEU	3.2
2	V	26	GLU	3.2
1	Q	456	THR	3.2
1	W	293	THR	3.2
1	U	29	ASP	3.2
1	U	361	ASP	3.2
1	K	250	GLU	3.2
1	S	185	THR	3.2
1	Q	282	GLY	3.2
1	W	210	GLY	3.2
2	T	20	GLY	3.2
2	X	99[A]	ASP	3.2
1	U	117	ALA	3.2
1	W	438	ALA	3.2
1	W	54	PHE	3.2
2	X	128	PHE	3.2
1	G	18	ASN	3.2
1	U	135	ASN	3.2
1	Q	22	GLU	3.1
1	W	368	GLU	3.1
2	X	40	HIS	3.1
1	U	189	ASP	3.1
1	W	297	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	U	47	GLU	3.1
1	C	196	VAL	3.1
1	O	313	GLY	3.1
1	O	421	GLY	3.1
1	S	297	THR	3.1
1	Q	311	HIS	3.1
1	W	253	LEU	3.1
1	M	281	PRO	3.1
1	S	312	THR	3.1
1	S	31	GLU	3.1
1	U	159	GLY	3.1
1	O	261	LYS	3.1
1	U	195	ASP	3.1
1	Q	455	ALA	3.1
1	S	422	HIS	3.1
1	W	310	GLY	3.1
1	S	175	ASN	3.1
1	S	176	TRP	3.1
2	X	76	ASP	3.1
2	J	16	SER	3.1
1	G	105	MET	3.1
1	Q	249	PRO	3.0
1	W	250	GLU	3.0
1	U	59	LEU	3.0
1	K	307	GLN	3.0
1	W	154	ASP	3.0
2	D	160	ASP	3.0
1	U	295	TYR	3.0
1	W	453	SER	3.0
2	T	16	SER	3.0
1	W	52	ARG	3.0
1	W	439	ARG	3.0
1	W	325	THR	3.0
1	O	257	GLN	3.0
1	I	298	GLU	3.0
1	U	452	PRO	3.0
1	S	442	TYR	3.0
1	U	279	ASP	3.0
2	T	52	LYS	3.0
1	W	457	LEU	3.0
1	U	121	SER	3.0
1	W	332	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	W	252	ASP	3.0
1	W	339	ILE	3.0
1	S	365	GLU	3.0
1	I	257	GLN	3.0
1	Q	18	ASN	3.0
1	O	457	LEU	2.9
1	U	448	MET	2.9
2	F	162	ASN	2.9
2	J	160	ASP	2.9
1	G	100	CYS	2.9
1	Q	253	LEU	2.9
1	Q	427	GLY	2.9
1	U	445	TRP	2.9
1	W	58	TRP	2.9
1	W	281	PRO	2.9
1	U	364	ALA	2.9
2	V	10	LYS	2.9
1	Q	140	LYS	2.9
1	U	30	GLN	2.9
1	S	56	ARG	2.9
1	S	283	SER	2.9
1	S	432	VAL	2.9
2	F	117	VAL	2.9
2	J	15	PRO	2.9
2	N	8	PHE	2.9
1	S	20	THR	2.9
1	U	123	HIS	2.9
1	Q	298	GLU	2.9
1	W	206	VAL	2.9
1	O	423	PRO	2.9
1	W	105	MET	2.9
1	G	310	GLY	2.9
1	W	336	ILE	2.9
1	G	89	LYS	2.9
1	W	302	ALA	2.9
1	W	237	THR	2.8
1	M	196	VAL	2.8
1	S	269	TRP	2.8
1	S	24	ILE	2.8
1	U	271	GLY	2.8
1	W	53	VAL	2.8
1	W	61	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	T	7	HIS	2.8
1	S	203	ALA	2.8
1	C	258	ILE	2.8
1	E	140	LYS	2.8
1	I	258	ILE	2.8
1	U	108	CYS	2.8
1	I	251	MET	2.8
1	S	253	LEU	2.8
1	S	201	THR	2.8
1	S	452	PRO	2.8
1	U	25	ARG	2.8
1	O	307	GLN	2.8
1	G	156	ALA	2.8
1	I	421	GLY	2.8
1	O	445	TRP	2.8
2	B	7	HIS	2.8
2	L	7	HIS	2.8
2	D	117	VAL	2.8
1	S	224	ALA	2.7
1	W	31	GLU	2.8
1	S	271	GLY	2.7
1	W	283	SER	2.7
2	D	14	TRP	2.7
1	E	244	LEU	2.7
1	K	257	GLN	2.7
1	M	307	GLN	2.7
1	S	303	GLU	2.7
2	V	124	THR	2.7
1	K	178	VAL	2.7
1	W	429	VAL	2.7
2	X	52	LYS	2.7
1	W	289	GLY	2.7
1	K	22	GLU	2.7
1	W	305	ALA	2.7
2	X	43	TYR	2.7
1	C	83	VAL	2.7
1	U	196	VAL	2.7
1	Q	279	ASP	2.7
2	X	141	LEU	2.7
1	U	71	GLY	2.7
1	U	107	ILE	2.7
1	W	23	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	W	317	ARG	2.7
2	L	159	ALA	2.7
1	W	153	PHE	2.7
1	U	58	TRP	2.7
1	W	407	GLN	2.7
1	K	416	GLY	2.7
1	S	284	LEU	2.7
1	W	334	PRO	2.7
2	X	88	THR	2.7
1	U	438	ALA	2.6
1	U	118	PHE	2.6
1	M	19	TRP	2.6
1	W	134	VAL	2.6
1	U	306	GLU	2.6
2	T	67	ARG	2.6
1	E	249	PRO	2.6
1	S	32	LYS	2.6
1	Q	260	THR	2.6
1	Q	307	GLN	2.6
2	X	42	ALA	2.6
1	S	39	ILE	2.6
2	X	188	PHE	2.6
1	G	154	ASP	2.6
1	U	358	VAL	2.6
1	K	294	GLN	2.6
1	S	281	PRO	2.6
1	W	372	ARG	2.6
1	M	419	GLN	2.6
1	U	257	GLN	2.6
1	W	197	MET	2.6
1	M	459	PRO	2.6
1	W	277	TYR	2.6
1	S	304	LEU	2.6
1	W	318	ARG	2.6
1	U	220	TRP	2.6
1	C	256	ALA	2.6
1	S	446	MET	2.6
1	W	69	GLU	2.6
2	X	44	GLU	2.6
1	W	379	SER	2.6
1	S	53	VAL	2.6
1	U	206	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	Q	142	ALA	2.6
1	U	443	HIS	2.6
1	M	140	LYS	2.6
1	S	197	MET	2.6
1	U	447	ARG	2.6
1	W	70	THR	2.6
2	D	162	ASN	2.6
2	L	99[A]	ASP	2.6
1	G	416	GLY	2.6
1	K	196	VAL	2.6
2	B	117	VAL	2.6
2	X	75	GLY	2.6
1	S	333	LEU	2.5
1	U	458	LYS	2.5
1	W	309	LEU	2.5
1	W	357	LEU	2.5
1	C	257	GLN	2.5
1	Q	20	THR	2.5
1	S	26	GLY	2.5
2	P	52	LYS	2.5
2	H	67	ARG	2.5
2	X	119	VAL	2.5
1	S	54	PHE	2.5
1	S	229	SER	2.5
1	M	294	GLN	2.5
1	M	252	ASP	2.5
1	G	140	LYS	2.5
1	S	445	TRP	2.5
1	K	53	VAL	2.5
1	W	287	VAL	2.5
1	U	180	ALA	2.5
1	U	281	PRO	2.5
1	W	384	PHE	2.5
1	U	78	MET	2.5
1	U	183	LEU	2.5
1	W	109	ARG	2.5
1	U	303	GLU	2.5
1	O	419	GLN	2.5
1	M	453	SER	2.5
1	U	44	SER	2.5
1	M	256	ALA	2.5
1	W	349	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	U	34	LEU	2.5
1	W	187	LEU	2.5
2	X	49	LEU	2.5
1	A	456	THR	2.5
1	U	185	THR	2.5
1	U	32	LYS	2.5
2	N	162	ASN	2.5
1	S	447	ARG	2.5
1	Q	320	VAL	2.5
1	Q	415	LEU	2.5
1	A	22	GLU	2.5
1	S	406	SER	2.5
2	X	13	GLU	2.5
1	O	290	PRO	2.4
1	S	315	PRO	2.4
2	L	125	PRO	2.4
1	Q	286	ALA	2.4
1	W	362	ALA	2.4
1	E	445	TRP	2.4
1	W	454	TRP	2.4
2	R	17	LYS	2.4
1	M	303	GLU	2.4
1	Q	157	GLU	2.4
1	U	141	GLU	2.4
1	U	190	ALA	2.4
1	W	59	LEU	2.4
1	U	168	TYR	2.4
2	X	18	ALA	2.4
1	O	420	THR	2.4
1	U	325	THR	2.4
1	U	456	THR	2.4
2	L	117	VAL	2.4
1	W	27	LEU	2.4
1	W	60	LEU	2.4
1	U	446	MET	2.4
1	K	260	THR	2.4
1	U	339	ILE	2.4
2	V	66	ILE	2.4
1	C	95	VAL	2.4
1	U	84	VAL	2.4
1	W	315	PRO	2.4
1	S	132	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	S	254	SER	2.4
1	U	77	TYR	2.4
1	U	276	TRP	2.4
2	V	78	ASP	2.4
1	O	417	ARG	2.4
1	U	167	THR	2.4
1	W	185	THR	2.4
1	M	423	PRO	2.4
1	O	157	GLU	2.4
2	T	125	PRO	2.4
1	W	39	ILE	2.4
1	W	179	GLN	2.4
1	W	358	VAL	2.4
1	W	128	ASP	2.3
1	W	193	TYR	2.3
2	N	159	ALA	2.3
1	O	294	GLN	2.3
1	W	71	GLY	2.3
1	A	423	PRO	2.3
1	W	196	VAL	2.3
1	U	155	LYS	2.3
2	D	67	ARG	2.3
1	Q	365	GLU	2.3
1	S	280	GLU	2.3
1	C	421	GLY	2.3
1	S	346	GLY	2.3
1	U	104	GLY	2.3
1	Q	459	PRO	2.3
1	S	279	ASP	2.3
1	U	19	TRP	2.3
1	E	22	GLU	2.3
1	U	418	SER	2.3
1	I	53	VAL	2.3
1	W	330	CYS	2.3
1	W	223	ALA	2.3
1	C	97	LEU	2.3
1	E	260	THR	2.3
1	U	81	ASP	2.3
1	U	328	PRO	2.3
1	W	177	ASP	2.3
1	U	101	ARG	2.3
1	U	439	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	143	PHE	2.3
1	S	44	SER	2.3
2	H	16	SER	2.3
1	Q	179	GLN	2.3
1	S	294	GLN	2.3
1	W	30	GLN	2.3
1	W	214	TRP	2.3
1	E	246	GLY	2.3
1	U	427	GLY	2.3
1	U	432	VAL	2.3
2	J	117	VAL	2.3
2	R	70	GLU	2.3
1	S	23	ALA	2.3
2	X	45	ALA	2.3
1	U	423	PRO	2.3
1	W	238	THR	2.3
1	S	161	LEU	2.3
1	W	240	LEU	2.3
1	U	450	SER	2.3
1	U	193	TYR	2.3
1	U	428	ASN	2.3
1	M	365	GLU	2.3
1	O	303	GLU	2.3
1	W	311	HIS	2.3
2	T	17	LYS	2.3
2	X	67	ARG	2.3
1	S	448	MET	2.3
1	W	231	MET	2.3
1	O	310	GLY	2.2
1	S	275	GLY	2.2
1	M	448	MET	2.2
1	U	70	THR	2.2
1	W	296	TRP	2.2
2	R	16	SER	2.2
2	X	66	ILE	2.2
2	R	53	ASP	2.2
1	C	59	LEU	2.2
1	E	59	LEU	2.2
1	K	311	HIS	2.2
1	U	422	HIS	2.2
1	W	97	LEU	2.2
1	U	173	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	194	MET	2.2
1	O	455	ALA	2.2
1	S	308	ARG	2.2
1	W	38	ARG	2.2
1	W	241	SER	2.2
1	M	53	VAL	2.2
1	U	42	ASP	2.2
1	W	62	GLY	2.2
2	X	46	TRP	2.2
1	U	198	LEU	2.2
2	J	90	TYR	2.2
2	V	58	MET	2.2
1	G	22	GLU	2.2
1	U	41	ALA	2.2
1	G	53	VAL	2.2
1	I	196	VAL	2.2
1	K	89	LYS	2.2
1	W	244	LEU	2.2
1	G	307	GLN	2.2
1	W	201	THR	2.2
1	K	31	GLU	2.2
1	W	184	GLU	2.2
1	W	385	GLU	2.2
2	X	53	ASP	2.2
1	S	453	SER	2.2
1	U	192	PRO	2.2
1	U	60	LEU	2.2
1	U	97	LEU	2.2
2	X	79	LEU	2.2
1	W	41	ALA	2.2
1	W	434	ALA	2.2
1	S	49	GLU	2.2
2	H	10	LYS	2.2
1	U	366	ILE	2.1
1	W	243	ILE	2.1
1	W	441	MET	2.1
1	S	309	LEU	2.1
1	U	357	LEU	2.1
1	Q	189	ASP	2.1
1	W	445	TRP	2.1
1	K	54	PHE	2.1
2	V	12	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	311	HIS	2.1
1	U	120	CYS	2.1
2	X	86	HIS	2.1
1	W	371	ARG	2.1
1	S	319	MET	2.1
1	K	313	GLY	2.1
1	S	289	GLY	2.1
1	W	299	GLY	2.1
2	B	27	ILE	2.1
1	I	253	LEU	2.1
1	M	257	GLN	2.1
1	Q	255	GLN	2.1
1	W	450	SER	2.1
1	A	109	ARG	2.1
1	E	311	HIS	2.1
1	S	21	PRO	2.1
1	M	54	PHE	2.1
1	U	169	LYS	2.1
1	U	172	VAL	2.1
1	W	389	GLY	2.1
1	G	456	THR	2.1
1	W	395	ILE	2.1
1	W	198	LEU	2.1
2	V	19	ALA	2.1
1	K	140	LYS	2.1
1	U	110	SER	2.1
2	J	67	ARG	2.1
2	P	67	ARG	2.1
1	U	182	ASP	2.1
1	C	296	TRP	2.1
1	S	276	TRP	2.1
2	T	164	GLY	2.1
1	S	451	GLU	2.1
1	O	316	VAL	2.1
1	S	105	MET	2.1
1	U	85	MET	2.1
2	X	9	PHE	2.1
2	H	124	THR	2.1
1	K	417	ARG	2.1
1	S	439	ARG	2.1
2	F	67	ARG	2.1
2	N	27	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	409	LEU	2.1
1	S	444	HIS	2.1
1	S	363	PRO	2.1
1	U	436	GLU	2.1
1	W	426	PRO	2.1
1	U	275	GLY	2.1
1	I	420	THR	2.1
1	K	261	LYS	2.1
2	L	17	LYS	2.1
1	K	296	TRP	2.1
1	U	176	TRP	2.1
1	S	142	ALA	2.1
1	M	247	ILE	2.1
2	H	118	ILE	2.1
2	X	118	ILE	2.1
1	U	333	LEU	2.1
1	O	416	GLY	2.1
1	Q	261	LYS	2.1
1	U	282	GLY	2.1
2	R	10	LYS	2.1
2	X	164	GLY	2.1
1	S	200	ARG	2.0
1	M	251	MET	2.0
1	U	76	THR	2.0
1	W	233	HIS	2.0
1	S	68	PRO	2.0
1	W	397	LYS	2.0
1	K	421	GLY	2.0
1	Q	417	ARG	2.0
2	X	157	ARG	2.0
1	S	59	LEU	2.0
1	W	161	LEU	2.0
2	X	167	ILE	2.0
1	U	22	GLU	2.0
2	V	126	ASP	2.0
1	I	453	SER	2.0
1	C	140	LYS	2.0
1	Q	102	HIS	2.0
2	H	17	LYS	2.0
2	L	52	LYS	2.0
1	S	168	TYR	2.0
1	Q	318	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	157	GLU	2.0
1	W	242	GLY	2.0
1	W	158	TRP	2.0
1	W	220	TRP	2.0
1	S	177	ASP	2.0
1	M	39	ILE	2.0
1	S	318	ARG	2.0
1	G	306	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	BNL	E	462	12/12	0.70	0.24	6.06	47,50,52,52	0
5	BNL	S	462	12/12	0.66	0.63	3.79	56,57,58,58	12
5	BNL	Q	462	12/12	0.74	0.19	2.80	56,58,60,60	0
5	BNL	C	462	12/12	0.80	0.17	1.32	33,34,35,35	0
5	BNL	K	462	12/12	0.90	0.11	0.74	42,43,44,44	0
3	FES	S	460	4/4	0.85	0.17	0.44	82,83,84,86	0
5	BNL	M	462	12/12	0.90	0.12	0.39	49,50,52,52	0
5	BNL	I	462	12/12	0.91	0.11	0.32	32,32,33,33	0
5	BNL	O	462	12/12	0.90	0.10	-0.06	38,38,40,40	0
5	BNL	W	462	12/12	0.79	0.15	-0.64	80,81,83,83	0
3	FES	K	460	4/4	0.99	0.10	-0.91	23,24,24,24	0
3	FES	E	460	4/4	0.99	0.08	-1.24	24,24,24,25	0
4	FE2	E	461	1/1	0.94	0.06	-1.27	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FES	U	460	4/4	0.92	0.12	-1.41	65,66,67,67	4
3	FES	M	460	4/4	0.99	0.07	-1.46	24,24,24,24	0
3	FES	G	460	4/4	0.97	0.06	-1.64	33,34,35,35	0
3	FES	Q	460	4/4	0.99	0.05	-1.77	29,30,30,31	0
4	FE2	C	461	1/1	0.96	0.06	-1.99	25,25,25,25	0
3	FES	C	460	4/4	0.98	0.07	-2.20	26,26,26,26	0
3	FES	O	460	4/4	0.98	0.05	-2.32	33,34,34,34	0
3	FES	I	460	4/4	0.98	0.05	-2.47	28,28,28,28	0
3	FES	A	460	4/4	0.98	0.05	-2.77	26,26,26,26	0
3	FES	W	460	4/4	0.97	0.04	-2.95	55,56,57,57	0
4	FE2	S	461	1/1	0.97	0.06	-4.07	68,68,68,68	0
4	FE2	M	461	1/1	0.99	0.02	-5.08	29,29,29,29	0
4	FE2	W	461	1/1	0.88	0.06	-	75,75,75,75	0
4	FE2	A	461	1/1	1.00	0.08	-	24,24,24,24	0
4	FE2	U	461	1/1	0.95	0.12	-	62,62,62,62	0
4	FE2	G	461	1/1	1.00	0.05	-	23,23,23,23	0
4	FE2	O	461	1/1	0.99	0.07	-	26,26,26,26	0
4	FE2	I	461	1/1	0.99	0.04	-	25,25,25,25	0
4	FE2	Q	461	1/1	0.95	0.05	-	50,50,50,50	0
4	FE2	K	461	1/1	0.99	0.04	-	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.