



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:04 am BST

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

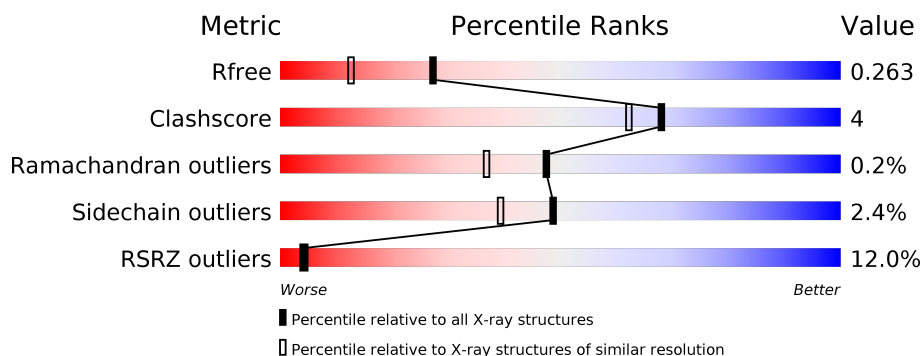
# 1 Overall quality at a glance

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))
$R_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (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  $\geq 3$ , 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	<div> <div></div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	459	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>
1	E	459	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>
1	G	459	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>
1	I	459	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	K	459	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>

Continued on next page...

Continued from previous page...

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	G	460	-	-	X	-
3	FES	Q	460	-	-	X	-
3	FES	W	460	-	-	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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

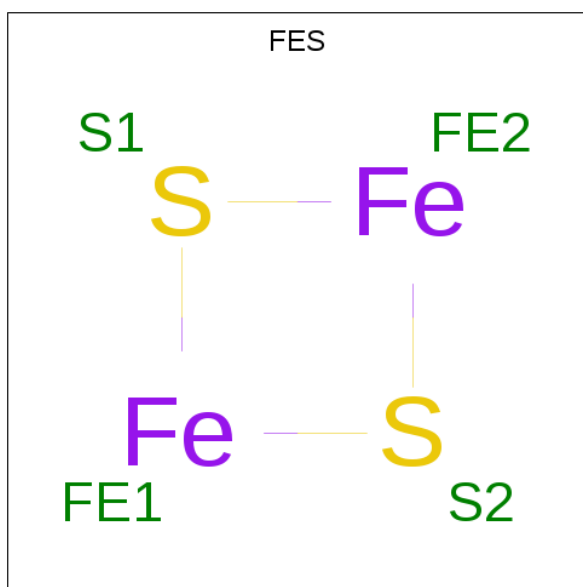
*Continued from previous page...*

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: Fe<sub>2</sub>S<sub>2</sub>).

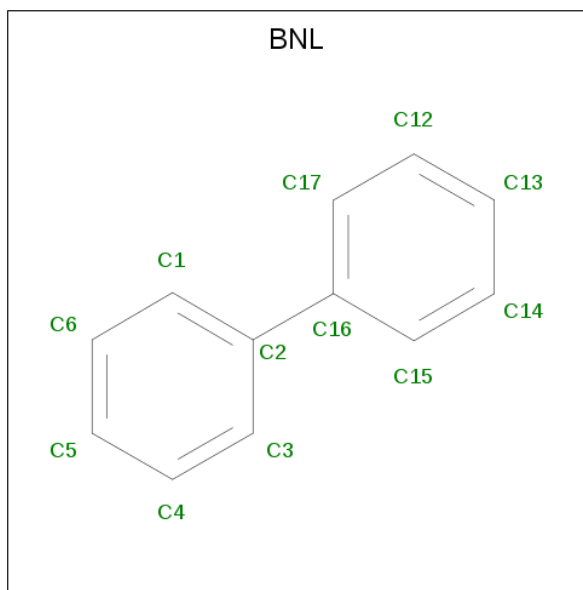


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	I	1	Total	Fe	S	0	0
			4	2	2		
3	K	1	Total	Fe	S	0	0
			4	2	2		
3	M	1	Total	Fe	S	0	0
			4	2	2		
3	O	1	Total	Fe	S	0	0
			4	2	2		
3	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:  $C_{12}H_{10}$ ).





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

*Continued on next page...*

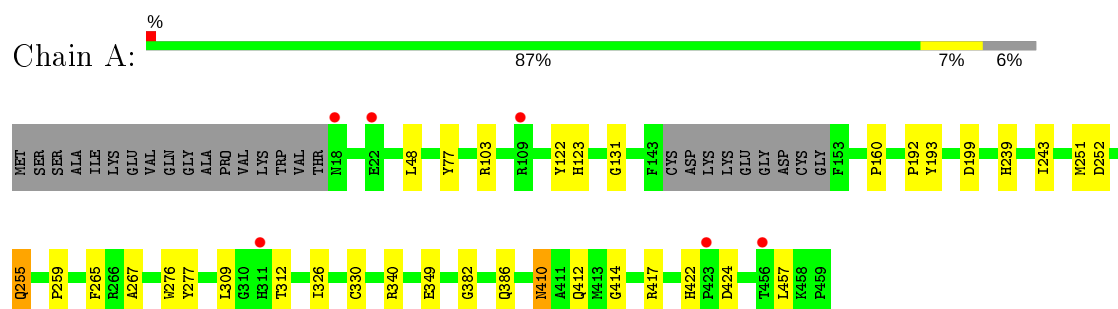
*Continued from previous page...*

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

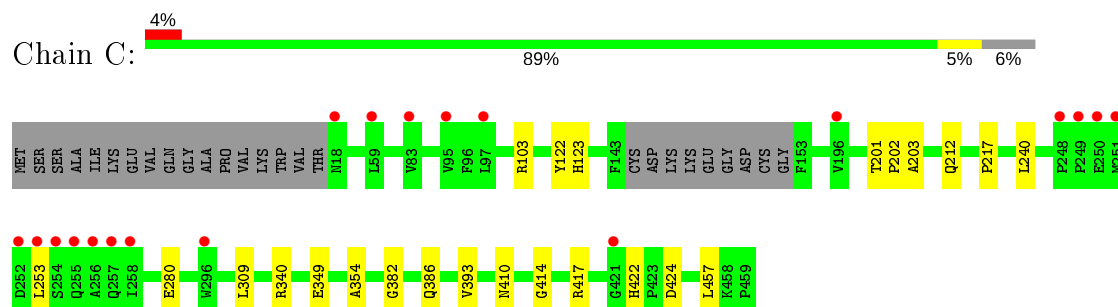
### 3 Residue-property plots [i](#)

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

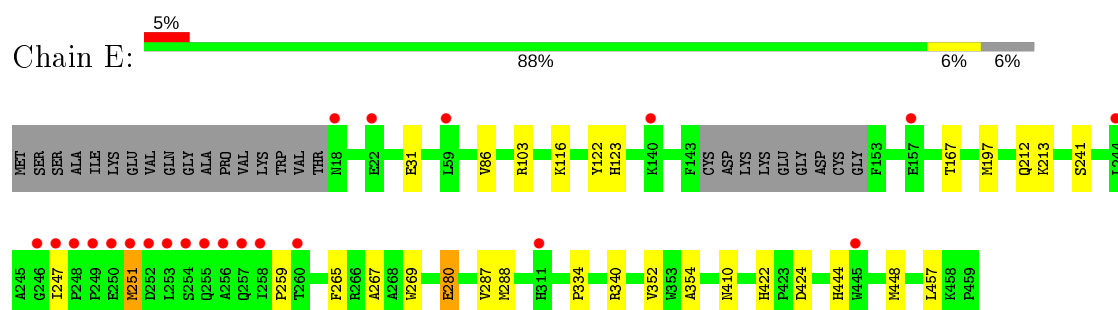
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



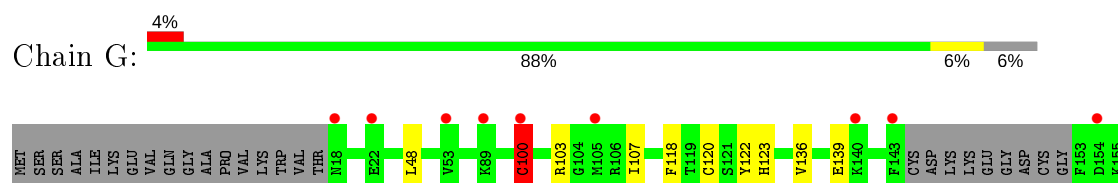
#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

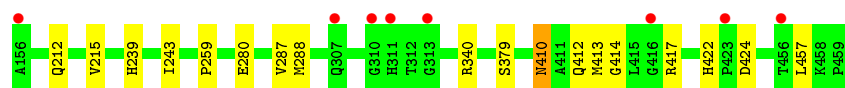


#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

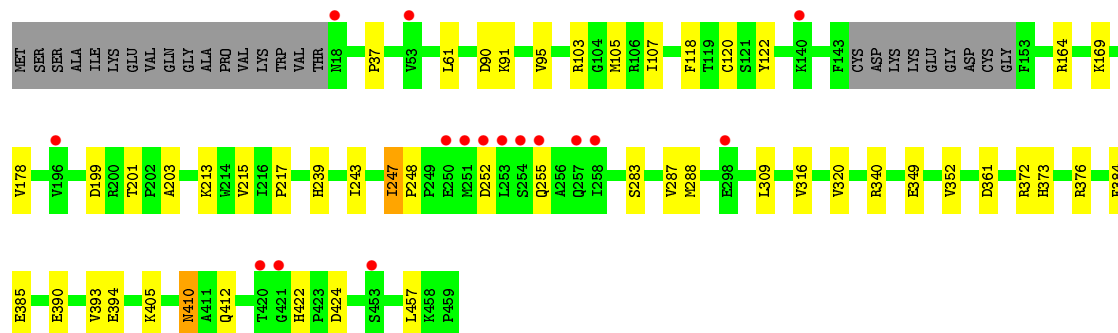
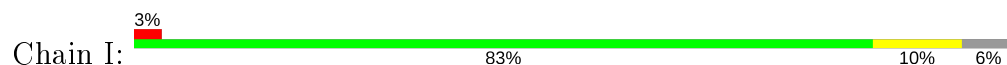


#### • Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

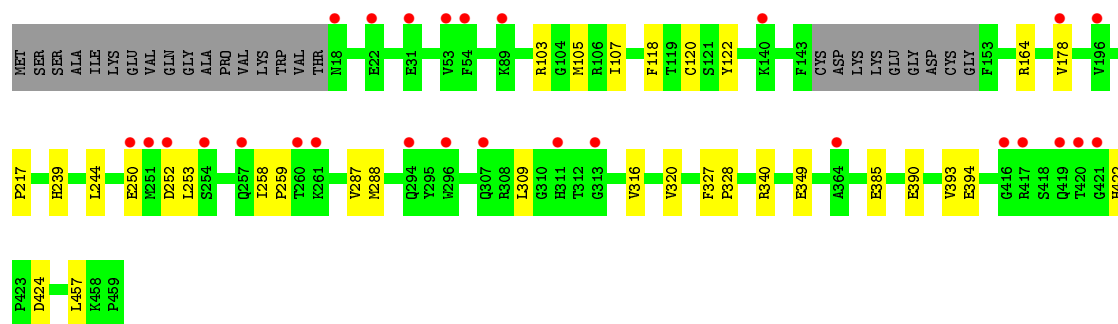
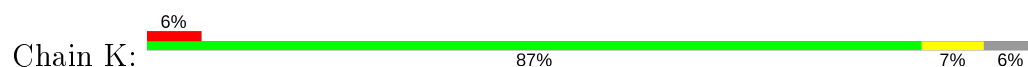




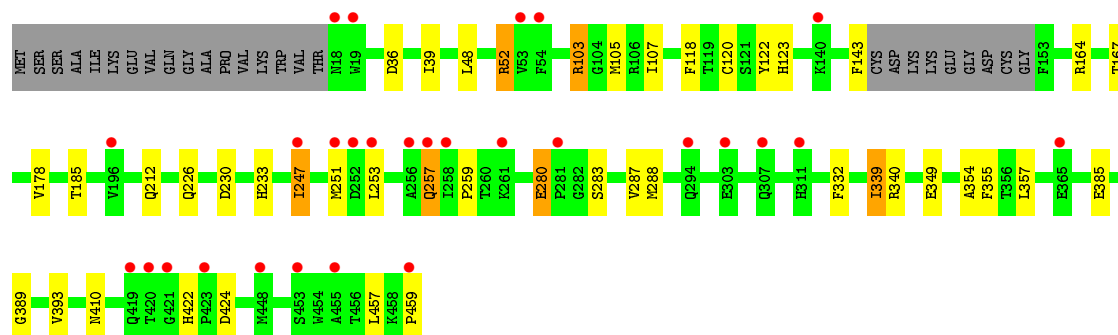
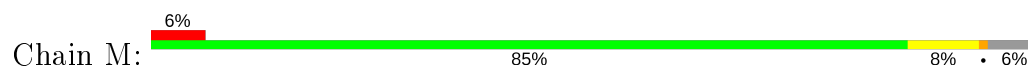
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



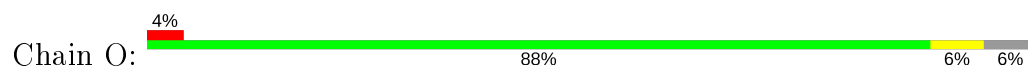
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

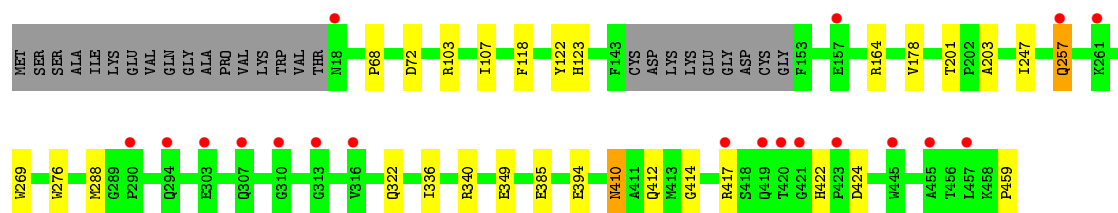


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

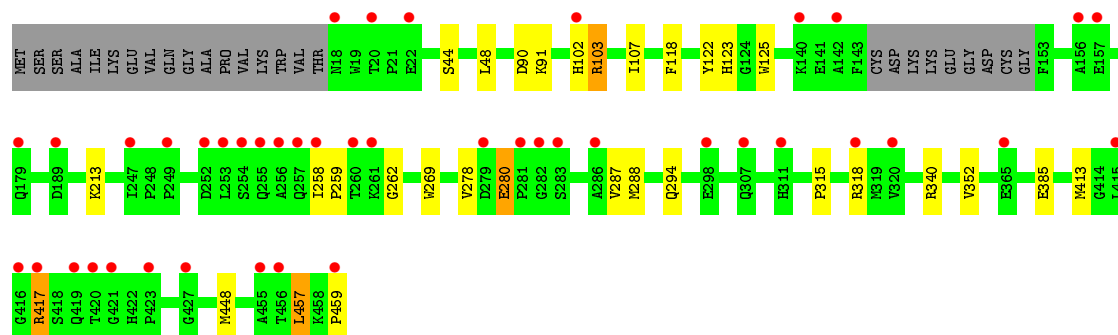
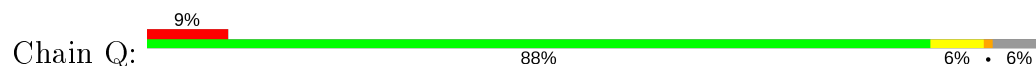


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

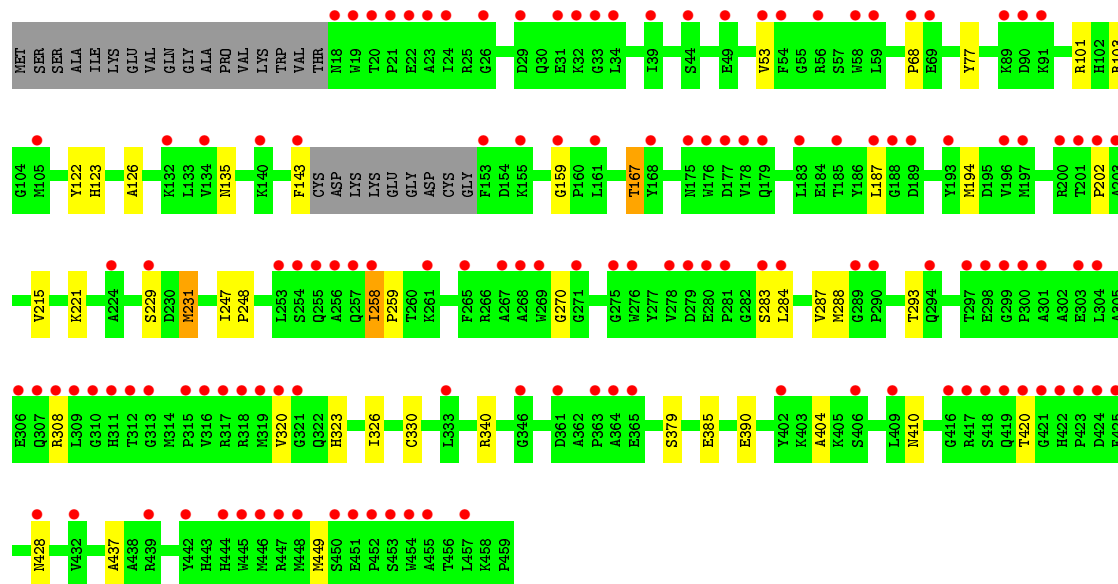
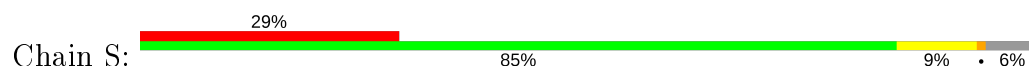




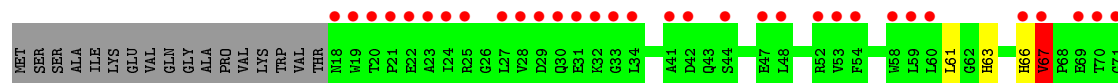
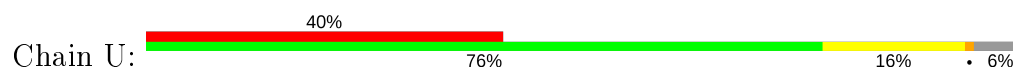
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

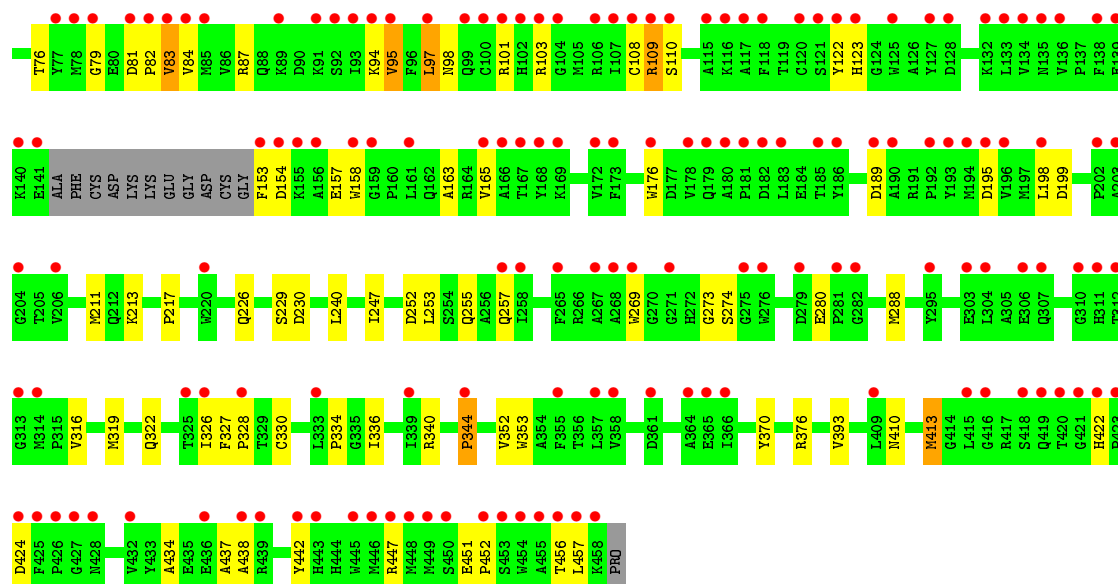


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

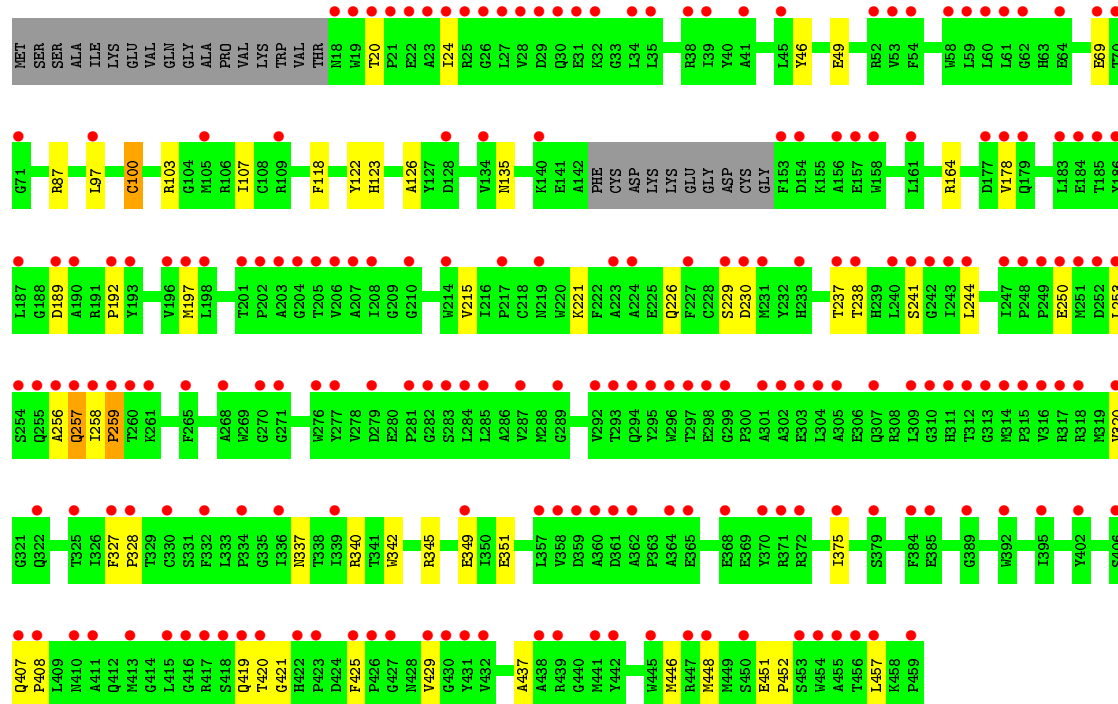
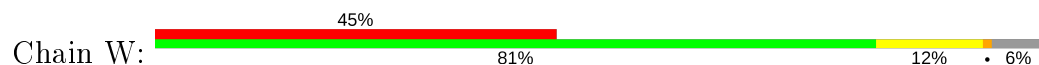


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

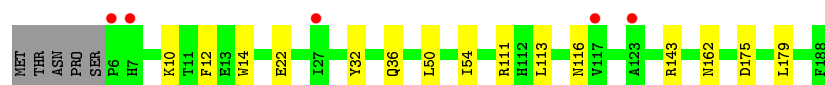
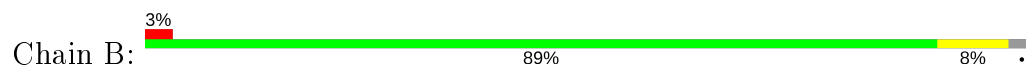




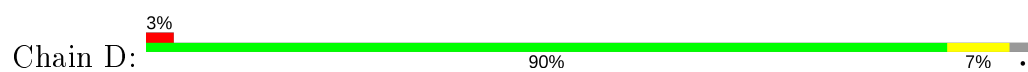
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



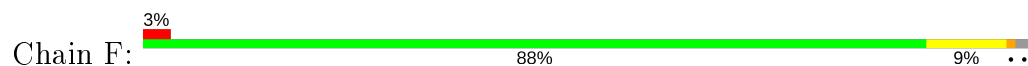
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



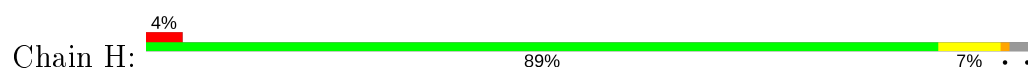
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



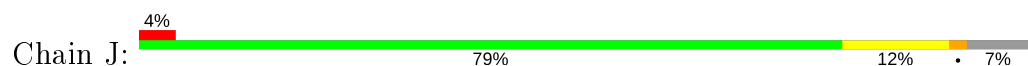
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



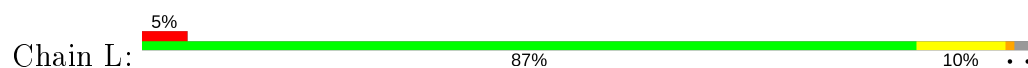
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



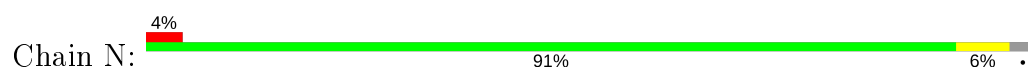
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



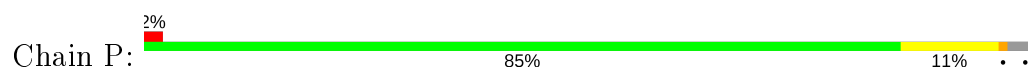
- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



- Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

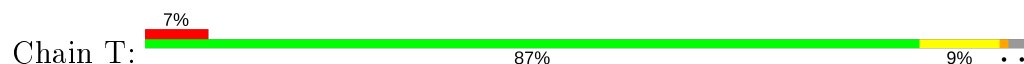




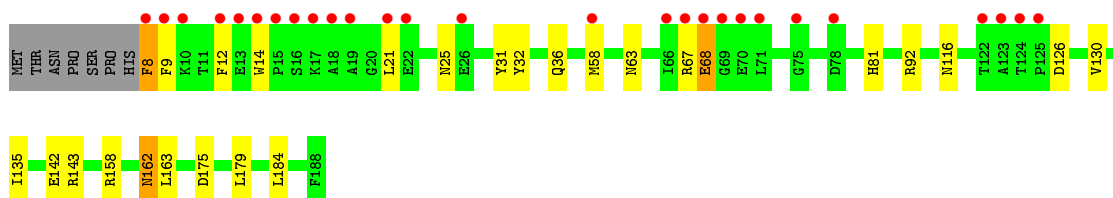
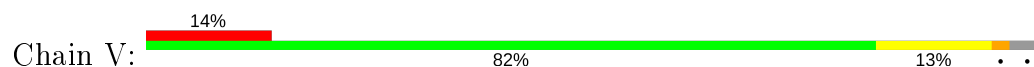
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



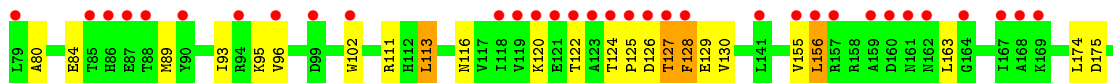
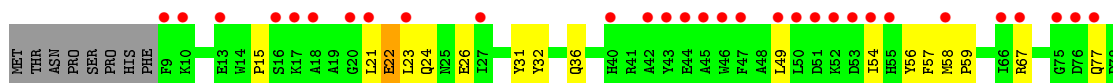
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• 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, $\alpha$ , $\beta$ , $\gamma$	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) 96.1 (23.33-1.88)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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:

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
-----	-------	-----	------	-------	---	-------------	----------

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	18	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

*Continued on next page...*

*Continued from previous page...*

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	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
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

*Continued on next page...*

*Continued from previous page...*

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	445	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 (445) 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

*Continued on next page...*

*Continued from previous page...*

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:G:120:CYS:SG	3:G:460:FES:FE1	1.69	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:287:VAL:CG1	1:K:288:MET:HE3	2.18	0.69
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
1:G:100:CYS:SG	3:G:460:FES:FE1	1.85	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
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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CE	2:N:81:HIS:CB	2.81	0.58
2:N:58:MET:HE1	2:N:184:LEU:HD13	1.86	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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:123:HIS:HB2	3:C:460:FES:S2	2.53	0.49
2:B:12:PHE:H	2:P:36:GLN:NE2	2.09	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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:X:58:MET:CE	2:X:174:LEU:HD22	2.48	0.44
2:V:12:PHE:H	2:X:36:GLN:HE21	1.64	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
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
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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

Continued from previous page...

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

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	430/459 (94%)	413 (96%)	17 (4%)	0	100	100
1	Q	429/459 (94%)	415 (97%)	13 (3%)	1 (0%)	47	37
1	S	429/459 (94%)	411 (96%)	17 (4%)	1 (0%)	47	37
1	U	426/459 (93%)	400 (94%)	22 (5%)	4 (1%)	17	7
1	W	428/459 (93%)	406 (95%)	19 (4%)	3 (1%)	22	11
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%)	25	14
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%)	29	17
2	R	179/188 (95%)	173 (97%)	5 (3%)	1 (1%)	25	14
2	T	180/188 (96%)	175 (97%)	5 (3%)	0	100	100
2	V	179/188 (95%)	170 (95%)	8 (4%)	1 (1%)	25	14
2	X	179/188 (95%)	169 (94%)	9 (5%)	1 (1%)	25	14
All	All	7315/7764 (94%)	7043 (96%)	258 (4%)	14 (0%)	47	37

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%)	55	47
1	C	353/372 (95%)	346 (98%)	7 (2%)	55	47
1	E	351/372 (94%)	343 (98%)	8 (2%)	50	41
1	G	351/372 (94%)	344 (98%)	7 (2%)	55	47
1	I	352/372 (95%)	343 (97%)	9 (3%)	46	36
1	K	351/372 (94%)	341 (97%)	10 (3%)	43	33
1	M	352/372 (95%)	338 (96%)	14 (4%)	31	19
1	O	352/372 (95%)	345 (98%)	7 (2%)	55	47
1	Q	351/372 (94%)	341 (97%)	10 (3%)	43	33
1	S	351/372 (94%)	342 (97%)	9 (3%)	46	36
1	U	349/372 (94%)	334 (96%)	15 (4%)	29	17
1	W	350/372 (94%)	345 (99%)	5 (1%)	67	62
2	B	163/167 (98%)	161 (99%)	2 (1%)	71	67
2	D	164/167 (98%)	163 (99%)	1 (1%)	86	86
2	F	165/167 (99%)	159 (96%)	6 (4%)	35	23
2	H	161/167 (96%)	160 (99%)	1 (1%)	86	86
2	J	155/167 (93%)	150 (97%)	5 (3%)	39	27
2	L	162/167 (97%)	161 (99%)	1 (1%)	86	86
2	N	162/167 (97%)	159 (98%)	3 (2%)	57	49
2	P	163/167 (98%)	160 (98%)	3 (2%)	59	52
2	R	160/167 (96%)	159 (99%)	1 (1%)	86	86
2	T	161/167 (96%)	156 (97%)	5 (3%)	40	29
2	V	160/167 (96%)	158 (99%)	2 (1%)	69	64
2	X	160/167 (96%)	153 (96%)	7 (4%)	28	16
All	All	6152/6468 (95%)	6007 (98%)	145 (2%)	49	39

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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	U	460	1	0,4,4	0.00	-	-		
3	FES	E	460	1	0,4,4	0.00	-	-		
3	FES	S	460	1,6	0,4,4	0.00	-	-		
3	FES	Q	460	1	0,4,4	0.00	-	-		
5	BNL	O	462	-	13,13,13	1.17	1 (7%)	16,16,16	0.62	0
5	BNL	I	462	-	13,13,13	1.14	1 (7%)	16,16,16	0.44	0
5	BNL	S	462	-	13,13,13	1.11	1 (7%)	16,16,16	0.62	0
3	FES	G	460	1	0,4,4	0.00	-	-		
5	BNL	C	462	-	13,13,13	1.09	1 (7%)	16,16,16	0.43	0
5	BNL	E	462	-	13,13,13	1.12	1 (7%)	16,16,16	0.68	0
5	BNL	M	462	-	13,13,13	1.12	1 (7%)	16,16,16	0.43	0
3	FES	C	460	1	0,4,4	0.00	-	-		
3	FES	A	460	1	0,4,4	0.00	-	-		
5	BNL	W	462	-	13,13,13	1.13	1 (7%)	16,16,16	0.51	0
3	FES	O	460	1	0,4,4	0.00	-	-		
3	FES	M	460	1	0,4,4	0.00	-	-		
5	BNL	Q	462	-	13,13,13	1.17	1 (7%)	16,16,16	0.49	0
5	BNL	K	462	-	13,13,13	1.15	1 (7%)	16,16,16	0.48	0
3	FES	I	460	1	0,4,4	0.00	-	-		
3	FES	K	460	1	0,4,4	0.00	-	-		
3	FES	W	460	1	0,4,4	0.00	-	-		

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	U	460	1	-	-	0/1/1/1
3	FES	E	460	1	-	-	0/1/1/1
5	BNL	S	462	-	-	0/4/4/4	0/2/2/2
5	BNL	Q	462	-	-	4/4/4/4	0/2/2/2
3	FES	O	460	1	-	-	0/1/1/1
3	FES	C	460	1	-	-	0/1/1/1
3	FES	I	460	1	-	-	0/1/1/1
3	FES	S	460	1,6	-	-	0/1/1/1
3	FES	G	460	1	-	-	0/1/1/1
5	BNL	E	462	-	-	4/4/4/4	0/2/2/2
3	FES	M	460	1	-	-	0/1/1/1
5	BNL	C	462	-	-	4/4/4/4	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	A	460	1	-	-	0/1/1/1
3	FES	W	460	1	-	-	0/1/1/1
5	BNL	O	462	-	-	0/4/4/4	0/2/2/2
5	BNL	M	462	-	-	0/4/4/4	0/2/2/2
3	FES	Q	460	1	-	-	0/1/1/1
5	BNL	K	462	-	-	0/4/4/4	0/2/2/2
5	BNL	I	462	-	-	0/4/4/4	0/2/2/2
3	FES	K	460	1	-	-	0/1/1/1
5	BNL	W	462	-	-	4/4/4/4	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	-3.81	1.39	1.49
5	O	462	BNL	C16-C2	-3.63	1.40	1.49
5	W	462	BNL	C16-C2	-3.59	1.40	1.49
5	Q	462	BNL	C16-C2	-3.58	1.40	1.49
5	K	462	BNL	C16-C2	-3.56	1.40	1.49
5	E	462	BNL	C16-C2	-3.51	1.40	1.49
5	M	462	BNL	C16-C2	-3.46	1.40	1.49
5	I	462	BNL	C16-C2	-3.27	1.40	1.49
5	C	462	BNL	C16-C2	-3.21	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	C15-C16-C2-C3
5	W	462	BNL	C17-C16-C2-C3
5	W	462	BNL	C17-C16-C2-C1
5	C	462	BNL	C15-C16-C2-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
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	U	460	FES	1	0
3	E	460	FES	1	0
3	S	460	FES	1	0
3	Q	460	FES	2	0
3	G	460	FES	3	0
5	C	462	BNL	3	0
5	E	462	BNL	1	0
5	M	462	BNL	1	0
3	C	460	FES	1	0
3	A	460	FES	1	0
3	O	460	FES	1	0
3	M	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	433/459 (94%)	0.08	6 (1%) 75 77	23, 26, 40, 53	11 (2%)
1	C	433/459 (94%)	0.24	19 (4%) 34 35	23, 26, 41, 87	15 (3%)
1	E	433/459 (94%)	0.13	22 (5%) 28 29	22, 29, 47, 96	12 (2%)
1	G	433/459 (94%)	0.08	17 (3%) 39 41	23, 29, 46, 63	16 (3%)
1	I	433/459 (94%)	0.04	16 (3%) 41 43	22, 30, 45, 61	16 (3%)
1	K	433/459 (94%)	0.18	27 (6%) 20 22	22, 33, 51, 64	15 (3%)
1	M	433/459 (94%)	0.22	28 (6%) 18 20	22, 33, 54, 65	16 (3%)
1	O	433/459 (94%)	0.11	19 (4%) 34 35	22, 36, 54, 68	20 (4%)
1	Q	433/459 (94%)	0.43	43 (9%) 7 8	25, 39, 65, 85	12 (2%)
1	S	433/459 (94%)	1.68	135 (31%) 0 0	43, 77, 113, 129	48 (11%)
1	U	430/459 (93%)	2.09	182 (42%) 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%) 54 56	24, 25, 31, 50	3 (1%)
2	D	183/188 (97%)	0.26	6 (3%) 46 47	24, 25, 33, 43	7 (3%)
2	F	184/188 (97%)	0.13	6 (3%) 46 47	24, 26, 33, 40	4 (2%)
2	H	181/188 (96%)	-0.00	8 (4%) 34 35	24, 26, 37, 47	3 (1%)
2	J	175/188 (93%)	0.19	8 (4%) 32 34	24, 26, 33, 67	8 (4%)
2	L	182/188 (96%)	0.02	9 (4%) 29 31	23, 27, 35, 58	4 (2%)
2	N	183/188 (97%)	0.04	8 (4%) 34 35	24, 27, 37, 58	6 (3%)
2	P	181/188 (96%)	-0.01	4 (2%) 62 63	23, 27, 38, 53	3 (1%)
2	R	181/188 (96%)	-0.03	9 (4%) 28 30	23, 30, 40, 48	3 (1%)
2	T	182/188 (96%)	0.40	13 (7%) 16 17	28, 41, 61, 68	3 (1%)
2	V	181/188 (96%)	0.68	27 (14%) 2 2	25, 44, 87, 107	11 (6%)
2	X	180/188 (95%)	1.78	65 (36%) 0 0	45, 72, 101, 111	21 (11%)

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	7368/7764 (94%)	0.53	887 (12%) 4 4	22, 32, 89, 129	381 (5%)

All (887) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	418	SER	21.2
1	U	409	LEU	13.4
1	W	284	LEU	12.0
1	U	100	CYS	11.7
1	W	230	ASP	11.6
1	S	258	ILE	11.1
1	U	99	GLN	10.2
1	U	269	TRP	9.9
1	S	364	ALA	9.9
1	W	258	ILE	9.8
2	X	122	THR	9.7
2	X	125	PRO	9.4
1	W	442	TYR	9.3
1	U	355	PHE	9.3
1	U	109	ARG	9.2
1	U	67	VAL	9.2
1	S	321	GLY	8.9
1	U	153	PHE	8.9
1	U	158	TRP	8.6
1	W	364	ALA	8.5
1	S	455	ALA	8.3
1	E	251	MET	8.2
1	W	257	GLN	8.2
2	V	8	PHE	7.9
1	W	26	GLY	7.9
1	W	249	PRO	7.9
1	S	313	GLY	7.7
1	E	256	ALA	7.6
1	U	82	PRO	7.6
1	U	449	MET	7.4
1	S	202	PRO	7.4
1	W	224	ALA	7.4
2	X	102	TRP	7.4
1	W	312	THR	7.3
1	U	95	VAL	7.2
1	S	420	THR	7.2
2	V	123	ALA	7.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	V	67	ARG	7.2
1	U	442	TYR	7.1
1	Q	257	GLN	7.1
2	X	168	ALA	7.1
1	U	79	GLY	7.1
1	Q	421	GLY	7.0
1	W	419	GLN	6.9
1	S	416	GLY	6.8
1	S	18	ASN	6.8
1	U	457	LEU	6.7
1	W	19	TRP	6.7
1	U	103	ARG	6.6
1	E	254	SER	6.6
1	U	455	ALA	6.6
1	W	34	LEU	6.4
1	E	250	GLU	6.4
1	U	140	LYS	6.4
1	U	178	VAL	6.4
1	W	22	GLU	6.3
1	W	260	THR	6.3
1	W	294	GLN	6.3
1	S	419	GLN	6.2
1	Q	258	ILE	6.2
1	C	255	GLN	6.1
1	W	316	VAL	6.1
1	S	159	GLY	6.1
1	U	93	ILE	6.1
1	S	311	HIS	6.0
2	X	54	ILE	6.0
1	U	313	GLY	6.0
1	W	422	HIS	6.0
1	S	178	VAL	6.0
1	U	156	ALA	5.9
1	W	256	ALA	5.9
1	W	202	PRO	5.8
1	S	153	PHE	5.8
1	W	455	ALA	5.8
1	W	20	THR	5.8
1	W	203	ALA	5.7
1	U	21	PRO	5.7
2	R	8	PHE	5.7
1	S	424	ASP	5.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	8	PHE	5.7
1	C	251	MET	5.6
1	U	132	LYS	5.6
1	C	254	SER	5.6
2	X	127	THR	5.6
2	V	18	ALA	5.6
1	W	420	THR	5.6
1	E	258	ILE	5.6
1	S	261	LYS	5.6
2	X	20	GLY	5.6
2	X	90	TYR	5.6
1	S	19	TRP	5.6
1	U	186	TYR	5.6
1	U	166	ALA	5.5
1	U	179	GLN	5.5
1	S	418	SER	5.5
2	V	125	PRO	5.4
1	U	83	VAL	5.4
1	U	419	GLN	5.4
1	W	413	MET	5.4
1	S	316	VAL	5.4
1	C	250	GLU	5.3
1	W	432	VAL	5.3
1	W	423	PRO	5.3
1	W	292	VAL	5.3
1	W	265	PHE	5.3
1	U	127	TYR	5.3
2	T	160	ASP	5.2
1	S	188	GLY	5.2
1	S	58	TRP	5.1
1	S	143	PHE	5.1
1	S	421	GLY	5.1
1	S	179	GLN	5.1
1	U	453	SER	5.1
1	W	328	PRO	5.1
2	X	155	VAL	5.1
1	W	189	ASP	5.1
1	U	18	ASN	5.1
1	S	183	LEU	5.1
2	V	69	GLY	5.0
1	U	138	PHE	5.0
1	M	253	LEU	5.0

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	U	311	HIS	5.0
2	X	16	SER	5.0
1	E	255	GLN	5.0
1	U	134	VAL	4.9
1	W	28	VAL	4.9
2	R	160	ASP	4.9
1	E	18	ASN	4.9
1	Q	281	PRO	4.9
1	U	94	LYS	4.9
1	S	189	ASP	4.9
1	U	91	LYS	4.9
1	U	106	ARG	4.9
2	X	87	GLU	4.8
1	U	420	THR	4.8
2	X	161	ASN	4.8
1	S	423	PRO	4.8
1	U	28	VAL	4.8
1	S	417	ARG	4.8
1	A	18	ASN	4.7
1	E	257	GLN	4.7
1	E	252	ASP	4.7
1	U	202	PRO	4.7
1	W	456	THR	4.7
1	S	310	GLY	4.7
1	U	181	PRO	4.7
1	S	255	GLN	4.7
2	T	159	ALA	4.7
1	U	165	VAL	4.7
1	U	89	LYS	4.7
2	N	6	PRO	4.7
1	S	268	ALA	4.6
1	W	276	TRP	4.6
1	U	307	GLN	4.6
2	X	17	LYS	4.6
1	U	421	GLY	4.6
1	I	255	GLN	4.6
1	Q	256	ALA	4.6
2	X	120	LYS	4.6
1	U	204	GLY	4.6
2	X	124	THR	4.6
1	W	361	ASP	4.6
1	S	90	ASP	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	J	14	TRP	4.5
2	X	162	ASN	4.5
1	U	454	TRP	4.5
2	V	75	GLY	4.5
1	Q	254	SER	4.5
2	X	27	ILE	4.5
2	X	156	LEU	4.5
1	C	252	ASP	4.5
1	I	254	SER	4.5
2	X	21	LEU	4.4
1	U	115	ALA	4.4
1	Q	419	GLN	4.4
1	U	425	PHE	4.4
1	E	248	PRO	4.4
1	M	18	ASN	4.4
1	Q	423	PRO	4.4
2	X	55	HIS	4.4
1	I	250	GLU	4.4
1	U	92	SER	4.4
1	W	303	GLU	4.4
1	S	307	GLN	4.4
1	W	415	LEU	4.4
1	W	157	GLU	4.4
2	X	160	ASP	4.4
1	U	33	GLY	4.3
1	S	256	ALA	4.3
1	W	295	TYR	4.3
1	W	285	LEU	4.3
2	T	21	LEU	4.3
2	T	126	ASP	4.3
2	L	160	ASP	4.3
1	U	54	PHE	4.3
2	X	47	PHE	4.3
1	U	66	HIS	4.3
2	X	77	GLN	4.3
1	W	425	PHE	4.3
2	V	9	PHE	4.3
1	W	18	ASN	4.3
1	W	207	ALA	4.3
1	M	421	GLY	4.2
1	W	430	GLY	4.2
1	W	402	TYR	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	252	ASP	4.2
1	W	359	ASP	4.2
1	S	265	PHE	4.2
1	S	454	TRP	4.2
2	V	17	LYS	4.2
1	U	122	TYR	4.2
2	B	6	PRO	4.2
1	W	140	LYS	4.2
1	W	279	ASP	4.1
1	U	415	LEU	4.1
2	F	160	ASP	4.1
1	S	278	VAL	4.1
2	P	160[A]	ASP	4.1
1	M	258	ILE	4.1
1	W	227	PHE	4.1
2	L	8	PHE	4.1
1	W	410	ASN	4.1
1	W	183	LEU	4.0
1	W	307	GLN	4.0
2	N	7	HIS	4.0
2	X	51	ASP	4.0
2	X	23	LEU	4.0
2	X	94	ARG	4.0
2	V	16	SER	4.0
1	W	411	ALA	4.0
2	N	123	ALA	4.0
1	W	259	PRO	4.0
1	U	268	ALA	4.0
1	S	193	TYR	4.0
1	W	298	GLU	4.0
1	W	370	TYR	3.9
1	U	52	ARG	3.9
1	S	140	LYS	3.9
1	C	248	PRO	3.9
1	U	416	GLY	3.9
1	W	217	PRO	3.9
1	K	252	ASP	3.9
1	S	306	GLU	3.9
1	W	261	LYS	3.9
1	U	344	PRO	3.9
2	X	121	GLU	3.9
1	S	402	TYR	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	S	89	LYS	3.9
1	U	365	GLU	3.9
2	X	187	PHE	3.9
1	E	253	LEU	3.9
1	W	271	GLY	3.9
1	W	156	ALA	3.8
1	M	311	HIS	3.8
1	K	419	GLN	3.8
1	W	313	GLY	3.8
2	X	123	ALA	3.8
1	U	20	THR	3.8
1	W	248	PRO	3.8
1	W	186	TYR	3.8
1	W	268	ALA	3.8
1	W	204	GLY	3.8
1	C	253	LEU	3.8
1	Q	156	ALA	3.8
1	K	420	THR	3.8
1	W	408	PRO	3.8
1	U	314	MET	3.8
1	Q	247	ILE	3.8
1	S	298	GLU	3.8
1	C	18	ASN	3.8
1	W	327	PHE	3.8
1	U	424	ASP	3.7
1	W	255	GLN	3.8
1	W	270	GLY	3.7
1	Q	416	GLY	3.7
1	W	375	ILE	3.7
1	S	257	GLN	3.7
1	W	282	GLY	3.7
1	U	116	LYS	3.7
2	X	10	LYS	3.7
1	U	48	LEU	3.7
1	W	251	MET	3.7
2	X	58	MET	3.7
1	W	459	PRO	3.7
1	W	301	ALA	3.7
2	H	8	PHE	3.7
1	S	134	VAL	3.7
2	T	162	ASN	3.7
1	W	208	ILE	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	W	417	ARG	3.7
1	W	314	MET	3.7
1	W	360	ALA	3.7
1	U	426	PRO	3.7
1	S	69	GLU	3.7
1	U	312	THR	3.6
1	W	431	TYR	3.6
1	W	304	LEU	3.6
1	W	178	VAL	3.6
1	M	420	THR	3.6
2	J	162	ASN	3.6
1	U	267	ALA	3.6
1	W	192	PRO	3.6
2	X	159	ALA	3.6
1	M	261	LYS	3.6
2	V	14	TRP	3.6
1	U	203	ALA	3.6
1	W	45	LEU	3.6
1	S	425	PHE	3.6
1	W	24	ILE	3.6
1	S	33	GLY	3.6
2	V	71	LEU	3.6
1	S	155	LYS	3.6
1	E	247	ILE	3.5
1	S	317	ARG	3.5
1	U	304	LEU	3.5
1	W	365	GLU	3.5
2	R	76	ASP	3.5
2	V	122	THR	3.5
1	U	133	LEU	3.5
1	W	64	GLU	3.5
1	W	21	PRO	3.5
1	I	140	LYS	3.5
1	K	254	SER	3.5
1	W	229	SER	3.5
1	S	267	ALA	3.5
1	S	361	ASP	3.5
1	U	128	ASP	3.5
1	W	32	LYS	3.5
1	W	254	SER	3.5
1	Q	420	THR	3.5
1	M	455	ALA	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	310	GLY	3.5
2	X	126	ASP	3.5
1	S	290	PRO	3.5
1	U	69	GLU	3.5
1	S	299	GLY	3.4
1	W	416	GLY	3.4
1	W	190	ALA	3.4
2	V	70	GLU	3.4
1	S	187	LEU	3.4
1	S	300	PRO	3.4
1	I	18	ASN	3.4
1	W	427	GLY	3.4
2	X	50	LEU	3.4
1	W	447	ARG	3.4
1	S	457	LEU	3.4
2	X	85	THR	3.4
1	U	53	VAL	3.4
1	W	35	LEU	3.4
1	W	406	SER	3.4
1	C	249	PRO	3.4
2	H	123	ALA	3.4
1	U	326	ILE	3.4
1	W	205	THR	3.4
1	S	196	VAL	3.4
2	V	15	PRO	3.3
1	U	139	GLU	3.3
1	U	23	ALA	3.3
2	F	14	TRP	3.3
1	O	18	ASN	3.3
1	U	258	ILE	3.3
1	U	31	GLU	3.3
1	A	311	HIS	3.3
1	K	364	ALA	3.3
1	W	448	MET	3.3
1	W	247	ILE	3.3
1	U	136	VAL	3.3
1	K	251	MET	3.3
1	G	423	PRO	3.3
1	S	34	LEU	3.3
2	F	5	SER	3.3
1	S	91	LYS	3.3
2	R	67	ARG	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	V	22	GLU	3.3
1	W	320	VAL	3.3
1	S	22	GLU	3.3
1	S	301	ALA	3.3
1	W	29	ASP	3.3
2	V	26	GLU	3.2
2	V	68	GLU	3.2
1	U	125	TRP	3.2
1	W	253	LEU	3.2
1	U	102	HIS	3.2
1	K	250	GLU	3.2
1	U	29	ASP	3.2
2	N	160	ASP	3.2
1	W	368	GLU	3.2
1	K	18	ASN	3.2
2	X	128	PHE	3.2
1	U	117	ALA	3.2
2	B	123	ALA	3.2
1	S	29	ASP	3.2
1	W	392	TRP	3.2
2	X	99[A]	ASP	3.2
1	U	135	ASN	3.2
1	W	52	ARG	3.2
1	O	313	GLY	3.2
2	V	13	GLU	3.2
1	G	18	ASN	3.2
1	S	176	TRP	3.2
1	Q	311	HIS	3.2
1	Q	456	THR	3.2
1	U	189	ASP	3.2
1	U	361	ASP	3.2
2	D	6	PRO	3.2
2	T	20	GLY	3.2
1	S	450	SER	3.2
2	V	21	LEU	3.1
1	S	185	THR	3.1
1	S	297	THR	3.1
1	U	159	GLY	3.1
1	W	438	ALA	3.1
2	J	16	SER	3.1
1	Q	22	GLU	3.1
1	U	47	GLU	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	265	PHE	3.1
1	W	54	PHE	3.1
1	Q	249	PRO	3.1
1	W	297	THR	3.1
1	U	195	ASP	3.1
1	S	175	ASN	3.1
1	S	312	THR	3.1
1	O	421	GLY	3.1
1	Q	282	GLY	3.1
1	W	210	GLY	3.1
1	W	310	GLY	3.1
1	C	196	VAL	3.1
1	O	261	LYS	3.1
1	W	293	THR	3.1
1	Q	283	SER	3.1
2	X	76	ASP	3.1
1	S	31	GLU	3.1
1	W	453	SER	3.1
2	T	16	SER	3.1
1	W	457	LEU	3.1
1	W	339	ILE	3.1
1	Q	455	ALA	3.1
1	W	439	ARG	3.1
1	U	279	ASP	3.0
1	W	252	ASP	3.0
1	S	422	HIS	3.0
1	G	105	MET	3.0
1	G	100	CYS	3.0
2	D	160	ASP	3.0
1	M	281	PRO	3.0
1	U	121	SER	3.0
2	X	169	LYS	3.0
1	K	307	GLN	3.0
1	I	298	GLU	3.0
1	W	154	ASP	3.0
1	W	332	PHE	3.0
1	U	452	PRO	3.0
1	U	295	TYR	3.0
1	O	257	GLN	3.0
1	S	365	GLU	3.0
1	W	250	GLU	3.0
1	O	457	LEU	3.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	X	40	HIS	3.0
1	S	442	TYR	3.0
1	S	432	VAL	3.0
1	Q	253	LEU	3.0
2	T	52	LYS	3.0
1	S	20	THR	3.0
1	W	281	PRO	3.0
1	U	59	LEU	2.9
1	W	325	THR	2.9
1	Q	140	LYS	2.9
2	V	10	LYS	2.9
1	U	448	MET	2.9
2	J	160	ASP	2.9
1	Q	18	ASN	2.9
2	F	162	ASN	2.9
1	Q	427	GLY	2.9
1	W	206	VAL	2.9
1	W	336	ILE	2.9
1	O	423	PRO	2.9
1	W	105	MET	2.9
2	J	15	PRO	2.9
1	U	445	TRP	2.9
2	F	117	VAL	2.9
1	I	257	GLN	2.9
1	U	364	ALA	2.9
1	W	61	LEU	2.9
1	G	310	GLY	2.9
1	S	203	ALA	2.9
2	N	8	PHE	2.9
1	S	283	SER	2.8
1	U	123	HIS	2.8
1	W	237	THR	2.8
1	S	269	TRP	2.8
1	W	58	TRP	2.8
2	D	14	TRP	2.8
1	I	251	MET	2.8
1	Q	298	GLU	2.8
1	S	224	ALA	2.8
1	W	302	ALA	2.8
1	S	56	ARG	2.8
2	T	7	HIS	2.8
1	G	89	LYS	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	S	201	THR	2.8
1	U	108	CYS	2.8
1	W	153	PHE	2.8
2	L	7	HIS	2.8
1	E	244	LEU	2.8
1	S	253	LEU	2.8
1	O	307	GLN	2.8
1	C	258	ILE	2.8
1	S	24	ILE	2.8
1	I	421	GLY	2.8
1	S	452	PRO	2.8
1	U	107	ILE	2.8
1	W	283	SER	2.8
1	M	196	VAL	2.8
1	G	156	ALA	2.8
2	X	141	LEU	2.8
1	I	258	ILE	2.8
1	U	25	ARG	2.8
2	X	43	TYR	2.8
1	S	303	GLU	2.8
2	V	124	THR	2.7
1	U	30	GLN	2.7
1	E	140	LYS	2.7
1	W	334	PRO	2.7
2	D	117	VAL	2.7
2	B	7	HIS	2.7
1	W	31	GLU	2.7
1	S	39	ILE	2.7
1	O	445	TRP	2.7
1	U	271	GLY	2.7
1	W	289	GLY	2.7
1	M	307	GLN	2.7
1	K	22	GLU	2.7
1	W	53	VAL	2.7
1	W	134	VAL	2.7
1	U	180	ALA	2.7
1	C	83	VAL	2.7
1	W	317	ARG	2.7
1	Q	279	ASP	2.7
1	S	284	LEU	2.7
1	Q	307	GLN	2.7
1	W	407	GLN	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	71	GLY	2.7
2	L	159	ALA	2.7
1	G	154	ASP	2.7
1	K	178	VAL	2.7
1	K	257	GLN	2.7
1	S	53	VAL	2.7
1	W	277	TYR	2.7
1	S	271	GLY	2.7
1	U	438	ALA	2.6
2	X	52	LYS	2.6
1	K	416	GLY	2.6
1	M	19	TRP	2.6
1	U	196	VAL	2.6
1	U	206	VAL	2.6
1	U	358	VAL	2.6
1	W	429	VAL	2.6
1	U	447	ARG	2.6
1	W	318	ARG	2.6
2	T	67	ARG	2.6
1	E	249	PRO	2.6
1	S	281	PRO	2.6
1	W	70	THR	2.6
2	X	88	THR	2.6
1	W	23	ALA	2.6
1	S	26	GLY	2.6
1	U	306	GLU	2.6
1	W	372	ARG	2.6
1	S	32	LYS	2.6
1	U	458	LYS	2.6
2	X	119	VAL	2.6
1	K	294	GLN	2.6
1	U	58	TRP	2.6
1	W	69	GLU	2.6
1	C	256	ALA	2.6
1	Q	142	ALA	2.6
2	X	42	ALA	2.6
2	X	75	GLY	2.6
1	S	54	PHE	2.6
1	S	229	SER	2.6
2	X	44	GLU	2.6
1	S	304	LEU	2.6
1	M	252	ASP	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	294	GLN	2.6
1	M	419	GLN	2.6
1	S	446	MET	2.6
1	W	197	MET	2.6
1	Q	20	THR	2.6
1	Q	260	THR	2.6
1	U	118	PHE	2.6
1	S	333	LEU	2.6
1	W	305	ALA	2.6
1	U	220	TRP	2.6
1	S	197	MET	2.6
1	Q	286	ALA	2.5
1	W	379	SER	2.5
1	M	459	PRO	2.5
1	U	257	GLN	2.5
1	G	416	GLY	2.5
1	G	140	LYS	2.5
1	W	287	VAL	2.5
2	B	117	VAL	2.5
1	S	406	SER	2.5
1	C	257	GLN	2.5
1	O	419	GLN	2.5
1	U	34	LEU	2.5
1	W	187	LEU	2.5
1	W	309	LEU	2.5
1	W	357	LEU	2.5
2	X	49	LEU	2.5
2	P	52	LYS	2.5
2	H	67	ARG	2.5
1	K	196	VAL	2.5
2	D	162	ASN	2.5
2	X	188	PHE	2.5
1	M	140	LYS	2.5
1	U	443	HIS	2.5
1	A	456	THR	2.5
1	S	445	TRP	2.5
1	U	44	SER	2.5
1	W	128	ASP	2.5
2	L	99[A]	ASP	2.5
1	U	190	ALA	2.5
1	W	362	ALA	2.5
1	S	447	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	W	109	ARG	2.5
2	X	13	GLU	2.5
1	M	453	SER	2.5
2	L	125	PRO	2.5
1	Q	320	VAL	2.5
1	U	78	MET	2.5
1	W	384	PHE	2.5
2	N	162	ASN	2.5
1	A	22	GLU	2.5
1	U	303	GLU	2.5
1	S	315	PRO	2.4
1	M	256	ALA	2.4
1	K	53	VAL	2.4
1	W	349	GLU	2.4
1	W	358	VAL	2.4
1	U	185	THR	2.4
1	Q	415	LEU	2.4
1	W	60	LEU	2.4
1	W	193	TYR	2.4
1	U	32	LYS	2.4
1	U	281	PRO	2.4
1	W	315	PRO	2.4
2	X	18	ALA	2.4
1	O	420	THR	2.4
1	U	325	THR	2.4
1	E	445	TRP	2.4
1	W	454	TRP	2.4
1	M	303	GLU	2.4
1	O	290	PRO	2.4
1	Q	157	GLU	2.4
1	U	104	GLY	2.4
1	S	132	LYS	2.4
1	S	254	SER	2.4
2	R	17	LYS	2.4
1	U	141	GLU	2.4
1	U	456	THR	2.4
1	M	423	PRO	2.4
1	U	183	LEU	2.4
1	U	77	TYR	2.4
1	U	168	TYR	2.4
1	U	450	SER	2.4
1	U	339	ILE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Q	459	PRO	2.4
1	G	143	PHE	2.4
1	S	279	ASP	2.4
1	U	446	MET	2.4
1	K	260	THR	2.4
1	W	185	THR	2.4
1	O	157	GLU	2.4
1	S	346	GLY	2.4
1	W	330	CYS	2.4
1	O	294	GLN	2.4
1	C	95	VAL	2.4
2	L	117	VAL	2.4
1	S	161	LEU	2.3
2	D	67	ARG	2.3
1	S	23	ALA	2.3
1	E	22	GLU	2.3
1	U	167	THR	2.3
1	E	246	GLY	2.3
1	W	179	GLN	2.3
2	T	125	PRO	2.3
2	V	66	ILE	2.3
1	Q	365	GLU	2.3
1	S	280	GLU	2.3
1	W	223	ALA	2.3
2	N	159	ALA	2.3
1	E	260	THR	2.3
1	O	417	ARG	2.3
1	U	19	TRP	2.3
1	U	155	LYS	2.3
1	U	276	TRP	2.3
2	T	17	LYS	2.3
1	W	39	ILE	2.3
1	W	71	GLY	2.3
1	W	97	LEU	2.3
1	A	423	PRO	2.3
1	W	177	ASP	2.3
2	V	78	ASP	2.3
1	U	418	SER	2.3
2	R	16	SER	2.3
1	Q	179	GLN	2.3
1	U	428	ASN	2.3
2	J	117	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	W	243	ILE	2.3
2	R	70	GLU	2.3
1	U	81	ASP	2.3
1	O	455	ALA	2.3
1	U	101	ARG	2.3
1	U	439	ARG	2.3
1	C	97	LEU	2.3
1	W	59	LEU	2.3
1	S	44	SER	2.3
1	M	365	GLU	2.3
1	U	422	HIS	2.3
2	X	67	ARG	2.3
1	M	448	MET	2.3
1	S	448	MET	2.3
1	W	214	TRP	2.3
1	W	296	TRP	2.3
1	S	21	PRO	2.3
1	S	294	GLN	2.3
1	U	70	THR	2.3
1	U	328	PRO	2.3
1	U	423	PRO	2.3
1	W	238	THR	2.3
1	G	22	GLU	2.3
2	H	16	SER	2.3
1	W	240	LEU	2.3
1	K	311	HIS	2.3
1	U	193	TYR	2.2
1	W	62	GLY	2.2
1	Q	255	GLN	2.2
1	U	194	MET	2.2
1	W	30	GLN	2.2
1	O	303	GLU	2.2
1	I	53	VAL	2.2
1	U	432	VAL	2.2
1	W	41	ALA	2.2
1	W	201	THR	2.2
2	X	46	TRP	2.2
1	W	27	LEU	2.2
1	C	421	GLY	2.2
1	S	275	GLY	2.2
1	W	231	MET	2.2
1	S	453	SER	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	W	241	SER	2.2
1	M	53	VAL	2.2
1	U	84	VAL	2.2
1	W	196	VAL	2.2
1	G	311	HIS	2.2
1	W	311	HIS	2.2
1	U	366	ILE	2.2
2	X	66	ILE	2.2
1	O	310	GLY	2.2
1	W	389	GLY	2.2
1	C	59	LEU	2.2
1	E	59	LEU	2.2
1	U	198	LEU	2.2
2	X	79	LEU	2.2
1	W	38	ARG	2.2
2	J	90	TYR	2.2
1	U	42	ASP	2.2
1	U	173	PHE	2.2
2	R	53	ASP	2.2
1	K	31	GLU	2.2
1	S	49	GLU	2.2
2	X	45	ALA	2.2
1	S	308	ARG	2.2
1	W	244	LEU	2.2
1	W	445	TRP	2.2
1	U	85	MET	2.2
2	V	58	MET	2.2
1	K	89	LYS	2.2
2	H	10	LYS	2.2
1	E	311	HIS	2.2
1	S	444	HIS	2.2
1	U	427	GLY	2.2
1	W	184	GLU	2.2
1	M	257	GLN	2.2
1	S	309	LEU	2.2
2	X	86	HIS	2.2
1	K	313	GLY	2.2
1	S	289	GLY	2.2
2	T	164	GLY	2.2
1	S	200	ARG	2.2
1	Q	189	ASP	2.2
2	X	53	ASP	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	120	CYS	2.2
1	S	451	GLU	2.1
1	U	60	LEU	2.1
1	W	385	GLU	2.1
1	U	275	GLY	2.1
1	S	276	TRP	2.1
2	V	12	PHE	2.1
1	I	196	VAL	2.1
1	S	363	PRO	2.1
1	S	319	MET	2.1
1	K	140	LYS	2.1
1	W	242	GLY	2.1
1	W	299	GLY	2.1
2	X	118	ILE	2.1
1	G	307	GLN	2.1
1	U	41	ALA	2.1
1	W	450	SER	2.1
1	U	192	PRO	2.1
1	M	54	PHE	2.1
2	X	9	PHE	2.1
1	G	53	VAL	2.1
1	S	320	VAL	2.1
1	U	172	VAL	2.1
1	S	105	MET	2.1
1	G	456	THR	2.1
2	H	124	THR	2.1
2	B	27	ILE	2.1
1	S	409	LEU	2.1
1	U	97	LEU	2.1
1	U	357	LEU	2.1
2	V	19	ALA	2.1
1	S	439	ARG	2.1
1	U	110	SER	2.1
2	J	67	ARG	2.1
2	R	10	LYS	2.1
1	U	182	ASP	2.1
1	C	296	TRP	2.1
1	W	441	MET	2.1
1	A	109	ARG	2.1
1	K	417	ARG	2.1
1	W	371	ARG	2.1
2	P	67	ARG	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	W	395	ILE	2.1
2	X	167	ILE	2.1
1	I	253	LEU	2.1
1	U	333	LEU	2.1
1	W	233	HIS	2.1
1	W	426	PRO	2.1
2	X	164	GLY	2.1
1	I	420	THR	2.1
1	K	261	LYS	2.1
1	Q	417	ARG	2.1
1	U	169	LYS	2.1
1	K	54	PHE	2.1
1	K	296	TRP	2.1
1	O	316	VAL	2.1
1	U	154	ASP	2.1
1	Q	102	HIS	2.1
1	U	436	GLU	2.1
1	M	247	ILE	2.1
2	H	118	ILE	2.1
1	W	161	LEU	2.1
1	S	318	ARG	2.0
2	F	67	ARG	2.0
1	U	22	GLU	2.0
1	S	428	ASN	2.0
1	W	219	ASN	2.0
2	X	96	VAL	2.0
1	U	176	TRP	2.0
1	W	158	TRP	2.0
1	S	68	PRO	2.0
2	L	17	LYS	2.0
1	K	421	GLY	2.0
1	U	282	GLY	2.0
1	W	25	ARG	2.0
1	U	24	ILE	2.0
2	N	27	ILE	2.0
1	M	251	MET	2.0
1	W	322	GLN	2.0
2	H	17	LYS	2.0
1	S	168	TYR	2.0
1	Q	318	ARG	2.0
2	X	157	ARG	2.0
1	G	313	GLY	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Q	252	ASP	2.0
1	S	177	ASP	2.0
1	S	59	LEU	2.0
1	U	27	LEU	2.0
1	U	161	LEU	2.0
1	W	198	LEU	2.0
1	Q	261	LYS	2.0
2	L	52	LYS	2.0
1	I	453	SER	2.0
1	E	157	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	BNL	S	462	12/12	0.66	0.63	56,57,58,58	12
5	BNL	E	462	12/12	0.70	0.24	47,50,52,52	0
5	BNL	Q	462	12/12	0.74	0.19	56,58,60,60	0
5	BNL	W	462	12/12	0.79	0.15	80,81,83,83	0
5	BNL	C	462	12/12	0.80	0.17	33,34,35,35	0
3	FES	S	460	4/4	0.85	0.17	82,83,84,86	0
4	FE2	W	461	1/1	0.88	0.07	75,75,75,75	0
5	BNL	M	462	12/12	0.89	0.12	49,50,52,52	0
5	BNL	K	462	12/12	0.90	0.11	42,43,44,44	0
5	BNL	I	462	12/12	0.91	0.11	32,32,33,33	0
5	BNL	O	462	12/12	0.91	0.10	38,38,40,40	0
3	FES	U	460	4/4	0.92	0.12	65,66,67,67	4
4	FE2	Q	461	1/1	0.94	0.05	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FE2	E	461	1/1	0.94	0.06	31,31,31,31	0
4	FE2	U	461	1/1	0.95	0.12	62,62,62,62	0
4	FE2	C	461	1/1	0.96	0.05	25,25,25,25	0
4	FE2	S	461	1/1	0.97	0.06	68,68,68,68	0
3	FES	G	460	4/4	0.97	0.06	33,34,35,35	0
3	FES	W	460	4/4	0.97	0.04	55,56,57,57	0
3	FES	O	460	4/4	0.98	0.05	33,34,34,34	0
3	FES	I	460	4/4	0.98	0.05	28,28,28,28	0
3	FES	A	460	4/4	0.98	0.05	26,26,26,26	0
4	FE2	M	461	1/1	0.99	0.02	29,29,29,29	0
4	FE2	I	461	1/1	0.99	0.04	25,25,25,25	0
3	FES	Q	460	4/4	0.99	0.05	29,30,30,31	0
3	FES	E	460	4/4	0.99	0.08	24,24,24,25	0
4	FE2	O	461	1/1	0.99	0.07	26,26,26,26	0
3	FES	C	460	4/4	0.99	0.07	26,26,26,26	0
3	FES	M	460	4/4	0.99	0.07	24,24,24,24	0
3	FES	K	460	4/4	0.99	0.10	23,24,24,24	0
4	FE2	K	461	1/1	0.99	0.04	30,30,30,30	0
4	FE2	A	461	1/1	1.00	0.08	24,24,24,24	0
4	FE2	G	461	1/1	1.00	0.05	23,23,23,23	0

## 6.5 Other polymers

There are no such residues in this entry.