



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 08:59 pm GMT

PDB ID : 1MMO  
Title : CRYSTAL STRUCTURE OF A BACTERIAL NON-HAEM IRON HYDROXYLASE THAT CATALYSES THE BIOLOGICAL OXIDATION OF METHANE  
Authors : Rosenzweig, A.C.; Frederick, C.A.; Lippard, S.J.; Nordlund, P.  
Deposited on : 1994-02-22  
Resolution : 2.20 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

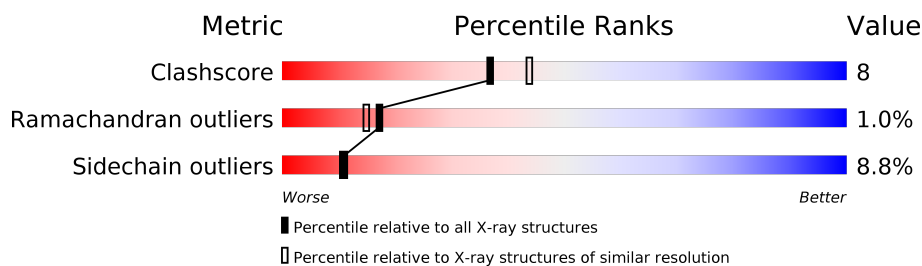
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	122078	5026 (2.20-2.20)
Ramachandran outliers	120005	4951 (2.20-2.20)
Sidechain outliers	119972	4952 (2.20-2.20)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	384	
1	C	384	
2	D	512	
2	E	512	
3	G	162	
3	H	162	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23859 atoms, of which 5642 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 METHANE MONOOXYGENASE HYDROLASE (BETA CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	384	Total	C	H	N	O	S	0	0	0
			3855	2024	705	544	574	8			
1	C	384	Total	C	H	N	O	S	0	0	0
			3855	2024	705	544	574	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	142	THR	ASP	CONFLICT	UNP P18798
B	143	SER	GLU	CONFLICT	UNP P18798
B	144	SER	PHE	CONFLICT	UNP P18798
B	145	CYS	ILE	CONFLICT	UNP P18798
C	142	THR	ASP	CONFLICT	UNP P18798
C	143	SER	GLU	CONFLICT	UNP P18798
C	144	SER	PHE	CONFLICT	UNP P18798
C	145	CYS	ILE	CONFLICT	UNP P18798

- Molecule 2 is a protein called METHANE MONOOXYGENASE HYDROLASE (ALPHA CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	512	Total	C	H	N	O	S	0	0	0
			5122	2680	936	721	767	18			
2	E	512	Total	C	H	N	O	S	0	0	0
			5122	2680	936	721	767	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	306	ASP	ASN	CONFLICT	UNP P22869
D	444	GLU	GLN	CONFLICT	UNP P22869

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Chain	Residue	Modelled	Actual	Comment	Reference
E	306	ASP	ASN	CONFLICT	UNP P22869
E	444	GLU	GLN	CONFLICT	UNP P22869

- Molecule 3 is a protein called METHANE MONOOXYGENASE HYDROLASE (GAMMA CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	162	Total	C	H	N	O	S	0	0	0
			1658	847	321	241	244	5			
3	H	162	Total	C	H	N	O	S	0	0	0
			1658	847	321	241	244	5			

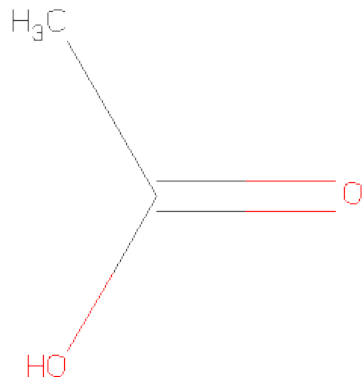
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	38	ASP	HIS	CONFLICT	UNP P11987
G	80	LYS	ASN	CONFLICT	UNP P11987
H	38	ASP	HIS	CONFLICT	UNP P11987
H	80	LYS	ASN	CONFLICT	UNP P11987

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Fe	0	0
			2	2		
4	E	2	Total	Fe	0	0
			2	2		

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

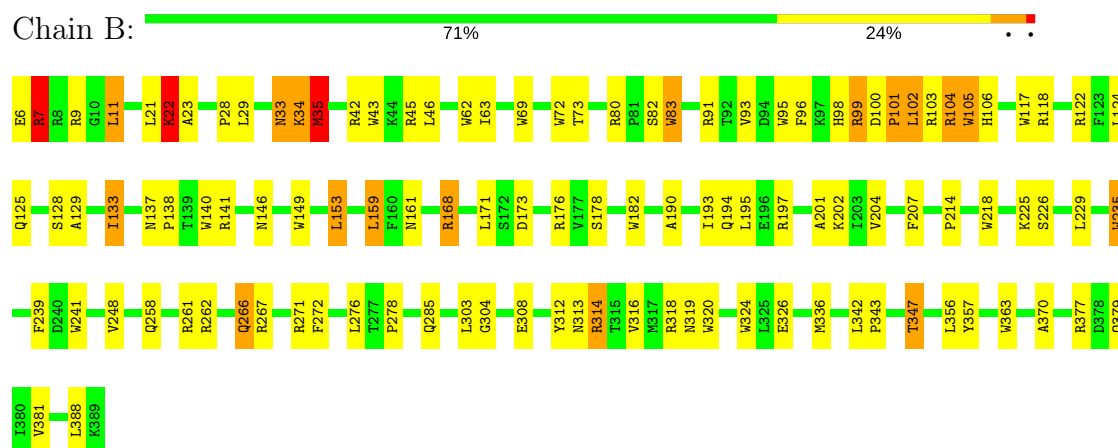
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	164	Total	H	O	0	0
			492	328	164		
6	C	142	Total	H	O	0	0
			426	284	142		
6	D	194	Total	H	O	0	0
			582	388	194		
6	E	199	Total	H	O	0	0
			597	398	199		
6	G	74	Total	H	O	0	0
			222	148	74		
6	H	86	Total	H	O	0	0
			258	172	86		

### 3 Residue-property plots

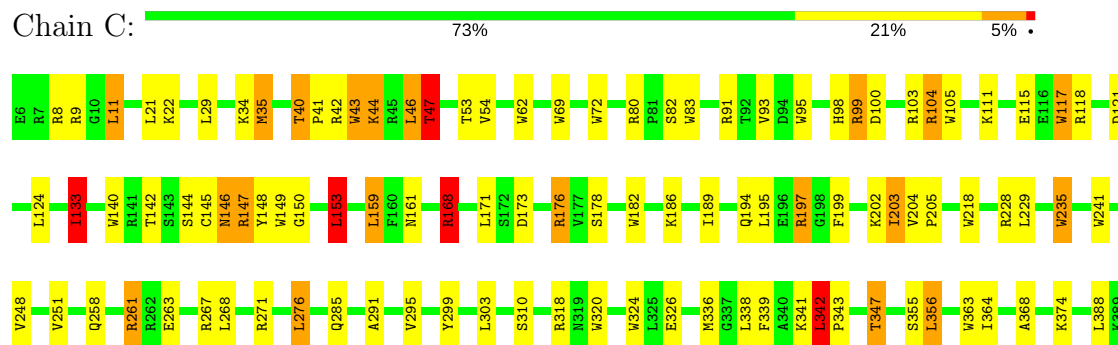
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

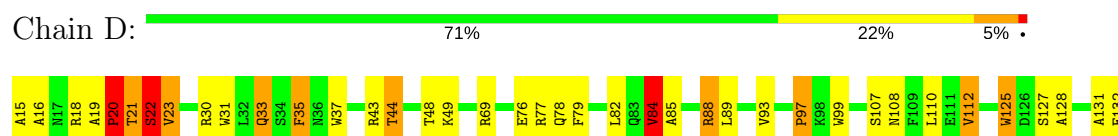
#### • Molecule 1: METHANE MONOOXYGENASE HYDROLASE (BETA CHAIN)

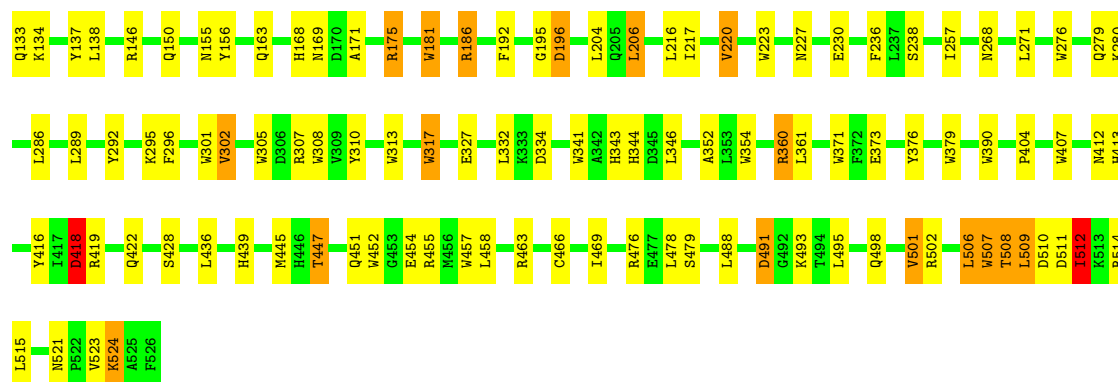


#### • Molecule 1: METHANE MONOOXYGENASE HYDROLASE (BETA CHAIN)



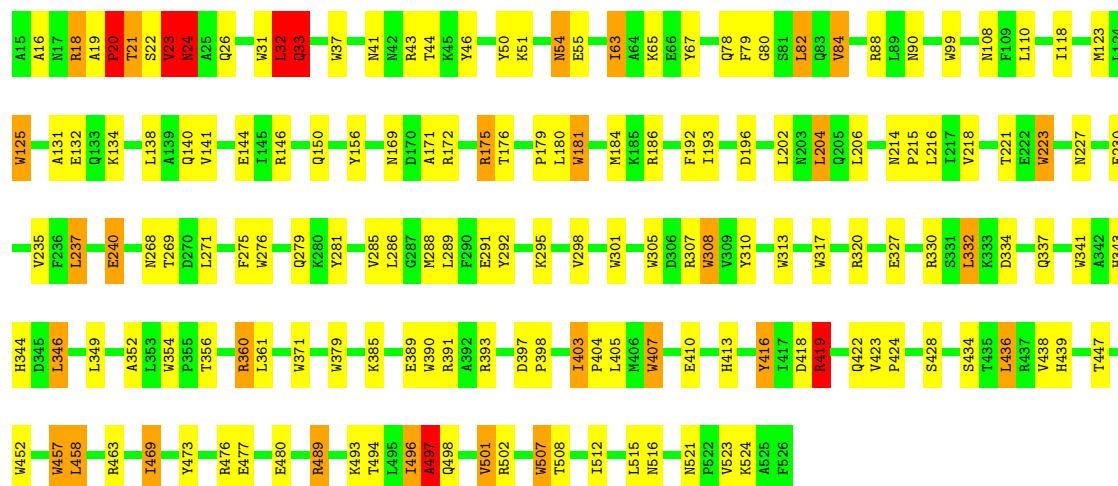
#### • Molecule 2: METHANE MONOOXYGENASE HYDROLASE (ALPHA CHAIN)





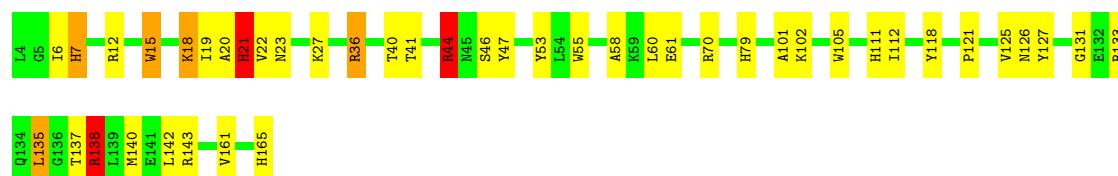
• Molecule 2: METHANE MONOOXYGENASE HYDROLASE (ALPHA CHAIN)

Chain E: 68% 25% 5% •



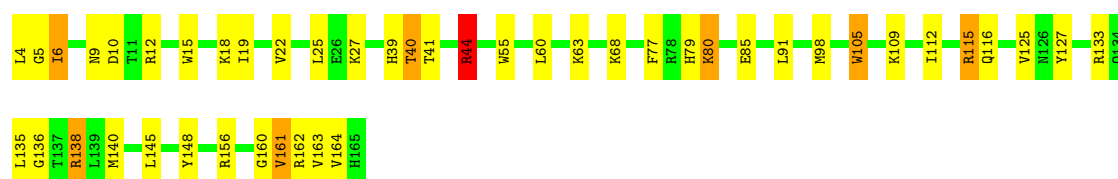
• Molecule 3: METHANE MONOOXYGENASE HYDROLASE (GAMMA CHAIN)

Chain G: 73% 22% • •



• Molecule 3: METHANE MONOOXYGENASE HYDROLASE (GAMMA CHAIN)

Chain H: 72% 23% • •



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.60Å 110.10Å 333.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, FE

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	B	0.83	0/3245	1.68	95/4407 (2.2%)
1	C	0.84	0/3245	1.72	89/4407 (2.0%)
2	D	0.85	0/4311	1.70	129/5855 (2.2%)
2	E	0.85	0/4311	1.67	119/5855 (2.0%)
3	G	0.85	0/1366	1.58	28/1840 (1.5%)
3	H	0.82	0/1366	1.52	22/1840 (1.2%)
All	All	0.84	0/17844	1.67	482/24204 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	2
2	E	0	3
All	All	0	6

There are no bond length outliers.

All (482) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	ARG	NE-CZ-NH2	-23.56	108.52	120.30
1	C	168	ARG	NE-CZ-NH1	21.25	130.92	120.30
1	C	118	ARG	NE-CZ-NH1	15.50	128.05	120.30
2	E	360	ARG	NE-CZ-NH1	14.50	127.55	120.30
2	D	175	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	C	118	ARG	NE-CZ-NH2	-13.64	113.48	120.30
1	C	104	ARG	NE-CZ-NH1	13.43	127.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	360	ARG	NE-CZ-NH2	-13.42	113.59	120.30
1	B	99	ARG	NE-CZ-NH2	-13.31	113.64	120.30
2	D	84	VAL	CG1-CB-CG2	-13.31	89.61	110.90
1	B	80	ARG	NE-CZ-NH2	-13.27	113.67	120.30
1	C	104	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	C	99	ARG	NE-CZ-NH1	12.49	126.55	120.30
2	E	419	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	B	9	ARG	NE-CZ-NH2	-12.01	114.30	120.30
1	B	168	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	B	99	ARG	NE-CZ-NH1	11.52	126.06	120.30
2	D	175	ARG	NE-CZ-NH1	11.43	126.01	120.30
3	G	133	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	B	43	TRP	CD1-CG-CD2	10.34	114.57	106.30
3	H	44	ARG	NE-CZ-NH2	-10.27	115.17	120.30
2	D	146	ARG	NE-CZ-NH2	-10.23	115.18	120.30
1	C	342	LEU	CA-CB-CG	10.17	138.70	115.30
1	B	118	ARG	NE-CZ-NH1	10.13	125.36	120.30
3	H	44	ARG	NE-CZ-NH1	10.10	125.35	120.30
2	D	88	ARG	NE-CZ-NH2	-10.05	115.27	120.30
2	D	476	ARG	NE-CZ-NH2	-9.64	115.48	120.30
2	E	31	TRP	CD1-CG-CD2	9.61	113.99	106.30
2	E	489	ARG	NE-CZ-NH2	-9.61	115.50	120.30
3	G	44	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	B	9	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	C	318	ARG	NE-CZ-NH2	-9.39	115.61	120.30
3	G	15	TRP	CD1-CG-CD2	9.04	113.53	106.30
2	D	507	TRP	CA-C-N	9.04	137.09	117.20
1	C	176	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	B	320	TRP	CD1-CG-CD2	8.96	113.47	106.30
1	B	218	TRP	CD1-CG-CD2	8.95	113.46	106.30
1	C	324	TRP	CD1-CG-CD2	8.90	113.42	106.30
1	B	80	ARG	NE-CZ-NH1	8.86	124.73	120.30
2	D	360	ARG	NE-CZ-NH1	8.85	124.72	120.30
2	E	181	TRP	CD1-CG-CD2	8.83	113.36	106.30
1	C	149	TRP	CD1-CG-CD2	8.76	113.31	106.30
1	C	105	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	B	140	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	B	149	TRP	CD1-CG-CD2	8.63	113.21	106.30
2	D	84	VAL	CA-CB-CG1	8.63	123.84	110.90
2	E	146	ARG	NE-CZ-NH2	-8.62	115.99	120.30
3	G	138	ARG	NE-CZ-NH1	8.62	124.61	120.30
2	D	452	TRP	CD1-CG-CD2	8.58	113.17	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	313	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	C	83	TRP	CD1-CG-CD2	8.53	113.13	106.30
1	B	43	TRP	CE2-CD2-CG	-8.49	100.51	107.30
1	B	95	TRP	CD1-CG-CD2	8.48	113.09	106.30
3	G	55	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	B	324	TRP	CD1-CG-CD2	8.43	113.05	106.30
2	E	276	TRP	CD1-CG-CD2	8.42	113.04	106.30
2	D	341	TRP	CD1-CG-CD2	8.41	113.03	106.30
2	D	407	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	B	140	TRP	CE2-CD2-CG	-8.35	100.62	107.30
2	D	301	TRP	CD1-CG-CD2	8.31	112.94	106.30
1	B	118	ARG	NE-CZ-NH2	-8.29	116.15	120.30
2	D	175	ARG	CA-CB-CG	8.29	131.64	113.40
1	C	43	TRP	CD1-CG-CD2	8.19	112.86	106.30
2	E	305	TRP	CD1-CG-CD2	8.18	112.85	106.30
2	E	37	TRP	CD1-CG-CD2	8.17	112.84	106.30
2	E	507	TRP	CD1-CG-CD2	8.15	112.82	106.30
2	E	419	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	E	31	TRP	CE2-CD2-CG	-8.11	100.81	107.30
3	G	112	ILE	O-C-N	-8.11	109.42	123.20
2	E	181	TRP	CE2-CD2-CG	-8.10	100.82	107.30
2	D	276	TRP	CD1-CG-CD2	8.07	112.76	106.30
2	E	354	TRP	CD1-CG-CD2	8.04	112.74	106.30
2	E	407	TRP	CD1-CG-CD2	8.04	112.73	106.30
2	E	175	ARG	NE-CZ-NH1	8.03	124.32	120.30
2	D	476	ARG	NE-CZ-NH1	8.02	124.31	120.30
2	D	99	TRP	CD1-CG-CD2	8.00	112.70	106.30
2	E	24	ASN	CA-C-N	-7.98	99.64	117.20
1	C	117	TRP	CD1-CG-CD2	7.98	112.68	106.30
1	B	62	TRP	CD1-CG-CD2	7.96	112.67	106.30
2	E	313	TRP	CD1-CG-CD2	7.94	112.66	106.30
1	B	324	TRP	CE2-CD2-CG	-7.93	100.95	107.30
1	B	149	TRP	CE2-CD2-CG	-7.93	100.96	107.30
2	E	37	TRP	CE2-CD2-CG	-7.91	100.97	107.30
3	G	112	ILE	CA-C-N	7.90	131.99	116.20
2	D	79	PHE	CA-C-N	7.89	131.99	116.20
1	C	147	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	B	153	LEU	CA-CB-CG	7.88	133.42	115.30
2	D	31	TRP	CD1-CG-CD2	7.86	112.59	106.30
3	H	105	TRP	CD1-CG-CD2	7.86	112.59	106.30
2	D	301	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	C	218	TRP	CD1-CG-CD2	7.84	112.57	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	379	TRP	CD1-CG-CD2	7.82	112.55	106.30
2	D	99	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	C	176	ARG	NE-CZ-NH1	7.81	124.20	120.30
2	D	305	TRP	CD1-CG-CD2	7.80	112.54	106.30
2	E	99	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	B	117	TRP	CD1-CG-CD2	7.79	112.54	106.30
2	D	308	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	C	140	TRP	CD1-CG-CD2	7.79	112.53	106.30
3	H	138	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	B	101	PRO	CA-C-N	7.79	134.33	117.20
1	C	241	TRP	CD1-CG-CD2	7.78	112.52	106.30
2	E	301	TRP	CD1-CG-CD2	7.78	112.52	106.30
2	E	371	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	B	62	TRP	CE2-CD2-CG	-7.75	101.10	107.30
2	E	313	TRP	CE2-CD2-CG	-7.74	101.11	107.30
1	C	149	TRP	CE2-CD2-CG	-7.74	101.11	107.30
1	C	105	TRP	CE2-CD2-CG	-7.68	101.16	107.30
3	G	44	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	105	TRP	CD1-CG-CD2	7.68	112.44	106.30
3	G	15	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	B	95	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	C	140	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	C	153	LEU	CA-CB-CG	7.64	132.88	115.30
2	E	418	ASP	O-C-N	-7.63	110.50	122.70
3	H	55	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	C	43	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	B	218	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	B	69	TRP	CD1-CG-CD2	7.58	112.37	106.30
1	C	320	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	B	72	TRP	CE2-CD2-CG	-7.58	101.24	107.30
2	D	354	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	B	105	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	B	241	TRP	CD1-CG-CD2	7.56	112.35	106.30
2	E	320	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	D	390	TRP	CD1-CG-CD2	7.55	112.34	106.30
3	G	55	TRP	CE2-CD2-CG	-7.52	101.28	107.30
2	D	125	TRP	CD1-CG-CD2	7.52	112.32	106.30
1	B	104	ARG	NE-CZ-NH1	7.50	124.05	120.30
2	E	457	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	C	62	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	C	69	TRP	CD1-CG-CD2	7.45	112.26	106.30
2	D	79	PHE	O-C-N	-7.44	110.56	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	223	TRP	CD1-CG-CD2	7.43	112.25	106.30
2	D	307	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	E	393	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	D	99	TRP	CG-CD2-CE3	7.42	140.57	133.90
2	E	276	TRP	CE2-CD2-CG	-7.42	101.37	107.30
1	B	377	ARG	NE-CZ-NH1	7.41	124.01	120.30
2	E	99	TRP	CE2-CD2-CG	-7.41	101.37	107.30
2	E	305	TRP	CE2-CD2-CG	-7.41	101.37	107.30
2	D	181	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	B	117	TRP	CE2-CD2-CG	-7.40	101.38	107.30
2	E	407	TRP	CE2-CD2-CG	-7.38	101.40	107.30
3	H	105	TRP	CE2-CD2-CG	-7.37	101.40	107.30
2	E	301	TRP	CE2-CD2-CG	-7.37	101.41	107.30
2	E	452	TRP	CD1-CG-CD2	7.37	112.19	106.30
3	H	15	TRP	CD1-CG-CD2	7.37	112.19	106.30
2	D	317	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	C	324	TRP	CE2-CD2-CG	-7.35	101.42	107.30
2	D	146	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	182	TRP	CD1-CG-CD2	7.34	112.18	106.30
2	D	313	TRP	CE2-CD2-CG	-7.33	101.43	107.30
1	B	363	TRP	CD1-CG-CD2	7.32	112.16	106.30
2	D	341	TRP	CE2-CD2-CG	-7.32	101.44	107.30
2	D	407	TRP	CE2-CD2-CG	-7.30	101.46	107.30
2	E	88	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	B	22	LYS	CA-CB-CG	7.27	129.39	113.40
1	C	363	TRP	CD1-CG-CD2	7.26	112.11	106.30
2	E	341	TRP	CD1-CG-CD2	7.26	112.11	106.30
2	E	371	TRP	CE2-CD2-CG	-7.26	101.49	107.30
2	D	457	TRP	CE2-CD2-CG	-7.23	101.52	107.30
2	E	507	TRP	CE2-CD2-CG	-7.23	101.52	107.30
2	E	452	TRP	CE2-CD2-CG	-7.23	101.52	107.30
2	D	457	TRP	CD1-CG-CD2	7.20	112.06	106.30
1	B	363	TRP	CE2-CD2-CG	-7.19	101.55	107.30
2	D	31	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	C	95	TRP	CD1-CG-CD2	7.17	112.03	106.30
2	D	37	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	B	168	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	C	363	TRP	CE2-CD2-CG	-7.13	101.60	107.30
2	E	317	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	B	235	TRP	CD1-CG-CD2	7.12	112.00	106.30
3	H	80	LYS	CA-CB-CG	7.12	129.06	113.40
2	D	125	TRP	CE2-CD2-CG	-7.11	101.61	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	37	TRP	CG-CD2-CE3	7.10	140.29	133.90
2	E	497	ALA	N-CA-CB	7.09	120.03	110.10
2	D	35	PHE	CB-CG-CD2	-7.08	115.84	120.80
2	D	37	TRP	CD1-CG-CD2	7.08	111.96	106.30
3	H	112	ILE	O-C-N	-7.06	111.20	123.20
1	B	320	TRP	CE2-CD2-CG	-7.04	101.67	107.30
3	H	15	TRP	CE2-CD2-CG	-7.04	101.67	107.30
2	D	452	TRP	CE2-CD2-CG	-7.03	101.67	107.30
3	H	112	ILE	CA-C-N	7.03	130.25	116.20
2	D	23	VAL	N-CA-C	-7.03	92.03	111.00
2	D	223	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	B	83	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	C	83	TRP	CE2-CD2-CG	-7.00	101.70	107.30
3	H	40	THR	N-CA-CB	-6.98	97.04	110.30
1	C	241	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	B	241	TRP	CE2-CD2-CG	-6.96	101.73	107.30
2	D	276	TRP	CE2-CD2-CG	-6.95	101.74	107.30
2	D	418	ASP	O-C-N	-6.95	111.58	122.70
2	E	125	TRP	CA-CB-CG	6.94	126.89	113.70
2	E	308	TRP	CD1-CG-CD2	6.94	111.85	106.30
2	E	354	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	C	95	TRP	CE2-CD2-CG	-6.93	101.75	107.30
1	B	72	TRP	CD1-CG-CD2	6.89	111.81	106.30
2	E	317	TRP	CE2-CD2-CG	-6.88	101.80	107.30
2	D	137	TYR	CB-CG-CD2	-6.88	116.88	121.00
2	D	305	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	B	69	TRP	CE2-CD2-CG	-6.85	101.82	107.30
1	C	69	TRP	CE2-CD2-CG	-6.85	101.82	107.30
2	D	354	TRP	CE2-CD2-CG	-6.83	101.83	107.30
2	E	223	TRP	CE2-CD2-CG	-6.83	101.83	107.30
3	G	55	TRP	CG-CD2-CE3	6.83	140.05	133.90
1	B	318	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	324	TRP	CG-CD2-CE3	6.82	140.03	133.90
2	E	20	PRO	CA-N-CD	-6.81	101.96	111.50
2	E	379	TRP	CD1-CG-CD2	6.81	111.75	106.30
1	C	168	ARG	CG-CD-NE	-6.80	97.52	111.80
2	D	507	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	B	117	TRP	CB-CG-CD1	-6.79	118.18	127.00
1	B	314	ARG	NE-CZ-NH2	-6.77	116.91	120.30
2	E	37	TRP	CG-CD2-CE3	6.76	139.99	133.90
2	D	379	TRP	CE2-CD2-CG	-6.76	101.89	107.30
2	D	21	THR	N-CA-C	-6.75	92.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	80	LYS	CB-CG-CD	-6.75	94.05	111.60
1	B	140	TRP	CG-CD2-CE3	6.75	139.97	133.90
2	E	84	VAL	CA-CB-CG2	-6.74	100.79	110.90
2	E	341	TRP	CE2-CD2-CG	-6.73	101.92	107.30
2	D	371	TRP	CD1-CG-CD2	6.73	111.68	106.30
2	E	390	TRP	CD1-CG-CD2	6.73	111.68	106.30
2	E	457	TRP	CE2-CD2-CG	-6.71	101.93	107.30
2	D	181	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	C	218	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	C	182	TRP	CD1-CG-CD2	6.69	111.65	106.30
2	D	390	TRP	CE2-CD2-CG	-6.67	101.96	107.30
2	D	502	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	C	320	TRP	CE2-CD2-CG	-6.65	101.98	107.30
2	D	308	TRP	CE2-CD2-CG	-6.65	101.98	107.30
2	E	184	MET	CG-SD-CE	6.64	110.82	100.20
1	C	72	TRP	CD1-CG-CD2	6.62	111.60	106.30
2	D	376	TYR	CB-CG-CD1	-6.61	117.03	121.00
2	D	419	ARG	NE-CZ-NH2	-6.61	117.00	120.30
2	E	379	TRP	CE2-CD2-CG	-6.61	102.01	107.30
2	D	317	TRP	CD1-CG-CD2	6.60	111.58	106.30
2	E	390	TRP	CE2-CD2-CG	-6.59	102.02	107.30
2	E	330	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	149	TRP	CG-CD2-CE3	6.58	139.83	133.90
1	B	101	PRO	O-C-N	-6.57	112.19	122.70
1	B	43	TRP	CG-CD1-NE1	-6.57	103.53	110.10
1	B	377	ARG	NE-CZ-NH2	-6.57	117.02	120.30
2	E	223	TRP	CD1-CG-CD2	6.56	111.55	106.30
2	D	507	TRP	CE2-CD2-CG	-6.54	102.07	107.30
2	D	371	TRP	CE2-CD2-CG	-6.53	102.07	107.30
2	D	491	ASP	CA-CB-CG	6.53	127.77	113.40
1	B	320	TRP	CG-CD1-NE1	-6.53	103.57	110.10
1	B	103	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	B	235	TRP	CE2-CD2-CG	-6.49	102.11	107.30
3	G	55	TRP	CB-CG-CD1	-6.47	118.58	127.00
1	B	95	TRP	CG-CD2-CE3	6.47	139.72	133.90
1	B	91	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	C	261	ARG	NE-CZ-NH2	-6.46	117.07	120.30
3	H	6	ILE	O-C-N	-6.45	112.39	122.70
1	C	117	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	C	103	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	D	407	TRP	CB-CG-CD1	-6.41	118.67	127.00
2	D	99	TRP	CB-CG-CD1	-6.40	118.67	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	D	514	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	149	TRP	CB-CG-CD1	-6.38	118.71	127.00
1	B	324	TRP	CB-CG-CD1	-6.37	118.72	127.00
3	G	6	ILE	CA-C-N	6.37	131.21	117.20
2	D	445	MET	CA-CB-CG	-6.37	102.48	113.30
1	B	83	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	C	72	TRP	CE2-CD2-CG	-6.35	102.22	107.30
2	E	37	TRP	CB-CG-CD1	-6.35	118.75	127.00
3	G	105	TRP	CD1-CG-CD2	6.34	111.38	106.30
3	G	105	TRP	CE2-CD2-CG	-6.34	102.23	107.30
2	E	476	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	D	84	VAL	CA-CB-CG2	-6.33	101.41	110.90
2	E	489	ARG	CG-CD-NE	-6.33	98.51	111.80
3	H	161	VAL	CA-CB-CG2	-6.32	101.42	110.90
1	B	122	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	D	507	TRP	N-CA-C	6.32	128.06	111.00
2	D	491	ASP	CB-CG-OD1	6.32	123.98	118.30
2	E	31	TRP	CG-CD1-NE1	-6.32	103.78	110.10
2	D	186	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	62	TRP	CE2-CD2-CG	-6.29	102.27	107.30
1	C	43	TRP	CG-CD2-CE3	6.28	139.55	133.90
1	B	168	ARG	CG-CD-NE	-6.26	98.65	111.80
1	C	235	TRP	CE2-CD2-CG	-6.26	102.29	107.30
1	C	47	THR	N-CA-CB	6.26	122.19	110.30
2	D	360	ARG	NE-CZ-NH2	-6.25	117.18	120.30
3	G	6	ILE	O-C-N	-6.25	112.70	122.70
3	G	133	ARG	CG-CD-NE	-6.25	98.68	111.80
1	B	262	ARG	NE-CZ-NH2	-6.25	117.18	120.30
2	E	146	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	E	463	ARG	NE-CZ-NH1	6.24	123.42	120.30
3	G	15	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	C	103	ARG	NE-CZ-NH1	6.23	123.42	120.30
3	H	55	TRP	CE2-CD2-CG	-6.20	102.34	107.30
1	C	35	MET	CA-C-N	6.19	128.58	116.20
3	H	115	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	C	99	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	324	TRP	CG-CD1-NE1	-6.16	103.94	110.10
2	D	507	TRP	O-C-N	-6.16	112.85	122.70
1	B	314	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	D	373	GLU	CA-CB-CG	6.13	126.89	113.40
2	E	473	TYR	CB-CG-CD2	-6.13	117.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	55	TRP	CG-CD1-NE1	-6.11	103.99	110.10
1	C	43	TRP	CB-CG-CD1	-6.11	119.06	127.00
2	E	307	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	182	TRP	CE2-CD2-CG	-6.10	102.42	107.30
2	D	307	ARG	NE-CZ-NH2	-6.10	117.25	120.30
3	G	118	TYR	CB-CG-CD2	-6.08	117.35	121.00
2	E	125	TRP	CD1-CG-CD2	6.08	111.17	106.30
3	G	53	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	C	168	ARG	CD-NE-CZ	6.08	132.11	123.60
1	C	91	ARG	NE-CZ-NH1	6.07	123.34	120.30
2	D	418	ASP	CA-C-N	6.07	130.56	117.20
2	D	37	TRP	CB-CG-CD1	-6.07	119.11	127.00
2	E	305	TRP	CB-CG-CD1	-6.06	119.12	127.00
2	E	496	ILE	N-CA-C	-6.05	94.67	111.00
2	D	512	ILE	CG1-CB-CG2	-6.04	98.11	111.40
1	C	80	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	D	156	TYR	CB-CG-CD1	-6.04	117.38	121.00
2	D	341	TRP	CG-CD1-NE1	-6.04	104.06	110.10
1	C	140	TRP	CG-CD2-CE3	6.03	139.32	133.90
2	D	21	THR	N-CA-CB	6.03	121.75	110.30
2	D	23	VAL	CA-CB-CG1	-6.03	101.86	110.90
1	C	342	LEU	N-CA-CB	-6.02	98.35	110.40
2	D	301	TRP	CB-CG-CD1	-6.01	119.18	127.00
1	B	105	TRP	CB-CG-CD1	-6.00	119.20	127.00
1	B	35	MET	N-CA-C	-6.00	94.81	111.00
1	C	149	TRP	CG-CD1-NE1	-5.99	104.11	110.10
2	E	502	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	C	168	ARG	CA-CB-CG	5.98	126.56	113.40
1	C	182	TRP	CE2-CD2-CG	-5.98	102.51	107.30
1	C	218	TRP	CB-CG-CD1	-5.98	119.23	127.00
2	E	181	TRP	CG-CD2-CE3	5.98	139.28	133.90
1	B	43	TRP	CB-CG-CD1	-5.97	119.23	127.00
2	D	69	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	E	31	TRP	CB-CG-CD1	-5.96	119.26	127.00
2	D	341	TRP	CB-CG-CD1	-5.95	119.26	127.00
2	E	452	TRP	CG-CD2-CE3	5.93	139.24	133.90
1	C	117	TRP	CG-CD1-NE1	-5.92	104.18	110.10
2	E	23	VAL	CA-CB-CG1	-5.91	102.04	110.90
1	C	235	TRP	CD1-CG-CD2	5.90	111.02	106.30
2	E	33	GLN	N-CA-CB	5.90	121.22	110.60
1	C	218	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	B	218	TRP	CG-CD1-NE1	-5.89	104.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	324	TRP	CG-CD1-NE1	-5.88	104.22	110.10
2	E	79	PHE	CA-C-N	5.88	127.96	116.20
2	E	354	TRP	CG-CD1-NE1	-5.88	104.22	110.10
2	D	305	TRP	CB-CG-CD1	-5.87	119.37	127.00
3	H	162	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	G	133	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	E	84	VAL	CA-CB-CG1	5.84	119.67	110.90
2	E	181	TRP	CG-CD1-NE1	-5.84	104.26	110.10
2	E	181	TRP	CB-CG-CD1	-5.82	119.44	127.00
1	B	117	TRP	CG-CD2-CE3	5.80	139.12	133.90
2	E	16	ALA	N-CA-C	-5.80	95.35	111.00
1	B	140	TRP	CB-CG-CD1	-5.79	119.47	127.00
1	B	43	TRP	CG-CD2-CE3	5.79	139.11	133.90
2	D	463	ARG	NE-CZ-NH1	5.79	123.19	120.30
2	D	313	TRP	CG-CD1-NE1	-5.77	104.33	110.10
2	E	416	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	C	149	TRP	CB-CG-CD1	-5.77	119.50	127.00
2	D	20	PRO	CA-N-CD	-5.76	103.43	111.50
2	E	156	TYR	CB-CG-CD1	-5.76	117.55	121.00
2	E	88	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	D	495	LEU	CA-CB-CG	5.75	128.52	115.30
1	C	342	LEU	CB-CA-C	5.75	121.11	110.20
2	D	407	TRP	CG-CD1-NE1	-5.74	104.36	110.10
2	D	463	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	228	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	105	TRP	CG-CD2-CE3	5.73	139.05	133.90
1	B	105	TRP	O-C-N	-5.72	113.54	122.70
1	B	168	ARG	CA-CB-CG	5.71	125.95	113.40
1	C	168	ARG	CB-CG-CD	5.71	126.43	111.60
2	E	476	ARG	NE-CZ-NH1	5.71	123.15	120.30
2	D	88	ARG	NE-CZ-NH1	5.69	123.15	120.30
2	E	341	TRP	CG-CD2-CE3	5.69	139.02	133.90
3	G	21	HIS	N-CA-CB	5.69	120.84	110.60
2	D	69	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	E	418	ASP	CA-C-N	5.65	129.63	117.20
1	B	149	TRP	CG-CD1-NE1	-5.64	104.46	110.10
3	G	47	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	B	176	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	E	79	PHE	O-C-N	-5.61	113.66	123.20
3	G	143	ARG	NE-CZ-NH2	-5.60	117.50	120.30
3	H	12	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	D	301	TRP	CG-CD2-CE3	5.60	138.94	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	TRP	CB-CG-CD1	-5.59	119.73	127.00
2	E	276	TRP	CG-CD1-NE1	-5.59	104.51	110.10
2	D	491	ASP	N-CA-CB	5.58	120.65	110.60
2	E	84	VAL	CG1-CB-CG2	-5.58	101.97	110.90
2	D	181	TRP	CG-CD1-NE1	-5.58	104.52	110.10
2	D	501	VAL	N-CA-CB	-5.57	99.24	111.50
2	E	391	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	168	ARG	CB-CG-CD	5.54	126.01	111.60
2	E	50	TYR	CB-CG-CD1	-5.54	117.67	121.00
2	E	240	GLU	CA-CB-CG	5.53	125.57	113.40
2	D	308	TRP	CG-CD1-NE1	-5.53	104.57	110.10
2	E	452	TRP	CB-CG-CD1	-5.52	119.82	127.00
1	C	197	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	235	TRP	CG-CD1-NE1	-5.48	104.62	110.10
2	E	37	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	C	105	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	C	83	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	C	133	ILE	CB-CA-C	-5.48	100.65	111.60
2	E	305	TRP	CG-CD2-CE3	5.47	138.82	133.90
2	E	501	VAL	N-CA-CB	-5.46	99.48	111.50
2	D	16	ALA	N-CA-C	-5.46	96.25	111.00
2	E	308	TRP	CE2-CD2-CG	-5.46	102.93	107.30
1	C	43	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	C	91	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	E	175	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	241	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	B	133	ILE	CB-CA-C	-5.42	100.75	111.60
2	E	341	TRP	CB-CG-CD1	-5.42	119.96	127.00
2	D	21	THR	O-C-N	5.41	131.35	122.70
3	G	7	HIS	CA-C-N	5.40	129.08	117.20
2	E	438	VAL	CG1-CB-CG2	-5.40	102.26	110.90
1	B	241	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	C	276	LEU	CA-CB-CG	5.39	127.71	115.30
2	E	305	TRP	CG-CD1-NE1	-5.39	104.71	110.10
2	E	99	TRP	CG-CD1-NE1	-5.38	104.72	110.10
3	G	36	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	62	TRP	CG-CD2-CE3	5.37	138.73	133.90
2	D	21	THR	CB-CA-C	-5.36	97.12	111.60
2	D	76	GLU	CA-CB-CG	5.36	125.19	113.40
1	B	95	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	C	147	ARG	CB-CG-CD	-5.36	97.68	111.60
1	C	149	TRP	CG-CD2-CE3	5.35	138.71	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	82	LEU	CA-CB-CG	5.35	127.59	115.30
2	D	31	TRP	CB-CG-CD1	-5.34	120.05	127.00
2	D	317	TRP	CB-CG-CD1	-5.34	120.05	127.00
2	E	31	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	B	72	TRP	CG-CD2-CE3	5.34	138.71	133.90
2	D	457	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	B	140	TRP	CG-CD1-NE1	-5.33	104.77	110.10
3	H	133	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	E	457	TRP	CB-CG-CD1	-5.32	120.08	127.00
1	C	140	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	B	312	TYR	CB-CG-CD1	-5.29	117.82	121.00
2	E	125	TRP	CE2-CD2-CG	-5.29	103.07	107.30
1	C	117	TRP	CB-CG-CD1	-5.28	120.13	127.00
1	C	69	TRP	CG-CD2-CE3	5.28	138.65	133.90
2	D	317	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	C	140	TRP	CB-CG-CD1	-5.27	120.15	127.00
2	D	220	VAL	CG1-CB-CG2	-5.27	102.47	110.90
2	D	407	TRP	CG-CD2-CE3	5.26	138.64	133.90
2	E	313	TRP	CG-CD2-CE3	5.25	138.63	133.90
2	E	32	LEU	CA-CB-CG	5.25	127.37	115.30
3	G	70	ARG	NE-CZ-NH2	-5.25	117.68	120.30
2	E	18	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	D	192	PHE	CB-CG-CD2	-5.21	117.15	120.80
2	D	341	TRP	CG-CD2-CE3	5.21	138.59	133.90
2	D	305	TRP	CG-CD1-NE1	-5.21	104.89	110.10
2	E	458	LEU	CA-CB-CG	5.20	127.26	115.30
2	D	181	TRP	CB-CG-CD1	-5.19	120.25	127.00
2	D	37	TRP	CG-CD1-NE1	-5.18	104.92	110.10
2	E	341	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	B	62	TRP	CB-CG-CD1	-5.16	120.29	127.00
2	E	308	TRP	CG-CD1-NE1	-5.16	104.94	110.10
3	H	162	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	E	172	ARG	NE-CZ-NH1	5.15	122.88	120.30
3	H	156	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	D	390	TRP	CG-CD1-NE1	-5.14	104.96	110.10
2	D	30	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	379	GLN	CA-CB-CG	-5.13	102.11	113.40
1	C	218	TRP	CG-CD2-CE3	5.13	138.51	133.90
2	E	313	TRP	CG-CD1-NE1	-5.11	104.99	110.10
2	E	371	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	C	356	LEU	CA-CB-CG	5.09	127.02	115.30
2	D	455	ARG	NE-CZ-NH1	5.09	122.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	C	105	TRP	CG-CD2-CE3	5.07	138.46	133.90
2	D	447	THR	N-CA-CB	-5.07	100.67	110.30
1	C	261	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	E	469	ILE	CA-CB-CG1	-5.06	101.39	111.00
2	D	301	TRP	CG-CD1-NE1	-5.06	105.04	110.10
2	D	99	TRP	CG-CD1-NE1	-5.06	105.04	110.10
2	D	31	TRP	CG-CD1-NE1	-5.04	105.06	110.10
2	E	407	TRP	CB-CG-CD1	-5.03	120.46	127.00
2	D	22	SER	CA-C-N	-5.02	106.16	117.20
2	D	502	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	E	301	TRP	CG-CD1-NE1	-5.01	105.09	110.10
2	D	313	TRP	CB-CG-CD1	-5.01	120.49	127.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	299	TYR	Sidechain
2	D	19	ALA	Peptide
2	D	22	SER	Mainchain
2	E	19	ALA	Peptide
2	E	24	ASN	Mainchain
2	E	67	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3150	705	2998	57	0
1	C	3150	705	2998	50	0
2	D	4186	936	3990	74	0
2	E	4186	936	3990	92	0
3	G	1337	321	1323	24	0
3	H	1337	321	1323	28	1
4	D	2	0	0	0	0
4	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	4	0	3	0	0
5	E	4	0	3	0	0
6	B	164	328	0	19	1
6	C	142	284	0	5	0
6	D	194	388	0	10	1
6	E	199	398	0	25	1
6	G	74	148	0	4	0
6	H	86	172	0	15	2
All	All	18217	5642	16628	288	3

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 8.

All (288) 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:D:171:ALA:O	2:D:175:ARG:HB2	1.77	0.84
2:E:44:THR:HB	6:E:640:HOH:O	1.84	0.78
2:E:507:TRP:HB3	6:E:700:HOH:O	1.83	0.77
1:C:267:ARG:HH22	1:C:347:THR:HG21	1.50	0.77
2:D:44:THR:HG23	2:D:127:SER:HA	1.68	0.75
2:E:63:ILE:HG21	6:E:670:HOH:O	1.86	0.75
2:E:403:ILE:HG21	6:E:721:HOH:O	1.87	0.75
2:D:416:TYR:HB3	2:D:447:THR:HG21	1.70	0.73
2:D:78:GLN:HE22	2:D:150:GLN:HE21	1.35	0.72
1:C:9:ARG:HD3	6:E:636:HOH:O	1.89	0.71
2:E:422:GLN:HA	6:E:638:HOH:O	1.89	0.71
2:E:237:LEU:HD13	6:E:693:HOH:O	1.89	0.71
1:B:159:LEU:HD13	6:B:524:HOH:O	1.91	0.71
1:B:370:ALA:HB2	6:B:422:HOH:O	1.89	0.70
1:B:190:ALA:HA	6:B:550:HOH:O	1.90	0.70
2:E:416:TYR:HB3	2:E:447:THR:HG21	1.73	0.70
6:B:474:HOH:O	2:D:35:PHE:HB2	1.92	0.70
2:E:286:LEU:HD13	6:E:696:HOH:O	1.93	0.68
2:E:216:LEU:HB2	6:E:696:HOH:O	1.94	0.68
2:E:403:ILE:HD13	2:E:515:LEU:HD11	1.75	0.66
2:E:44:THR:HG22	2:E:46:TYR:H	1.60	0.66
2:D:89:LEU:HD13	6:E:636:HOH:O	1.93	0.66
2:E:118:ILE:HA	6:E:681:HOH:O	1.96	0.66
1:C:194:GLN:HE22	1:C:197:ARG:HH11	1.41	0.66
2:E:171:ALA:O	2:E:175:ARG:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:227:ASN:HD21	2:E:295:LYS:H	1.43	0.66
2:D:108:ASN:HD21	2:D:175:ARG:HE	1.42	0.66
2:D:352:ALA:HA	2:D:404:PRO:HB2	1.77	0.65
1:B:193:ILE:HB	6:B:550:HOH:O	1.95	0.65
2:D:206:LEU:HD13	2:D:317:TRP:HE1	1.59	0.65
1:B:261:ARG:HE	1:B:285:GLN:HE22	1.45	0.64
1:B:267:ARG:HH22	1:B:347:THR:HG21	1.61	0.64
3:H:105:TRP:O	3:H:109:LYS:HD3	1.96	0.64
2:D:77:ARG:HB3	2:E:84:VAL:HG21	1.80	0.64
2:D:196:ASP:HB2	3:G:140:MET:HE1	1.79	0.64
2:E:202:LEU:HA	2:E:206:LEU:HB2	1.81	0.63
2:E:419:ARG:N	6:E:638:HOH:O	2.32	0.63
2:E:33:GLN:HA	2:E:131:ALA:HB3	1.80	0.62
1:C:124:LEU:HD12	2:E:21:THR:HG22	1.82	0.62
1:C:261:ARG:HE	1:C:285:GLN:HE22	1.48	0.62
2:D:155:ASN:HD22	2:D:168:HIS:HD2	1.48	0.62
1:B:258:GLN:HE21	1:B:261:ARG:HH21	1.47	0.62
3:H:145:LEU:HD22	6:H:244:HOH:O	2.00	0.61
2:D:479:SER:HB2	2:D:509:LEU:HD22	1.80	0.61
2:D:196:ASP:HB2	3:G:140:MET:CE	2.31	0.61
3:H:39:HIS:HD2	6:H:188:HOH:O	1.83	0.61
2:D:78:GLN:NE2	2:D:150:GLN:HE21	1.99	0.61
1:B:194:GLN:HE22	1:B:197:ARG:HH11	1.49	0.60
2:E:24:ASN:HA	6:E:616:HOH:O	2.01	0.60
2:E:352:ALA:HA	2:E:404:PRO:HB2	1.83	0.60
2:E:18:ARG:O	2:E:20:PRO:HD3	2.01	0.59
1:C:117:TRP:HH2	2:E:23:VAL:O	1.84	0.59
1:C:195:LEU:HD11	2:E:23:VAL:HA	1.84	0.59
2:E:457:TRP:HZ3	6:H:248:HOH:O	1.86	0.59
1:C:186:LYS:HD3	6:C:524:HOH:O	2.02	0.59
3:H:68:LYS:HB3	6:H:229:HOH:O	2.01	0.59
1:B:124:LEU:HD12	2:D:21:THR:HG23	1.85	0.58
2:E:269:THR:HG21	6:H:178:HOH:O	2.03	0.58
1:C:124:LEU:HB2	2:E:21:THR:HG23	1.86	0.58
2:E:22:SER:O	2:E:24:ASN:N	2.37	0.57
1:C:339:PHE:HA	1:C:342:LEU:HD13	1.86	0.57
2:E:227:ASN:ND2	2:E:295:LYS:H	2.01	0.57
2:D:506:LEU:HD12	6:D:588:HOH:O	2.03	0.57
3:G:19:ILE:O	3:G:22:VAL:HG22	2.04	0.57
2:E:141:VAL:HA	6:E:681:HOH:O	2.02	0.57
3:H:77:PHE:HE1	6:H:229:HOH:O	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LEU:O	1:C:47:THR:HG23	2.05	0.56
1:C:338:LEU:HD12	1:C:341:LYS:HD2	1.88	0.56
1:C:336:MET:HB3	1:C:388:LEU:HA	1.88	0.56
2:D:268:ASN:HD21	2:D:327:GLU:H	1.53	0.56
2:D:508:THR:N	6:D:666:HOH:O	2.37	0.55
2:E:292:TYR:OH	2:E:344:HIS:HD2	1.88	0.55
1:B:153:LEU:HA	6:B:550:HOH:O	2.07	0.55
1:C:47:THR:N	6:C:467:HOH:O	2.40	0.55
2:E:439:HIS:HB3	3:H:161:VAL:CG2	2.36	0.55
2:E:436:LEU:HD13	6:H:199:HOH:O	2.07	0.55
1:C:144:SER:HA	1:C:148:TYR:HD2	1.71	0.54
2:E:175:ARG:HD3	2:E:181:TRP:CZ2	2.42	0.54
3:H:4:LEU:HB3	6:H:185:HOH:O	2.07	0.54
1:B:159:LEU:HG	1:B:248:VAL:HG13	1.89	0.54
3:H:19:ILE:HA	6:H:221:HOH:O	2.06	0.54
1:B:304:GLY:HA2	6:B:546:HOH:O	2.07	0.54
2:D:21:THR:O	2:D:23:VAL:HG23	2.08	0.53
2:D:422:GLN:HA	6:D:582:HOH:O	2.08	0.53
2:E:360:ARG:HG2	2:E:498:GLN:HB2	1.90	0.53
1:C:53:THR:HG23	6:C:487:HOH:O	2.09	0.53
3:H:136:GLY:N	6:H:226:HOH:O	2.41	0.53
3:H:5:GLY:HA2	3:H:9:ASN:HB3	1.90	0.53
2:D:302:VAL:HB	6:D:699:HOH:O	2.07	0.53
2:D:84:VAL:HG13	2:D:88:ARG:HH21	1.74	0.53
2:E:489:ARG:NE	6:E:664:HOH:O	2.41	0.53
1:B:313:ASN:HB2	6:B:546:HOH:O	2.09	0.53
2:E:175:ARG:HD3	2:E:181:TRP:CE2	2.44	0.52
2:D:360:ARG:HG2	2:D:498:GLN:HB2	1.90	0.52
3:G:41:THR:O	3:G:44:ARG:HD2	2.09	0.52
2:E:21:THR:HG22	2:E:23:VAL:HG13	1.92	0.52
1:C:41:PRO:HB3	1:C:46:LEU:HA	1.92	0.52
2:D:85:ALA:O	2:D:89:LEU:HD23	2.10	0.52
2:E:439:HIS:HD2	3:H:163:VAL:HA	1.75	0.52
1:B:194:GLN:HE22	1:B:197:ARG:NH1	2.06	0.52
1:C:202:LYS:HD2	6:E:628:HOH:O	2.10	0.52
3:G:22:VAL:HG21	6:G:230:HOH:O	2.09	0.51
1:C:199:PHE:HA	6:E:628:HOH:O	2.10	0.51
2:D:227:ASN:HD21	2:D:296:PHE:H	1.57	0.51
2:E:108:ASN:HD21	2:E:175:ARG:HE	1.59	0.51
2:E:33:GLN:HE21	2:E:33:GLN:HA	1.74	0.51
1:B:73:THR:HA	2:D:466:CYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:308:TRP:HZ3	6:E:696:HOH:O	1.93	0.51
3:G:18:LYS:HD3	6:G:215:HOH:O	2.10	0.51
3:G:40:THR:HG21	6:G:174:HOH:O	2.10	0.51
2:E:33:GLN:NE2	2:E:132:GLU:H	2.09	0.51
1:C:11:LEU:HD12	2:E:230:GLU:HG3	1.93	0.51
1:B:314:ARG:HG3	6:B:546:HOH:O	2.11	0.51
1:B:82:SER:HA	6:B:485:HOH:O	2.09	0.51
2:D:479:SER:HB3	2:D:512:ILE:HG22	1.93	0.51
2:E:413:HIS:HD2	2:E:428:SER:OG	1.94	0.51
1:B:201:ALA:HA	1:B:207:PHE:HB3	1.93	0.50
2:D:33:GLN:HE21	2:D:131:ALA:HB3	1.75	0.50
2:E:439:HIS:HB3	3:H:161:VAL:HG21	1.92	0.50
2:E:477:GLU:O	2:E:480:GLU:HG2	2.10	0.50
2:D:292:TYR:OH	2:D:344:HIS:HD2	1.95	0.50
1:B:128:SER:HB2	2:D:20:PRO:HD2	1.93	0.50
1:B:42:ARG:HB2	1:B:99:ARG:HG3	1.93	0.50
2:E:288:MET:SD	2:E:346:LEU:HD13	2.52	0.50
3:G:15:TRP:HA	3:G:18:LYS:HG2	1.92	0.50
3:H:161:VAL:HB	6:H:248:HOH:O	2.11	0.50
2:D:112:VAL:HG21	2:D:181:TRP:HH2	1.76	0.50
2:E:214:ASN:HB3	2:E:215:PRO:HD3	1.94	0.50
1:B:101:PRO:O	1:B:102:LEU:HB2	2.11	0.50
1:C:203:ILE:HG22	1:C:204:VAL:HG23	1.92	0.50
1:C:291:ALA:O	1:C:295:VAL:HG13	2.12	0.49
2:D:175:ARG:HG2	2:D:181:TRP:CD2	2.47	0.49
1:B:106:HIS:N	6:B:424:HOH:O	2.45	0.49
2:D:507:TRP:O	2:D:511:ASP:HB2	2.12	0.49
1:B:266:GLN:HE22	1:B:278:PRO:HA	1.76	0.49
3:G:58:ALA:HB2	6:G:229:HOH:O	2.13	0.49
2:D:77:ARG:HA	2:E:80:GLY:HA2	1.95	0.49
1:C:117:TRP:CH2	2:E:23:VAL:O	2.65	0.49
1:C:42:ARG:HB2	1:C:99:ARG:HG3	1.95	0.48
1:C:258:GLN:HE21	1:C:261:ARG:HH21	1.61	0.48
2:D:48:THR:O	3:G:137:THR:HG23	2.12	0.48
1:C:54:VAL:HG13	6:C:436:HOH:O	2.13	0.48
2:D:89:LEU:HD22	6:E:636:HOH:O	2.13	0.48
2:E:434:SER:HA	6:E:662:HOH:O	2.14	0.48
2:E:269:THR:HG22	3:H:148:TYR:CE2	2.48	0.48
1:C:159:LEU:HG	1:C:248:VAL:HG13	1.95	0.48
2:D:216:LEU:O	2:D:220:VAL:HG23	2.13	0.48
2:E:23:VAL:HG23	2:E:24:ASN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:61:GLU:HG2	3:G:121:PRO:HD3	1.96	0.48
2:D:44:THR:CG2	2:D:127:SER:HA	2.43	0.48
1:B:146:ASN:O	1:B:214:PRO:HG3	2.14	0.48
1:B:98:HIS:HE1	1:B:178:SER:OG	1.97	0.48
1:B:124:LEU:HD11	1:B:195:LEU:HD21	1.96	0.48
1:B:357:TYR:CZ	1:B:381:VAL:HG21	2.49	0.48
1:C:261:ARG:NE	1:C:285:GLN:HE22	2.12	0.48
3:G:101:ALA:HB3	3:G:138:ARG:HH12	1.78	0.48
3:G:138:ARG:HG3	3:G:138:ARG:HH11	1.79	0.48
2:E:78:GLN:HE21	2:E:235:VAL:HA	1.79	0.48
3:H:22:VAL:O	3:H:63:LYS:HE3	2.14	0.48
2:E:78:GLN:HE22	2:E:150:GLN:HE21	1.60	0.47
2:D:196:ASP:N	6:D:640:HOH:O	2.46	0.47
1:C:161:ASN:HB3	1:C:235:TRP:CE2	2.48	0.47
1:C:189:ILE:HB	6:C:524:HOH:O	2.12	0.47
1:B:28:PRO:HA	2:D:163:GLN:O	2.15	0.47
1:B:33:ASN:H	1:B:33:ASN:HD22	1.63	0.47
3:G:44:ARG:HG3	3:G:46:SER:O	2.14	0.47
1:B:124:LEU:HD12	2:D:21:THR:CG2	2.45	0.47
2:E:54:ASN:O	2:E:55:GLU:HB2	2.15	0.47
1:B:225:LYS:HA	6:B:503:HOH:O	2.14	0.47
1:C:100:ASP:OD2	1:C:104:ARG:HD3	2.14	0.47
2:E:21:THR:HB	2:E:23:VAL:HG22	1.97	0.47
1:B:6:GLU:N	6:B:538:HOH:O	2.48	0.46
2:D:521:ASN:HB3	2:D:524:LYS:HD3	1.97	0.46
1:B:11:LEU:HD12	2:D:230:GLU:HG3	1.96	0.46
2:E:108:ASN:ND2	2:E:175:ARG:HH21	2.13	0.46
1:B:6:GLU:O	1:B:7:ARG:HB3	2.15	0.46
1:B:22:LYS:HE2	1:B:23:ALA:N	2.31	0.46
3:G:40:THR:HG22	3:G:41:THR:HG23	1.98	0.46
1:B:100:ASP:OD2	1:B:104:ARG:HD3	2.15	0.46
1:B:239:PHE:HB2	3:G:126:ASN:HA	1.98	0.46
1:C:98:HIS:HE1	1:C:178:SER:OG	1.99	0.46
1:B:129:ALA:O	2:D:15:ALA:N	2.49	0.46
2:E:223:TRP:CE2	2:E:298:VAL:HB	2.51	0.46
3:H:116:GLN:HG3	6:H:203:HOH:O	2.15	0.46
2:E:179:PRO:HD2	6:E:632:HOH:O	2.16	0.46
1:B:161:ASN:HB3	1:B:235:TRP:CE2	2.51	0.46
1:B:336:MET:HB3	1:B:388:LEU:HA	1.97	0.46
2:D:227:ASN:HD21	2:D:295:LYS:H	1.63	0.46
2:D:493:LYS:HD2	2:D:493:LYS:HA	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:ASN:ND2	2:D:175:ARG:HH21	2.13	0.45
2:D:439:HIS:HE1	2:D:454:GLU:OE2	1.99	0.45
2:D:84:VAL:HG13	2:D:88:ARG:NH2	2.31	0.45
1:C:82:SER:HB3	2:E:193:ILE:HD11	1.99	0.45
2:E:51:LYS:HD2	2:E:51:LYS:N	2.31	0.45
1:C:342:LEU:HA	1:C:343:PRO:HD3	1.91	0.45
2:D:413:HIS:HD2	2:D:428:SER:OG	2.00	0.45
3:H:79:HIS:HD2	3:H:127:TYR:OH	1.99	0.45
2:D:493:LYS:HE3	2:D:508:THR:HG23	1.99	0.45
2:D:33:GLN:NE2	2:D:132:GLU:H	2.15	0.45
2:E:140:GLN:O	2:E:144:GLU:HG2	2.17	0.45
2:E:385:LYS:O	2:E:389:GLU:HG2	2.18	0.44
1:C:364:ILE:HA	1:C:368:ALA:HB3	1.99	0.44
1:B:161:ASN:HD21	2:D:134:LYS:HD3	1.82	0.44
2:D:493:LYS:CE	2:D:508:THR:HG23	2.46	0.44
2:E:175:ARG:HG3	2:E:176:THR:N	2.32	0.44
1:B:42:ARG:CB	1:B:99:ARG:HG3	2.47	0.44
1:C:111:LYS:O	1:C:115:GLU:HG3	2.17	0.44
3:H:41:THR:O	3:H:44:ARG:HD2	2.17	0.44
2:D:493:LYS:NZ	2:D:510:ASP:H	2.16	0.44
2:E:275:PHE:CZ	2:E:332:LEU:HD23	2.52	0.44
3:H:40:THR:HG22	3:H:41:THR:HG23	2.00	0.44
1:B:225:LYS:O	1:B:226:SER:HB2	2.17	0.44
3:G:138:ARG:NH1	3:G:142:LEU:HD11	2.33	0.44
1:C:146:ASN:ND2	1:C:197:ARG:HH21	2.15	0.43
1:C:168:ARG:HD3	2:E:123:MET:SD	2.58	0.43
2:E:407:TRP:HA	2:E:410:GLU:HG2	1.99	0.43
2:D:498:GLN:NE2	6:D:588:HOH:O	2.51	0.43
2:E:291:GLU:HB2	6:E:726:HOH:O	2.19	0.43
3:G:79:HIS:HD2	3:G:127:TYR:OH	2.01	0.43
3:H:115:ARG:HB2	6:H:203:HOH:O	2.19	0.43
2:D:33:GLN:HA	2:D:131:ALA:HB3	2.00	0.43
2:D:49:LYS:HD3	3:G:140:MET:HB3	2.00	0.43
2:E:423:VAL:HA	2:E:424:PRO:HD3	1.90	0.43
1:B:96:PHE:O	1:B:99:ARG:NH2	2.52	0.43
1:C:161:ASN:HD21	2:E:134:LYS:HD3	1.83	0.43
2:D:44:THR:HB	6:D:690:HOH:O	2.18	0.43
1:B:202:LYS:HZ2	2:D:22:SER:C	2.22	0.43
1:C:42:ARG:CB	1:C:99:ARG:HG3	2.49	0.43
2:D:257:ILE:HB	6:D:673:HOH:O	2.19	0.43
2:E:32:LEU:O	2:E:33:GLN:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:GLN:HE22	1:C:197:ARG:NH1	2.13	0.42
2:E:496:ILE:O	2:E:497:ALA:HB3	2.19	0.42
3:G:7:HIS:HA	3:G:12:ARG:NH1	2.34	0.42
2:D:108:ASN:HD21	2:D:175:ARG:HH21	1.68	0.42
2:E:494:THR:HA	2:E:508:THR:HA	2.00	0.42
1:C:268:LEU:HD23	1:C:271:ARG:HD2	2.00	0.42
6:B:474:HOH:O	2:D:131:ALA:CB	2.68	0.42
2:E:268:ASN:ND2	2:E:327:GLU:H	2.17	0.42
3:G:131:GLY:O	3:G:135:LEU:HB2	2.20	0.42
1:C:263:GLU:HB3	1:C:355:SER:HB2	2.01	0.42
1:C:204:VAL:HA	1:C:205:PRO:HD2	1.80	0.42
2:E:218:VAL:O	2:E:221:THR:HB	2.20	0.42
2:E:22:SER:HB2	6:E:628:HOH:O	2.20	0.42
2:E:512:ILE:HG12	6:E:700:HOH:O	2.19	0.42
2:D:343:HIS:H	2:D:343:HIS:CD2	2.38	0.42
2:E:268:ASN:HD21	2:E:327:GLU:H	1.67	0.42
3:H:160:GLY:HA2	6:H:235:HOH:O	2.20	0.42
1:C:117:TRP:CE3	2:E:65:LYS:HD3	2.55	0.42
1:C:150:GLY:O	1:C:153:LEU:HB3	2.20	0.42
2:D:108:ASN:HD21	2:D:175:ARG:NE	2.11	0.42
1:B:128:SER:CB	2:D:20:PRO:HD2	2.49	0.42
3:G:36:ARG:O	3:G:40:THR:HB	2.20	0.42
3:H:19:ILE:HG12	3:H:60:LEU:HD13	2.00	0.42
1:B:272:PHE:HZ	6:B:531:HOH:O	2.03	0.42
2:D:217:ILE:HG23	2:D:236:PHE:HB3	2.02	0.42
2:E:21:THR:CG2	2:E:23:VAL:HG13	2.48	0.42
2:E:196:ASP:HB2	3:H:140:MET:SD	2.60	0.41
1:B:125:GLN:HG3	2:D:21:THR:OG1	2.20	0.41
2:D:422:GLN:N	6:D:582:HOH:O	2.46	0.41
1:C:40:THR:HA	1:C:41:PRO:HD3	1.72	0.41
2:E:439:HIS:HB3	3:H:161:VAL:HG22	2.02	0.41
1:B:316:VAL:O	1:B:319:ASN:HB3	2.20	0.41
1:B:267:ARG:HH22	1:B:347:THR:CG2	2.31	0.41
1:C:133:ILE:HG12	1:C:203:ILE:HG23	2.02	0.41
2:D:128:ALA:HB1	2:D:133:GLN:HB3	2.03	0.41
1:C:121:ASP:HA	2:E:21:THR:HG21	2.03	0.41
2:E:281:TYR:CZ	2:E:285:VAL:HG21	2.55	0.41
2:E:397:ASP:HA	2:E:398:PRO:HD2	1.88	0.41
2:E:269:THR:HG22	3:H:148:TYR:HE2	1.86	0.41
2:E:286:LEU:HB3	6:E:580:HOH:O	2.20	0.41
2:E:521:ASN:HB3	2:E:524:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HD2	1:B:204:VAL:HG21	2.02	0.41
1:B:195:LEU:HG	2:D:23:VAL:HG11	2.02	0.41
2:E:343:HIS:CD2	2:E:343:HIS:H	2.39	0.41
3:H:98:MET:O	3:H:138:ARG:NH1	2.54	0.41
1:B:137:ASN:HA	1:B:138:PRO:HD3	1.96	0.40
1:B:314:ARG:N	6:B:546:HOH:O	2.53	0.40
1:B:63:ILE:HD12	6:B:400:HOH:O	2.20	0.40
3:G:20:ALA:O	3:G:21:HIS:CB	2.69	0.40
1:C:43:TRP:O	1:C:44:LYS:HB2	2.21	0.40
3:H:80:LYS:HB2	3:H:85:GLU:O	2.22	0.40
1:B:105:TRP:N	6:B:424:HOH:O	2.54	0.40
6:B:418:HOH:O	2:D:195:GLY:HA2	2.22	0.40
3:G:138:ARG:CG	3:G:138:ARG:HH11	2.35	0.40
3:H:10:ASP:HB2	6:H:190:HOH:O	2.21	0.40
1:B:34:LYS:HB3	1:B:35:MET:H	1.75	0.40
2:D:418:ASP:C	6:D:582:HOH:O	2.59	0.40
2:E:192:PHE:CE1	2:E:204:LEU:HA	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:27:LYS:HZ1	6:H:249:HOH:H1[4_465]	1.28	0.32
6:B:521:HOH:O	6:H:169:HOH:H1[1_545]	1.52	0.08
6:D:672:HOH:O	6:E:673:HOH:H2[3_645]	1.60	0.00

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	382/384 (100%)	359 (94%)	19 (5%)	4 (1%)	<b>17</b> <b>15</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	382/384 (100%)	368 (96%)	10 (3%)	4 (1%)	17	15
2	D	510/512 (100%)	481 (94%)	22 (4%)	7 (1%)	12	9
2	E	510/512 (100%)	482 (94%)	23 (4%)	5 (1%)	17	15
3	G	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	27	28
3	H	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	27	28
All	All	2104/2116 (99%)	2002 (95%)	80 (4%)	22 (1%)	17	15

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	MET
1	C	46	LEU
1	C	47	THR
2	D	22	SER
2	D	196	ASP
2	D	508	THR
2	E	23	VAL
2	E	33	GLN
3	H	6	ILE
1	B	34	LYS
2	D	418	ASP
2	D	491	ASP
1	B	7	ARG
1	B	83	TRP
2	E	41	ASN
3	G	21	HIS
1	C	40	THR
2	D	20	PRO
2	E	497	ALA
1	C	251	VAL
2	E	20	PRO
2	D	97	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	B	318/318 (100%)	293 (92%)	25 (8%)	13	13
1	C	318/318 (100%)	288 (91%)	30 (9%)	9	9
2	D	432/432 (100%)	389 (90%)	43 (10%)	8	7
2	E	432/432 (100%)	392 (91%)	40 (9%)	10	9
3	G	140/140 (100%)	128 (91%)	12 (9%)	11	11
3	H	140/140 (100%)	133 (95%)	7 (5%)	27	33
All	All	1780/1780 (100%)	1623 (91%)	157 (9%)	11	11

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	ARG
1	B	11	LEU
1	B	21	LEU
1	B	22	LYS
1	B	29	LEU
1	B	33	ASN
1	B	45	ARG
1	B	46	LEU
1	B	93	VAL
1	B	102	LEU
1	B	133	ILE
1	B	159	LEU
1	B	168	ARG
1	B	171	LEU
1	B	173	ASP
1	B	229	LEU
1	B	266	GLN
1	B	276	LEU
1	B	303	LEU
1	B	308	GLU
1	B	326	GLU
1	B	342	LEU
1	B	343	PRO
1	B	347	THR
1	B	356	LEU
1	C	8	ARG
1	C	11	LEU
1	C	21	LEU

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Mol	Chain	Res	Type
1	C	22	LYS
1	C	29	LEU
1	C	34	LYS
1	C	35	MET
1	C	44	LYS
1	C	93	VAL
1	C	133	ILE
1	C	142	THR
1	C	145	CYS
1	C	146	ASN
1	C	147	ARG
1	C	153	LEU
1	C	159	LEU
1	C	168	ARG
1	C	171	LEU
1	C	173	ASP
1	C	176	ARG
1	C	203	ILE
1	C	229	LEU
1	C	276	LEU
1	C	303	LEU
1	C	310	SER
1	C	326	GLU
1	C	342	LEU
1	C	347	THR
1	C	356	LEU
1	C	374	LYS
2	D	18	ARG
2	D	33	GLN
2	D	43	ARG
2	D	44	THR
2	D	82	LEU
2	D	84	VAL
2	D	93	VAL
2	D	97	PRO
2	D	107	SER
2	D	110	LEU
2	D	112	VAL
2	D	125	TRP
2	D	138	LEU
2	D	169	ASN
2	D	186	ARG

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Mol	Chain	Res	Type
2	D	204	LEU
2	D	206	LEU
2	D	238	SER
2	D	271	LEU
2	D	279	GLN
2	D	280	LYS
2	D	286	LEU
2	D	289	LEU
2	D	302	VAL
2	D	310	TYR
2	D	332	LEU
2	D	334	ASP
2	D	346	LEU
2	D	361	LEU
2	D	412	ASN
2	D	436	LEU
2	D	451	GLN
2	D	458	LEU
2	D	469	ILE
2	D	478	LEU
2	D	488	LEU
2	D	501	VAL
2	D	506	LEU
2	D	509	LEU
2	D	512	ILE
2	D	515	LEU
2	D	523	VAL
2	D	524	LYS
2	E	21	THR
2	E	24	ASN
2	E	26	GLN
2	E	32	LEU
2	E	33	GLN
2	E	43	ARG
2	E	54	ASN
2	E	63	ILE
2	E	82	LEU
2	E	90	ASN
2	E	110	LEU
2	E	125	TRP
2	E	138	LEU
2	E	169	ASN

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Mol	Chain	Res	Type
2	E	180	LEU
2	E	186	ARG
2	E	204	LEU
2	E	237	LEU
2	E	240	GLU
2	E	271	LEU
2	E	279	GLN
2	E	289	LEU
2	E	310	TYR
2	E	332	LEU
2	E	334	ASP
2	E	337	GLN
2	E	346	LEU
2	E	349	LEU
2	E	356	THR
2	E	361	LEU
2	E	403	ILE
2	E	405	LEU
2	E	419	ARG
2	E	436	LEU
2	E	458	LEU
2	E	469	ILE
2	E	493	LYS
2	E	501	VAL
2	E	516	ASN
2	E	523	VAL
3	G	18	LYS
3	G	23	ASN
3	G	27	LYS
3	G	44	ARG
3	G	60	LEU
3	G	102	LYS
3	G	111	HIS
3	G	125	VAL
3	G	135	LEU
3	G	138	ARG
3	G	161	VAL
3	G	165	HIS
3	H	18	LYS
3	H	25	LEU
3	H	44	ARG
3	H	91	LEU

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Mol	Chain	Res	Type
3	H	125	VAL
3	H	135	LEU
3	H	164	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	ASN
1	B	98	HIS
1	B	155	ASN
1	B	161	ASN
1	B	194	GLN
1	B	258	GLN
1	B	266	GLN
1	B	283	GLN
1	B	285	GLN
1	C	98	HIS
1	C	146	ASN
1	C	155	ASN
1	C	161	ASN
1	C	194	GLN
1	C	220	ASN
1	C	258	GLN
1	C	283	GLN
1	C	285	GLN
2	D	33	GLN
2	D	78	GLN
2	D	90	ASN
2	D	100	ASN
2	D	108	ASN
2	D	116	ASN
2	D	168	HIS
2	D	169	ASN
2	D	227	ASN
2	D	249	ASN
2	D	252	GLN
2	D	268	ASN
2	D	273	ASN
2	D	278	GLN
2	D	279	GLN
2	D	343	HIS
2	D	344	HIS

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Mol	Chain	Res	Type
2	D	413	HIS
2	D	439	HIS
2	E	33	GLN
2	E	78	GLN
2	E	90	ASN
2	E	100	ASN
2	E	108	ASN
2	E	155	ASN
2	E	168	HIS
2	E	169	ASN
2	E	227	ASN
2	E	249	ASN
2	E	268	ASN
2	E	273	ASN
2	E	278	GLN
2	E	344	HIS
2	E	413	HIS
2	E	439	HIS
3	G	7	HIS
3	G	45	ASN
3	G	79	HIS
3	G	144	ASN
3	H	7	HIS
3	H	39	HIS
3	H	45	ASN
3	H	79	HIS
3	H	144	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ACY	D	1	4	1,3,3	2.33	1 (100%)	0,3,3	0.00	-
5	ACY	E	527	4	1,3,3	1.76	0	0,3,3	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
5	ACY	D	1	4	-	0/0/0/0	0/0/0/0
5	ACY	E	527	4	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	ACY	CH3-C	2.33	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.