Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 06:07 PM GMT

PDB ID	:	1FCB
Title	:	MOLECULAR STRUCTURE OF FLAVOCYTOCHROME B2 AT 2.4 ANGSTROMS RESOLUTION
Authors	:	Mathews, F.S.; Xia, Z.-X.
Deposited on	:	1990-01-16
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
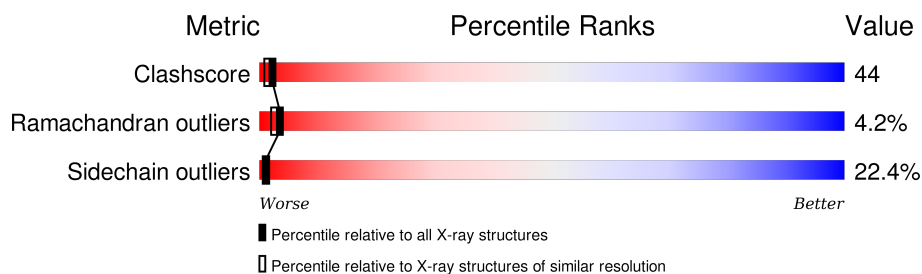with specific help available everywhere you see the (i) symbol.

---

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Clashscore		44
Ramachandran outliers		4.2%
Sidechain outliers		22.4%

Worse   *Better*

∎ Percentile relative to all X-ray structures

⬚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	A	511	35% 33% 19% 10% ·
1	B	511	26% 29% 17% 6% 22%

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	FMN	A	570	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7342 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 FLAVOCYTOCHROME B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total 3841	C 2446	N 652	O 728	S 15	0	0	0
1	B	400	Total 3107	C 1968	N 529	O 599	S 11	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
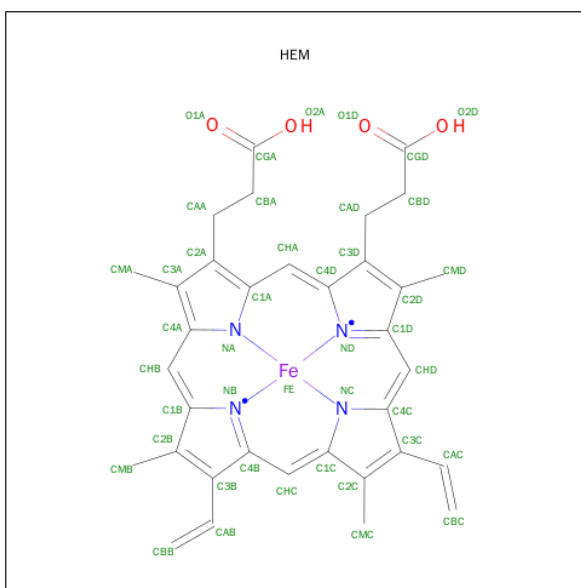
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).
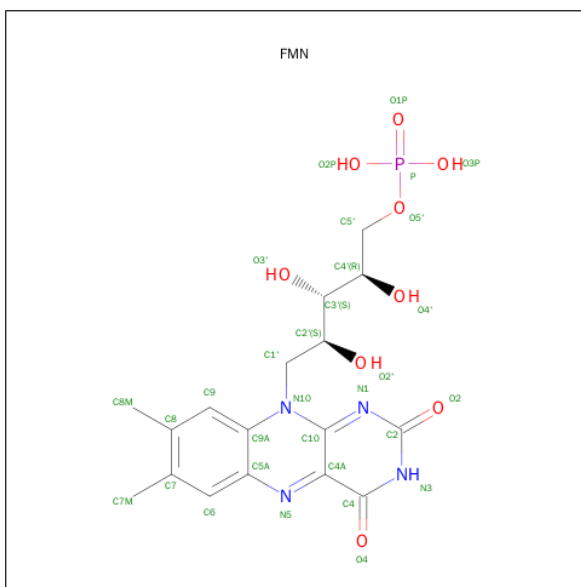
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).
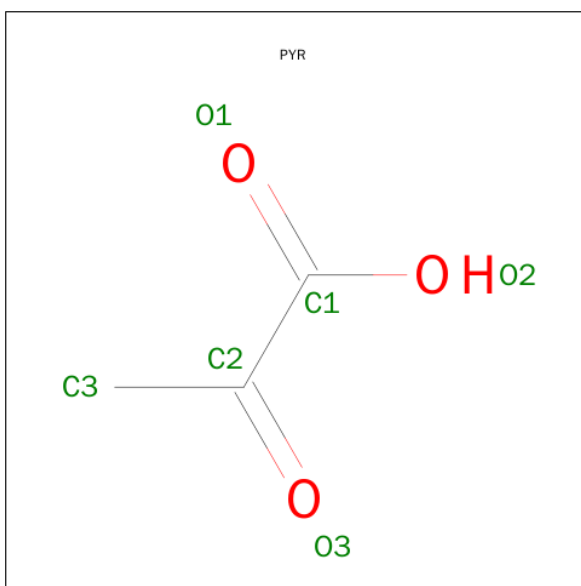
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	182	Total O 182 182	0	0
5	B	101	Total O 101 101	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: FLAVOCYTOCHROME B2

Chain A:

35%   33%   19%   10%

- Molecule 1: FLAVOCYTOCHROME B2

Chain B:

26%   29%   17%   6%   22%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	165.51Å 165.51Å 113.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å²)	35.0	wwPDB-VP

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: FMN, HEM, PYR

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	1.00	2/3916 (0.1%)	2.80	286/5303 (5.4%)
1	B	0.97	0/3156	2.83	233/4263 (5.5%)
All	All	0.99	2/7072 (0.0%)	2.81	519/9566 (5.4%)

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	A	0	4
1	B	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLU	CD-OE1	-5.64	1.19	1.25
1	A	232	SER	CB-OG	-5.27	1.35	1.42

All (519) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	353	ARG	NE-CZ-NH1	41.59	141.09	120.30
1	B	259	ARG	NE-CZ-NH2	32.94	136.77	120.30
1	A	155	ARG	NE-CZ-NH2	32.52	136.56	120.30
1	A	376	ARG	NE-CZ-NH1	30.93	135.76	120.30
1	A	353	ARG	NE-CZ-NH2	-26.04	107.28	120.30
1	B	382	ARG	CD-NE-CZ	25.74	159.64	123.60
1	A	414	ARG	NE-CZ-NH1	-22.71	108.95	120.30

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	163	ARG	NE-CZ-NH2	-22.31	109.15	120.30
1	A	108	ARG	CD-NE-CZ	21.72	154.01	123.60
1	A	289	ARG	CD-NE-CZ	20.73	152.63	123.60
1	A	163	ARG	NE-CZ-NH2	-19.79	110.41	120.30
1	B	486	ARG	NE-CZ-NH1	19.52	130.06	120.30
1	B	155	ARG	CD-NE-CZ	19.38	150.73	123.60
1	B	155	ARG	NE-CZ-NH2	-19.16	110.72	120.30
1	B	251	TYR	CB-CG-CD1	18.47	132.08	121.00
1	B	175	ARG	NE-CZ-NH1	-17.69	111.46	120.30
1	A	398	ARG	NE-CZ-NH1	17.39	129.00	120.30
1	A	444	ARG	NE-CZ-NH1	-17.35	111.62	120.30
1	B	455	ARG	NE-CZ-NH2	17.33	128.96	120.30
1	B	155	ARG	NE-CZ-NH1	17.18	128.89	120.30
1	B	259	ARG	NE-CZ-NH1	-17.16	111.72	120.30
1	B	353	ARG	NE-CZ-NH2	-16.92	111.84	120.30
1	B	182	ASP	CB-CG-OD1	16.80	133.42	118.30
1	A	214	ARG	NE-CZ-NH2	-16.48	112.06	120.30
1	B	175	ARG	NE-CZ-NH2	16.20	128.40	120.30
1	A	120	ASP	CB-CG-OD2	-15.59	104.27	118.30
1	B	173	ASP	CB-CG-OD1	15.55	132.30	118.30
1	B	353	ARG	CD-NE-CZ	15.41	145.17	123.60
1	B	413	ARG	CD-NE-CZ	14.79	144.31	123.60
1	A	240	GLU	CA-CB-CG	14.51	145.32	113.40
1	B	476	ASP	CB-CG-OD1	-14.32	105.41	118.30
1	B	353	ARG	NE-CZ-NH1	14.27	127.43	120.30
1	A	465	LEU	CA-CB-CG	14.23	148.02	115.30
1	B	414	ARG	NE-CZ-NH2	14.13	127.37	120.30
1	A	479	ASP	CB-CG-OD2	-14.12	105.59	118.30
1	A	163	ARG	CD-NE-CZ	14.00	143.20	123.60
1	B	292	ASP	CB-CG-OD1	-13.96	105.73	118.30
1	A	259	ARG	NE-CZ-NH1	13.78	127.19	120.30
1	B	292	ASP	CB-CG-OD2	13.73	130.66	118.30
1	B	282	ASP	CB-CG-OD1	12.84	129.85	118.30
1	A	24	ASP	CB-CG-OD1	-12.79	106.79	118.30
1	B	391	THR	CA-CB-CG2	12.77	130.28	112.40
1	B	251	TYR	CB-CG-CD2	-12.73	113.36	121.00
1	A	353	ARG	CB-CG-CD	12.62	144.40	111.60
1	B	353	ARG	CB-CG-CD	12.53	144.18	111.60
1	A	452	GLU	CA-CB-CG	12.43	140.75	113.40
1	A	165	PHE	CB-CG-CD2	12.37	129.46	120.80
1	A	214	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	B	173	ASP	CB-CG-OD2	-12.28	107.25	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ARG	CA-CB-CG	12.14	140.11	113.40
1	A	173	ASP	CB-CG-OD1	11.80	128.92	118.30
1	B	414	ARG	NE-CZ-NH1	-11.72	114.44	120.30
1	B	353	ARG	CA-CB-CG	11.68	139.10	113.40
1	A	382	ARG	CD-NE-CZ	11.39	139.55	123.60
1	A	479	ASP	CB-CG-OD1	11.39	128.55	118.30
1	A	292	ASP	CB-CG-OD1	-11.37	108.07	118.30
1	A	486	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	B	390	GLU	OE1-CD-OE2	-11.23	109.83	123.30
1	B	463	ARG	CD-NE-CZ	-11.12	108.04	123.60
1	A	155	ARG	NH1-CZ-NH2	-11.01	107.29	119.40
1	A	173	ASP	CB-CG-OD2	-10.99	108.41	118.30
1	B	409	ASP	CB-CG-OD2	10.98	128.19	118.30
1	B	182	ASP	CB-CG-OD2	-10.80	108.58	118.30
1	A	376	ARG	NH1-CZ-NH2	-10.78	107.54	119.40
1	A	408	VAL	CA-CB-CG2	10.73	126.99	110.90
1	B	124	ASN	CB-CA-C	-10.54	89.33	110.40
1	A	368	VAL	CA-CB-CG2	10.50	126.65	110.90
1	A	130	TYR	CB-CG-CD1	10.47	127.28	121.00
1	A	130	TYR	CB-CG-CD2	-10.42	114.75	121.00
1	A	365	VAL	CG1-CB-CG2	10.36	127.48	110.90
1	A	433	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	B	263	ASP	CB-CG-OD2	-10.30	109.03	118.30
1	A	472	GLU	CG-CD-OE2	-10.24	97.81	118.30
1	B	127	ASP	CB-CG-OD1	10.08	127.38	118.30
1	B	390	GLU	CA-CB-CG	10.07	135.56	113.40
1	B	188	VAL	O-C-N	10.00	138.70	122.70
1	A	327	ASP	CB-CG-OD2	9.94	127.25	118.30
1	A	398	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	A	175	ARG	CD-NE-CZ	9.88	137.43	123.60
1	A	38	ARG	NE-CZ-NH1	-9.84	115.38	120.30
1	A	259	ARG	NH1-CZ-NH2	-9.83	108.59	119.40
1	A	245	ASP	CB-CG-OD1	9.82	127.14	118.30
1	B	452	GLU	CA-CB-CG	9.77	134.89	113.40
1	A	289	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	A	152	VAL	CA-CB-CG1	9.71	125.47	110.90
1	A	48	ASP	CB-CG-OD1	9.68	127.01	118.30
1	B	405	GLU	CG-CD-OE1	9.66	137.62	118.30
1	B	259	ARG	CD-NE-CZ	-9.66	110.08	123.60
1	A	38	ARG	CD-NE-CZ	-9.59	110.17	123.60
1	A	190	VAL	CA-CB-CG1	9.57	125.25	110.90
1	B	151	GLU	CG-CD-OE1	9.49	137.28	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	472	GLU	OE1-CD-OE2	9.47	134.67	123.30
1	B	115	LEU	CB-CA-C	9.44	128.13	110.20
1	B	120	ASP	CB-CG-OD2	-9.43	109.81	118.30
1	A	379	ASP	CB-CG-OD1	9.36	126.73	118.30
1	B	429	VAL	CA-CB-CG1	9.35	124.92	110.90
1	A	155	ARG	NE-CZ-NH1	-9.17	115.71	120.30
1	A	244	SER	N-CA-CB	9.13	124.19	110.50
1	A	486	ARG	CD-NE-CZ	9.12	136.37	123.60
1	A	437	TYR	CB-CG-CD2	-9.06	115.56	121.00
1	A	376	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	B	413	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	B	112	LEU	CA-CB-CG	9.00	136.01	115.30
1	A	237	GLU	CB-CA-C	-8.99	92.42	110.40
1	A	109	LYS	CB-CA-C	8.97	128.34	110.40
1	A	353	ARG	NH1-CZ-NH2	-8.95	109.56	119.40
1	A	405	GLU	CG-CD-OE1	8.94	136.18	118.30
1	A	414	ARG	NH1-CZ-NH2	8.93	129.22	119.40
1	A	353	ARG	CA-CB-CG	8.88	132.93	113.40
1	A	465	LEU	C-N-CA	8.83	140.85	122.30
1	B	444	ARG	NE-CZ-NH1	-8.79	115.90	120.30
1	A	57	ASP	CB-CG-OD2	-8.77	110.40	118.30
1	B	376	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	278	PHE	CB-CG-CD2	8.67	126.87	120.80
1	B	493	ASP	CB-CG-OD2	-8.62	110.54	118.30
1	A	456	ASP	CB-CG-OD1	8.60	126.04	118.30
1	B	108	ARG	CD-NE-CZ	8.57	135.60	123.60
1	B	397	GLN	CB-CA-C	-8.51	93.37	110.40
1	B	320	ARG	CD-NE-CZ	-8.49	111.71	123.60
1	A	444	ARG	CG-CD-NE	-8.48	94.00	111.80
1	B	414	ARG	CD-NE-CZ	-8.46	111.76	123.60
1	A	232	SER	N-CA-CB	-8.41	97.89	110.50
1	A	240	GLU	OE1-CD-OE2	-8.39	113.23	123.30
1	B	163	ARG	NH1-CZ-NH2	8.32	128.56	119.40
1	A	38	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	A	492	ASN	CB-CA-C	8.24	126.88	110.40
1	A	137	THR	N-CA-CB	-8.21	94.70	110.30
1	A	402	ASP	CB-CG-OD1	8.19	125.67	118.30
1	B	330	LEU	CA-CB-CG	8.17	134.10	115.30
1	B	184	LEU	N-CA-CB	-8.14	94.12	110.40
1	A	386	GLU	N-CA-CB	8.12	125.22	110.60
1	B	152	VAL	CA-CB-CG1	8.11	123.07	110.90
1	B	463	ARG	N-CA-CB	-8.07	96.07	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	VAL	CB-CA-C	8.05	126.69	111.40
1	A	222	LYS	N-CA-CB	8.05	125.09	110.60
1	B	166	PHE	O-C-N	8.00	135.50	122.70
1	B	386	GLU	O-C-N	-7.99	109.92	122.70
1	B	104	GLU	CB-CA-C	-7.97	94.46	110.40
1	A	178	ASP	CB-CG-OD1	7.97	125.47	118.30
1	A	496	TYR	N-CA-CB	-7.94	96.31	110.60
1	A	72	ASP	CB-CG-OD2	-7.88	111.20	118.30
1	B	231	ALA	N-CA-CB	-7.88	99.08	110.10
1	B	386	GLU	CG-CD-OE1	7.87	134.04	118.30
1	A	464	LEU	O-C-N	-7.85	110.14	122.70
1	B	197	THR	N-CA-CB	-7.79	95.49	110.30
1	B	378	LEU	CB-CG-CD2	7.79	124.24	111.00
1	B	402	ASP	CB-CG-OD1	7.75	125.27	118.30
1	B	211	ASP	CB-CG-OD2	7.75	125.27	118.30
1	A	499	VAL	CA-CB-CG2	7.74	122.51	110.90
1	A	232	SER	CB-CA-C	-7.67	95.53	110.10
1	A	129	GLU	OE1-CD-OE2	-7.66	114.11	123.30
1	B	488	VAL	CA-C-N	7.66	131.52	116.20
1	B	266	VAL	CA-CB-CG2	-7.63	99.45	110.90
1	A	411	GLY	C-N-CA	7.62	140.76	121.70
1	B	121	ASN	O-C-N	7.60	134.86	122.70
1	B	390	GLU	CG-CD-OE1	7.60	133.50	118.30
1	B	282	ASP	OD1-CG-OD2	-7.59	108.88	123.30
1	B	488	VAL	CA-C-O	-7.57	104.21	120.10
1	A	197	THR	OG1-CB-CG2	7.52	127.30	110.00
1	B	226	MET	CG-SD-CE	-7.51	88.18	100.20
1	A	207	GLU	CG-CD-OE1	7.50	133.31	118.30
1	A	409	ASP	C-N-CA	7.48	138.00	122.30
1	B	476	ASP	O-C-N	7.46	134.64	122.70
1	B	355	GLU	CG-CD-OE1	7.42	133.14	118.30
1	A	329	SER	CA-C-O	-7.41	104.53	120.10
1	A	495	LEU	CB-CA-C	7.40	124.27	110.20
1	B	413	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	B	209	GLU	CG-CD-OE1	7.40	133.09	118.30
1	B	462	MET	CA-CB-CG	-7.39	100.73	113.30
1	B	166	PHE	CB-CG-CD1	-7.39	115.63	120.80
1	B	433	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	179	ILE	O-C-N	-7.38	110.89	122.70
1	A	429	VAL	CA-CB-CG1	7.37	121.96	110.90
1	A	58	VAL	CA-CB-CG2	7.35	121.93	110.90
1	A	58	VAL	N-CA-CB	-7.35	95.33	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	MET	N-CA-CB	7.33	123.80	110.60
1	B	456	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	368	VAL	CA-CB-CG1	7.30	121.85	110.90
1	A	209	GLU	OE1-CD-OE2	-7.29	114.56	123.30
1	A	504	THR	CA-CB-CG2	7.27	122.57	112.40
1	B	250	TRP	CA-CB-CG	7.26	127.50	113.70
1	A	202	LEU	CA-CB-CG	7.24	131.94	115.30
1	A	115	LEU	CB-CA-C	7.23	123.94	110.20
1	B	150	ASP	CB-CG-OD2	7.20	124.78	118.30
1	B	259	ARG	NH1-CZ-NH2	-7.18	111.50	119.40
1	A	230	LEU	CA-CB-CG	7.17	131.80	115.30
1	A	384	PRO	O-C-N	-7.17	111.22	122.70
1	A	380	PHE	CB-CG-CD2	7.17	125.82	120.80
1	B	175	ARG	CD-NE-CZ	-7.16	113.57	123.60
1	B	214	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	442	TYR	CB-CG-CD1	7.15	125.29	121.00
1	A	486	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	259	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	B	410	GLY	C-N-CA	7.14	137.29	122.30
1	B	486	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	268	ASN	CB-CG-OD1	7.07	135.74	121.60
1	B	463	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	404	LEU	CA-CB-CG	7.05	131.51	115.30
1	A	8	LYS	N-CA-CB	-7.04	97.93	110.60
1	A	380	PHE	CB-CA-C	7.02	124.44	110.40
1	A	462	MET	CA-CB-CG	-7.01	101.39	113.30
1	A	104	GLU	CB-CG-CD	-7.00	95.30	114.20
1	B	496	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	A	413	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	497	ASN	CA-CB-CG	6.98	128.75	113.40
1	A	297	PHE	CA-CB-CG	6.95	130.58	113.90
1	B	399	ASN	O-C-N	6.95	133.82	122.70
1	B	226	MET	O-C-N	6.92	133.77	122.70
1	B	465	LEU	CA-CB-CG	6.92	131.21	115.30
1	A	487	THR	N-CA-CB	-6.89	97.21	110.30
1	A	405	GLU	CG-CD-OE2	-6.88	104.55	118.30
1	A	176	LYS	CA-CB-CG	6.87	128.51	113.40
1	A	359	LYS	CD-CE-NZ	-6.84	95.97	111.70
1	B	144	TYR	CB-CG-CD1	6.83	125.10	121.00
1	B	331	THR	N-CA-CB	-6.83	97.32	110.30
1	B	355	GLU	OE1-CD-OE2	-6.83	115.10	123.30
1	B	444	ARG	NE-CZ-NH2	6.83	123.72	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LEU	CB-CA-C	6.83	123.17	110.20
1	A	436	LEU	CB-CG-CD2	-6.81	99.42	111.00
1	B	256	ASN	O-C-N	6.81	133.59	122.70
1	B	427	LYS	CD-CE-NZ	-6.79	96.08	111.70
1	B	161	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	A	120	ASP	CB-CG-OD1	6.78	124.40	118.30
1	B	186	SER	CA-CB-OG	6.78	129.51	111.20
1	B	442	TYR	CB-CG-CD1	6.78	125.07	121.00
1	A	8	LYS	N-CA-C	6.78	129.29	111.00
1	B	348	ILE	CA-CB-CG2	6.77	124.44	110.90
1	B	233	CYS	O-C-N	6.74	133.48	122.70
1	B	408	VAL	CA-CB-CG1	6.74	121.00	110.90
1	A	339	LYS	CA-CB-CG	6.73	128.20	113.40
1	B	163	ARG	CG-CD-NE	-6.72	97.69	111.80
1	B	237	GLU	CG-CD-OE1	6.71	131.72	118.30
1	A	151	GLU	CG-CD-OE2	6.70	131.69	118.30
1	A	444	ARG	CD-NE-CZ	-6.70	114.22	123.60
1	A	243	PRO	CA-C-N	6.68	131.90	117.20
1	A	26	TRP	N-CA-CB	6.66	122.59	110.60
1	B	197	THR	OG1-CB-CG2	6.66	125.32	110.00
1	A	297	PHE	N-CA-CB	6.66	122.58	110.60
1	A	182	ASP	CB-CG-OD1	6.65	124.28	118.30
1	B	191	PRO	C-N-CA	6.62	138.25	121.70
1	A	237	GLU	CG-CD-OE1	6.60	131.50	118.30
1	B	278	PHE	CB-CG-CD1	-6.60	116.18	120.80
1	B	253	LEU	N-CA-C	6.59	128.79	111.00
1	B	294	LYS	CB-CA-C	6.59	123.58	110.40
1	A	318	ALA	CB-CA-C	6.56	119.94	110.10
1	B	139	GLN	OE1-CD-NE2	6.56	136.99	121.90
1	A	297	PHE	O-C-N	6.52	133.13	122.70
1	B	272	LEU	O-C-N	6.52	134.28	123.20
1	A	368	VAL	N-CA-CB	-6.51	97.18	111.50
1	A	161	TYR	CG-CD1-CE1	-6.51	116.09	121.30
1	A	363	ILE	CA-CB-CG2	6.51	123.91	110.90
1	A	197	THR	CA-CB-CG2	6.50	121.50	112.40
1	A	212	VAL	CA-CB-CG2	6.50	120.65	110.90
1	B	396	GLU	CG-CD-OE1	6.50	131.30	118.30
1	B	249	GLN	N-CA-CB	6.50	122.29	110.60
1	A	251	TYR	CB-CG-CD1	6.49	124.90	121.00
1	A	277	LEU	O-C-N	6.49	133.08	122.70
1	B	189	ASP	CB-CG-OD2	6.48	124.13	118.30
1	A	89	PRO	N-CA-C	-6.46	95.29	112.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	437	TYR	CG-CD1-CE1	-6.46	116.13	121.30
1	B	455	ARG	NE-CZ-NH1	-6.43	117.09	120.30
1	A	210	LYS	CB-CG-CD	-6.42	94.90	111.60
1	A	361	ALA	O-C-N	-6.42	112.44	122.70
1	B	355	GLU	CA-CB-CG	6.41	127.50	113.40
1	A	493	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	A	24	ASP	OD1-CG-OD2	6.38	135.42	123.30
1	A	327	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	B	405	GLU	CG-CD-OE2	-6.34	105.61	118.30
1	A	320	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	386	GLU	CG-CD-OE2	-6.33	105.64	118.30
1	B	486	ARG	CA-CB-CG	6.32	127.30	113.40
1	A	170	ILE	CA-CB-CG2	6.32	123.53	110.90
1	A	379	ASP	CA-CB-CG	-6.31	99.51	113.40
1	A	205	PRO	O-C-N	-6.31	112.60	122.70
1	A	248	ILE	CA-CB-CG2	6.29	123.48	110.90
1	A	192	PHE	CG-CD2-CE2	6.28	127.71	120.80
1	A	163	ARG	NH1-CZ-NH2	6.27	126.30	119.40
1	A	106	ILE	CB-CA-C	6.27	124.13	111.60
1	B	237	GLU	CA-CB-CG	6.22	127.09	113.40
1	A	45	GLY	CA-C-O	-6.22	109.41	120.60
1	A	104	GLU	CG-CD-OE2	-6.21	105.88	118.30
1	A	266	VAL	CA-CB-CG1	6.19	120.19	110.90
1	B	130	TYR	CB-CG-CD1	6.19	124.72	121.00
1	B	193	TYR	CB-CG-CD2	6.19	124.72	121.00
1	A	243	PRO	CA-C-O	-6.19	105.35	120.20
1	B	253	LEU	N-CA-CB	-6.18	98.04	110.40
1	B	508	PHE	N-CA-CB	6.18	121.72	110.60
1	A	131	LEU	CB-CG-CD1	6.17	121.49	111.00
1	B	260	LYS	N-CA-CB	6.16	121.69	110.60
1	A	365	VAL	CA-CB-CG1	6.16	120.14	110.90
1	A	236	GLU	CA-CB-CG	6.16	126.94	113.40
1	A	431	LEU	CA-CB-CG	6.15	129.45	115.30
1	B	200	CYS	CA-C-O	-6.15	107.18	120.10
1	B	476	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	454	LEU	CB-CA-C	6.15	121.88	110.20
1	A	495	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	A	108	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	B	136	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	402	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	214	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	B	437	TYR	CB-CG-CD2	6.12	124.67	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	158	HIS	CA-CB-CG	-6.11	103.21	113.60
1	A	190	VAL	N-CA-CB	-6.10	98.08	111.50
1	B	237	GLU	CG-CD-OE2	-6.09	106.11	118.30
1	A	268	ASN	OD1-CG-ND2	-6.08	107.91	121.90
1	B	336	GLU	OE1-CD-OE2	6.07	130.59	123.30
1	A	40	LEU	CB-CG-CD2	-6.07	100.68	111.00
1	B	143	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	A	407	PHE	CB-CG-CD1	-6.06	116.56	120.80
1	A	400	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	378	LEU	CB-CG-CD1	6.05	121.29	111.00
1	A	124	ASN	CB-CA-C	6.05	122.50	110.40
1	A	142	ALA	CB-CA-C	-6.05	101.02	110.10
1	A	236	GLU	N-CA-CB	6.04	121.48	110.60
1	B	151	GLU	OE1-CD-OE2	-6.04	116.05	123.30
1	B	459	GLU	CA-CB-CG	6.04	126.69	113.40
1	A	329	SER	CB-CA-C	6.03	121.56	110.10
1	A	476	ASP	CA-CB-CG	-6.02	100.15	113.40
1	A	484	LYS	N-CA-CB	6.00	121.40	110.60
1	B	255	VAL	CG1-CB-CG2	6.00	120.49	110.90
1	A	112	LEU	CB-CG-CD1	-5.99	100.82	111.00
1	B	382	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	B	105	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	325	PHE	CB-CG-CD2	-5.98	116.62	120.80
1	A	101	GLU	C-N-CA	5.96	136.59	121.70
1	B	162	HIS	CA-CB-CG	-5.95	103.48	113.60
1	B	459	GLU	N-CA-CB	5.95	121.31	110.60
1	A	15	GLU	CG-CD-OE1	5.94	130.17	118.30
1	B	151	GLU	CG-CD-OE2	-5.92	106.45	118.30
1	B	326	ILE	CB-CA-C	5.92	123.43	111.60
1	A	151	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	481	SER	CB-CA-C	5.90	121.31	110.10
1	A	255	VAL	CA-CB-CG1	5.89	119.74	110.90
1	A	320	ARG	CD-NE-CZ	-5.89	115.35	123.60
1	B	501	GLU	OE1-CD-OE2	5.88	130.35	123.30
1	B	437	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	B	162	HIS	N-CA-CB	5.83	121.09	110.60
1	A	339	LYS	N-CA-CB	-5.82	100.13	110.60
1	A	292	ASP	N-CA-CB	-5.81	100.14	110.60
1	B	228	SER	O-C-N	5.81	131.99	122.70
1	A	455	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	104	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	A	251	TYR	CB-CG-CD2	-5.80	117.52	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	155	ARG	CA-CB-CG	-5.79	100.67	113.40
1	A	437	TYR	CD1-CG-CD2	5.78	124.26	117.90
1	B	397	GLN	CG-CD-OE1	-5.78	110.05	121.60
1	B	135	THR	CA-CB-OG1	-5.77	96.89	109.00
1	B	486	ARG	NH1-CZ-NH2	-5.77	113.06	119.40
1	B	405	GLU	OE1-CD-OE2	-5.76	116.39	123.30
1	A	192	PHE	CB-CG-CD2	5.76	124.83	120.80
1	B	100	GLY	C-N-CA	5.76	136.09	121.70
1	B	404	LEU	N-CA-CB	-5.74	98.93	110.40
1	A	164	ILE	O-C-N	5.73	131.87	122.70
1	A	390	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	B	124	ASN	OD1-CG-ND2	-5.72	108.74	121.90
1	A	472	GLU	CB-CG-CD	-5.71	98.78	114.20
1	B	402	ASP	N-CA-CB	5.70	120.86	110.60
1	B	140	ALA	N-CA-CB	5.70	118.07	110.10
1	A	402	ASP	CB-CA-C	5.69	121.78	110.40
1	B	167	LYS	CG-CD-CE	5.68	128.94	111.90
1	A	127	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	381	SER	C-N-CA	5.66	135.85	121.70
1	A	262	THR	O-C-N	5.66	131.75	122.70
1	B	161	TYR	CG-CD1-CE1	-5.66	116.78	121.30
1	A	366	SER	CB-CA-C	-5.65	99.36	110.10
1	B	139	GLN	CB-CG-CD	-5.65	96.91	111.60
1	B	326	ILE	CA-C-O	5.65	131.96	120.10
1	A	155	ARG	CD-NE-CZ	-5.64	115.70	123.60
1	A	507	GLU	N-CA-C	5.64	126.24	111.00
1	A	163	ARG	CG-CD-NE	-5.63	99.97	111.80
1	A	130	TYR	O-C-N	-5.63	113.69	122.70
1	A	139	GLN	CB-CA-C	5.62	121.64	110.40
1	A	317	GLY	O-C-N	-5.62	113.71	122.70
1	A	24	ASP	CA-CB-CG	-5.62	101.05	113.40
1	A	372	ASN	CB-CA-C	5.62	121.63	110.40
1	A	337	GLU	CA-CB-CG	-5.61	101.05	113.40
1	B	233	CYS	CA-C-O	-5.61	108.32	120.10
1	B	266	VAL	CB-CA-C	5.61	122.06	111.40
1	A	216	CYS	CA-CB-SG	5.60	124.07	114.00
1	B	190	VAL	O-C-N	5.60	131.73	121.10
1	B	486	ARG	N-CA-C	-5.60	95.89	111.00
1	A	265	LEU	CD1-CG-CD2	5.59	127.28	110.50
1	A	356	ASP	CB-CG-OD2	-5.59	113.26	118.30
1	A	249	GLN	N-CA-CB	5.59	120.66	110.60
1	A	291	LYS	CB-CA-C	-5.59	99.22	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ILE	O-C-N	5.59	131.65	122.70
1	A	337	GLU	OE1-CD-OE2	5.59	130.01	123.30
1	B	276	ALA	CA-C-N	-5.58	104.92	117.20
1	A	163	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	157	ASN	C-N-CA	5.57	135.63	121.70
1	A	440	SER	O-C-N	-5.57	113.79	122.70
1	A	490	VAL	CA-CB-CG1	5.56	119.24	110.90
1	B	390	GLU	CB-CA-C	-5.56	99.28	110.40
1	A	376	ARG	CD-NE-CZ	5.56	131.38	123.60
1	A	257	SER	CB-CA-C	-5.55	99.56	110.10
1	B	237	GLU	N-CA-CB	5.54	120.58	110.60
1	A	115	LEU	N-CA-C	-5.54	96.04	111.00
1	A	408	VAL	N-CA-CB	-5.53	99.33	111.50
1	B	473	LEU	CB-CA-C	5.53	120.72	110.20
1	B	188	VAL	CA-C-O	-5.53	108.48	120.10
1	B	258	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	B	397	GLN	CB-CG-CD	-5.53	97.23	111.60
1	A	115	LEU	N-CA-CB	5.52	121.45	110.40
1	A	23	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	255	VAL	CG1-CB-CG2	5.51	119.72	110.90
1	B	420	LYS	N-CA-CB	5.51	120.52	110.60
1	B	103	LYS	N-CA-CB	-5.51	100.68	110.60
1	B	169	LYS	CB-CA-C	-5.51	99.38	110.40
1	A	414	ARG	CD-NE-CZ	5.50	131.30	123.60
1	A	51	LYS	CA-CB-CG	5.50	125.50	113.40
1	A	444	ARG	NH1-CZ-NH2	5.50	125.45	119.40
1	A	365	VAL	CA-CB-CG2	-5.49	102.66	110.90
1	B	444	ARG	CD-NE-CZ	5.49	131.28	123.60
1	A	93	VAL	CA-CB-CG1	5.49	119.13	110.90
1	A	104	GLU	CA-CB-CG	5.49	125.47	113.40
1	A	359	LYS	CB-CA-C	-5.49	99.43	110.40
1	B	252	GLN	CB-CG-CD	5.47	125.83	111.60
1	A	255	VAL	CA-C-O	5.47	131.59	120.10
1	B	472	GLU	CG-CD-OE2	-5.47	107.35	118.30
1	B	196	ALA	CA-C-O	5.46	131.57	120.10
1	B	165	PHE	CB-CG-CD1	-5.46	116.98	120.80
1	B	166	PHE	CA-C-O	-5.46	108.63	120.10
1	B	270	GLU	CB-CA-C	-5.46	99.48	110.40
1	B	260	LYS	O-C-N	5.46	131.43	122.70
1	A	380	PHE	N-CA-CB	5.44	120.40	110.60
1	A	508	PHE	N-CA-CB	5.44	120.40	110.60
1	A	165	PHE	CG-CD2-CE2	5.44	126.79	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	LEU	O-C-N	5.43	131.38	122.70
1	A	491	PRO	CA-C-N	5.42	129.12	117.20
1	A	179	ILE	C-N-CA	5.41	135.23	121.70
1	A	506	THR	N-CA-CB	5.39	120.54	110.30
1	B	276	ALA	O-C-N	5.39	131.32	122.70
1	A	429	VAL	CA-CB-CG2	5.38	118.96	110.90
1	B	337	GLU	OE1-CD-OE2	5.38	129.75	123.30
1	B	487	THR	N-CA-CB	-5.37	100.09	110.30
1	A	73	LYS	N-CA-CB	-5.37	100.94	110.60
1	A	166	PHE	CB-CA-C	-5.37	99.66	110.40
1	A	197	THR	N-CA-CB	-5.37	100.10	110.30
1	B	422	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	A	184	LEU	N-CA-CB	-5.35	99.70	110.40
1	A	318	ALA	N-CA-CB	5.35	117.59	110.10
1	B	147	GLY	N-CA-C	-5.35	99.73	113.10
1	B	263	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	354	THR	CA-CB-OG1	-5.35	97.77	109.00
1	A	365	VAL	CB-CA-C	5.34	121.56	111.40
1	A	507	GLU	CA-CB-CG	5.34	125.15	113.40
1	B	159	ASN	O-C-N	5.34	131.25	122.70
1	B	431	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	B	326	ILE	O-C-N	-5.32	114.20	122.70
1	B	500	TYR	CB-CA-C	-5.30	99.80	110.40
1	B	191	PRO	O-C-N	-5.29	114.23	122.70
1	A	297	PHE	CB-CA-C	-5.27	99.85	110.40
1	A	413	ARG	CB-CG-CD	5.27	125.31	111.60
1	B	139	GLN	CG-CD-NE2	-5.27	104.06	116.70
1	A	475	PRO	N-CA-CB	5.26	109.61	103.30
1	B	486	ARG	CD-NE-CZ	5.26	130.96	123.60
1	A	491	PRO	C-N-CA	-5.26	108.56	121.70
1	A	161	TYR	CD1-CE1-CZ	5.25	124.53	119.80
1	A	170	ILE	O-C-N	-5.25	114.30	122.70
1	B	101	GLU	N-CA-CB	-5.24	101.17	110.60
1	A	40	LEU	CB-CA-C	5.24	120.15	110.20
1	A	194	VAL	CA-CB-CG2	5.24	118.75	110.90
1	B	291	LYS	O-C-N	5.23	131.07	122.70
1	A	236	GLU	CB-CG-CD	5.23	128.31	114.20
1	B	138	LYS	CA-CB-CG	-5.23	101.90	113.40
1	A	169	LYS	N-CA-CB	5.22	119.99	110.60
1	A	343	LYS	CA-CB-CG	-5.21	101.94	113.40
1	A	465	LEU	CB-CA-C	5.20	120.09	110.20
1	B	256	ASN	CB-CA-C	-5.20	100.00	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	379	ASP	OD1-CG-OD2	-5.20	113.43	123.30
1	B	103	LYS	O-C-N	5.19	131.00	122.70
1	A	6	MET	N-CA-C	-5.18	97.02	111.00
1	A	322	LEU	CA-CB-CG	5.18	127.20	115.30
1	A	205	PRO	CA-CB-CG	-5.17	94.19	104.00
1	A	461	SER	CA-CB-OG	-5.16	97.26	111.20
1	B	331	THR	CA-CB-CG2	5.16	119.62	112.40
1	A	111	GLN	CG-CD-OE1	-5.15	111.30	121.60
1	B	388	LEU	CB-CA-C	-5.15	100.41	110.20
1	B	479	ASP	C-N-CA	5.15	134.58	121.70
1	A	207	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	B	379	ASP	CA-CB-CG	-5.14	102.08	113.40
1	A	136	LEU	CB-CG-CD2	-5.14	102.27	111.00
1	B	115	LEU	N-CA-C	-5.13	97.14	111.00
1	A	156	GLU	OE1-CD-OE2	5.13	129.45	123.30
1	A	390	GLU	CA-CB-CG	5.12	124.67	113.40
1	B	149	ASN	N-CA-CB	-5.12	101.39	110.60
1	B	454	LEU	CB-CG-CD1	5.11	119.68	111.00
1	B	351	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	A	388	LEU	CB-CG-CD1	5.10	119.67	111.00
1	A	170	ILE	N-CA-CB	-5.10	99.07	110.80
1	A	117	PRO	O-C-N	5.09	130.78	121.10
1	A	237	GLU	CG-CD-OE2	-5.09	108.11	118.30
1	B	486	ARG	CB-CG-CD	-5.09	98.37	111.60
1	B	270	GLU	CG-CD-OE2	-5.09	108.13	118.30
1	A	359	LYS	O-C-N	5.08	130.83	122.70
1	B	368	VAL	N-CA-CB	-5.08	100.32	111.50
1	A	427	LYS	N-CA-CB	-5.07	101.48	110.60
1	A	184	LEU	CB-CG-CD1	5.05	119.59	111.00
1	B	250	TRP	CB-CA-C	5.05	120.50	110.40
1	B	348	ILE	O-C-N	-5.05	114.62	122.70
1	B	388	LEU	CD1-CG-CD2	5.05	125.64	110.50
1	B	509	GLU	CG-CD-OE2	-5.05	108.21	118.30
1	A	80	LYS	CB-CG-CD	5.04	124.72	111.60
1	A	467	VAL	C-N-CA	-5.04	109.10	121.70
1	B	220	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	A	262	THR	CA-CB-CG2	5.03	119.44	112.40
1	A	148	ALA	N-CA-CB	-5.02	103.07	110.10
1	B	253	LEU	CB-CA-C	-5.02	100.66	110.20
1	B	418	VAL	CG1-CB-CG2	-5.02	102.86	110.90
1	A	429	VAL	CB-CA-C	5.02	120.94	111.40
1	B	463	ARG	CG-CD-NE	5.02	122.34	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	B	385	ILE	N-CA-CB	5.02	122.34	110.80
1	A	166	PHE	CZ-CE2-CD2	-5.01	114.09	120.10
1	A	458	ILE	CB-CG1-CD1	5.01	127.92	113.90
1	B	191	PRO	N-CA-CB	-5.01	97.09	102.60
1	A	49	VAL	CA-CB-CG2	5.00	118.41	110.90
1	A	113	LYS	C-N-CA	-5.00	109.19	121.70
1	B	290	GLU	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ARG	Sidechain
1	A	353	ARG	Sidechain
1	A	376	ARG	Sidechain
1	A	38	ARG	Sidechain
1	B	163	ARG	Sidechain
1	B	463	ARG	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	A	3841	0	3899	403	2
1	B	3107	0	3156	259	0
2	A	43	0	30	9	0
3	A	31	0	17	0	0
3	B	31	0	18	2	0
4	B	6	0	3	0	0
5	A	182	0	0	9	0
5	B	101	0	0	11	0
All	All	7342	0	7123	628	2

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 44.

All (628) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LYS:O	1:A:10:LYS:HD3	1.18	1.33
1:A:24:ASP:HA	1:A:37:THR:CG2	1.60	1.27
1:A:1:GLU:N	1:A:71:ILE:HD12	1.49	1.27
1:A:1:GLU:H3	1:A:2:PRO:CD	1.50	1.25
1:A:24:ASP:CA	1:A:37:THR:HG21	1.66	1.25
1:A:24:ASP:O	1:A:37:THR:HG22	1.36	1.24
1:A:10:LYS:HZ3	1:A:85:GLN:NE2	1.37	1.22
1:A:26:TRP:CE3	1:A:81:LEU:HD23	1.75	1.21
1:A:33:VAL:HG23	1:A:82:GLY:O	1.37	1.20
1:A:1:GLU:N	1:A:71:ILE:CD1	2.05	1.18
1:A:1:GLU:N	1:A:2:PRO:HD2	1.51	1.17
1:B:398:ARG:O	1:B:399:ASN:HB2	1.45	1.14
1:B:396:GLU:HG3	1:B:401:LYS:HD3	1.28	1.11
1:A:113:LYS:CE	1:A:115:LEU:HD13	1.80	1.11
1:A:9:GLN:HG2	1:A:11:ILE:HD11	1.32	1.10
1:A:496:TYR:C	1:A:496:TYR:HD1	1.53	1.10
1:A:495:LEU:HD12	1:B:503:PRO:HB2	1.23	1.10
1:B:313:GLU:O	1:B:314:GLU:HB2	1.41	1.08
1:A:113:LYS:HE2	1:A:115:LEU:HD13	1.12	1.07
1:A:317:GLY:HA3	1:A:320:ARG:HH11	0.97	1.07
1:A:494:VAL:HG21	1:B:503:PRO:HD2	1.18	1.06
1:A:79:LYS:HD2	1:A:79:LYS:N	1.70	1.06
1:A:317:GLY:HA3	1:A:320:ARG:NH1	1.71	1.06
1:A:1:GLU:H1	1:A:71:ILE:CD1	1.63	1.06
1:A:1:GLU:CA	1:A:71:ILE:HD12	1.85	1.05
1:B:197:THR:CG2	1:B:436:LEU:HD21	1.86	1.05
1:A:226:MET:HE2	1:A:252:GLN:HB2	1.38	1.04
1:A:503:PRO:O	1:A:504:THR:HB	1.58	1.04
1:A:1:GLU:H3	1:A:2:PRO:HD2	0.97	1.04
1:A:10:LYS:O	1:A:10:LYS:CD	2.05	1.04
1:A:248:ILE:HD11	1:A:250:TRP:NE1	1.71	1.04
1:A:494:VAL:CG2	1:B:503:PRO:HD2	1.87	1.03
1:A:6:MET:HG2	1:A:7:ASN:H	1.24	1.03
1:A:491:PRO:HD3	5:A:732:HOH:O	1.57	1.02
1:A:146:SER:HB3	1:A:291:LYS:HD2	1.40	1.01
1:B:509:GLU:HG3	1:B:510:ASP:H	1.25	1.00
1:A:6:MET:HG2	1:A:7:ASN:N	1.71	1.00
1:A:35:ASP:OD1	1:A:37:THR:HG22	1.60	1.00
1:A:1:GLU:H1	1:A:71:ILE:HD12	1.02	0.99
1:B:509:GLU:CG	1:B:510:ASP:H	1.71	0.99
1:B:396:GLU:HG3	1:B:401:LYS:CD	1.91	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:THR:HG21	1:B:436:LEU:HD21	1.44	0.99
1:A:137:THR:HG22	1:A:140:ALA:H	1.24	0.98
1:A:496:TYR:CD1	1:A:496:TYR:C	2.31	0.98
1:A:102:THR:HG22	1:A:102:THR:O	1.62	0.98
1:B:108:ARG:C	1:B:112:LEU:HD23	1.85	0.97
1:A:10:LYS:NZ	1:A:85:GLN:NE2	2.12	0.97
1:A:257:SER:HB2	1:A:324:LYS:HG3	1.45	0.97
1:A:24:ASP:O	1:A:37:THR:CG2	2.12	0.96
1:A:35:ASP:OD1	1:A:37:THR:CG2	2.12	0.96
1:A:2:PRO:O	1:A:3:LYS:CE	2.14	0.96
1:B:313:GLU:O	1:B:314:GLU:CB	2.12	0.95
1:A:9:GLN:HG2	1:A:11:ILE:CD1	1.97	0.94
1:A:10:LYS:HZ3	1:A:85:GLN:HE22	1.08	0.94
1:A:29:ILE:HD12	1:A:58:VAL:HG12	1.47	0.94
1:A:24:ASP:C	1:A:37:THR:CG2	2.37	0.93
1:A:26:TRP:CE3	1:A:81:LEU:CD2	2.51	0.93
1:A:495:LEU:HD12	1:B:503:PRO:CB	1.97	0.93
1:A:69:ASN:H	1:A:69:ASN:HD22	1.15	0.92
1:A:110:GLU:O	1:A:113:LYS:CG	2.19	0.91
1:B:108:ARG:O	1:B:112:LEU:HD23	1.71	0.91
1:A:257:SER:CB	1:A:324:LYS:HG3	2.00	0.91
1:A:113:LYS:HE2	1:A:115:LEU:CD1	1.99	0.91
1:A:2:PRO:O	1:A:3:LYS:NZ	2.04	0.91
1:A:10:LYS:NZ	1:A:85:GLN:HE22	1.67	0.91
1:A:2:PRO:O	1:A:3:LYS:HE3	1.69	0.90
1:B:113:LYS:O	1:B:115:LEU:HD23	1.72	0.89
1:A:317:GLY:CA	1:A:320:ARG:HH11	1.85	0.89
1:A:113:LYS:O	1:A:113:LYS:HG3	1.72	0.89
1:A:9:GLN:O	1:A:10:LYS:HB3	1.73	0.88
5:A:593:HOH:O	1:B:491:PRO:HD3	1.70	0.88
1:B:197:THR:HG21	1:B:436:LEU:CD2	2.03	0.87
1:A:29:ILE:HD12	1:A:58:VAL:CG1	2.03	0.87
1:B:115:LEU:O	1:B:116:LEU:C	2.13	0.86
1:A:90:PRO:O	1:A:92:LEU:N	2.06	0.86
1:B:396:GLU:HG3	1:B:401:LYS:CE	2.06	0.86
1:A:226:MET:CE	1:A:252:GLN:HB2	2.06	0.86
1:B:113:LYS:C	1:B:115:LEU:H	1.76	0.85
1:A:11:ILE:O	1:A:85:GLN:HB2	1.76	0.85
1:A:33:VAL:CG2	1:A:82:GLY:O	2.22	0.85
1:A:2:PRO:C	1:A:3:LYS:HG2	1.96	0.85
1:B:113:LYS:C	1:B:115:LEU:N	2.29	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:GLU:HG3	1:B:510:ASP:N	1.91	0.85
1:A:113:LYS:O	1:A:114:SER:C	2.13	0.84
1:B:102:THR:C	1:B:103:LYS:HD2	1.96	0.84
1:A:155:ARG:HE	1:B:491:PRO:HB3	1.42	0.84
1:A:270:GLU:OE1	1:A:343:LYS:HE3	1.77	0.84
1:A:112:LEU:HD12	1:A:113:LYS:N	1.92	0.83
1:B:396:GLU:CG	1:B:401:LYS:HD3	2.07	0.83
1:A:146:SER:HB3	1:A:291:LYS:CD	2.09	0.82
1:A:496:TYR:O	1:A:496:TYR:HD1	1.61	0.82
1:A:510:ASP:H	1:B:115:LEU:HD13	1.41	0.82
1:A:9:GLN:O	1:A:10:LYS:CB	2.27	0.82
1:A:112:LEU:C	1:A:112:LEU:HD12	1.98	0.82
1:A:32:TYR:HE2	1:A:80:LYS:HB3	1.45	0.82
1:A:226:MET:HE2	1:A:252:GLN:CB	2.10	0.82
1:A:2:PRO:HG3	1:A:72:ASP:OD1	1.78	0.82
1:A:24:ASP:HA	1:A:37:THR:HG21	0.82	0.82
1:A:510:ASP:CA	1:B:115:LEU:CD1	2.58	0.81
1:A:22:PRO:O	1:A:24:ASP:N	2.13	0.81
1:A:510:ASP:N	1:B:115:LEU:HD13	1.93	0.81
1:A:6:MET:SD	1:A:8:LYS:HD2	2.20	0.81
1:A:1:GLU:CA	1:A:71:ILE:CD1	2.57	0.81
1:A:137:THR:HG22	1:A:140:ALA:N	1.96	0.80
1:A:1:GLU:N	1:A:2:PRO:CD	2.20	0.80
1:A:26:TRP:CZ3	1:A:81:LEU:HD23	2.16	0.80
1:A:24:ASP:CA	1:A:37:THR:CG2	2.41	0.79
1:A:510:ASP:CA	1:B:115:LEU:HD13	2.11	0.79
1:A:244:SER:HB2	1:A:246:LYS:H	1.46	0.79
1:A:110:GLU:O	1:A:113:LYS:HG3	1.82	0.79
1:A:50:ILE:HG23	2:A:560:HEM:CBC	2.12	0.79
1:A:6:MET:CG	1:A:7:ASN:N	2.44	0.79
1:A:110:GLU:O	1:A:113:LYS:HG2	1.83	0.78
1:A:16:VAL:CG1	1:A:88:MET:HE1	2.13	0.78
1:A:26:TRP:CZ3	1:A:81:LEU:CD2	2.66	0.78
1:A:130:TYR:CE2	1:A:134:GLN:NE2	2.50	0.78
1:B:248:ILE:HB	1:B:275:LYS:HD2	1.66	0.78
1:A:20:ASN:H	1:A:20:ASN:HD22	1.32	0.77
1:A:29:ILE:CD1	1:A:58:VAL:CG1	2.63	0.77
1:A:29:ILE:CD1	1:A:58:VAL:HG12	2.13	0.77
1:B:120:ASP:C	1:B:121:ASN:HD22	1.88	0.77
1:A:102:THR:O	1:A:104:GLU:N	2.18	0.77
1:A:257:SER:HB2	1:A:324:LYS:CG	2.15	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:CB	1:A:291:LYS:HD2	2.15	0.77
1:B:286:LEU:CD1	5:B:645:HOH:O	2.32	0.77
1:B:496:TYR:CD1	1:B:496:TYR:C	2.57	0.76
1:B:320:ARG:HG3	1:B:320:ARG:O	1.71	0.76
1:A:1:GLU:H2	1:A:71:ILE:CD1	1.98	0.76
1:A:248:ILE:CD1	1:A:250:TRP:NE1	2.49	0.76
1:B:312:VAL:O	1:B:314:GLU:N	2.18	0.76
1:A:78:GLU:C	1:A:79:LYS:HD2	2.05	0.75
1:A:101:GLU:OE2	1:A:138:LYS:HG3	1.87	0.75
1:A:88:MET:C	1:A:89:PRO:O	2.19	0.75
1:A:88:MET:O	1:A:89:PRO:C	2.24	0.75
1:A:24:ASP:HA	1:A:37:THR:CB	2.16	0.75
1:A:256:ASN:HD22	1:A:258:ASP:H	1.32	0.74
1:A:211:ASP:HB3	1:A:439:ASN:HD21	1.51	0.74
1:A:248:ILE:HD11	1:A:250:TRP:CE2	2.21	0.74
1:A:27:VAL:HG13	1:A:29:ILE:HD13	1.69	0.74
1:A:9:GLN:CG	1:A:11:ILE:CD1	2.65	0.74
1:B:509:GLU:CG	1:B:510:ASP:N	2.47	0.73
1:A:40:LEU:HD12	1:A:47:GLN:HG2	1.69	0.73
1:A:84:LEU:HD11	1:A:88:MET:HG2	1.67	0.73
1:A:113:LYS:CG	1:A:113:LYS:O	2.34	0.73
1:A:24:ASP:C	1:A:37:THR:HG22	2.03	0.73
1:A:1:GLU:N	1:A:71:ILE:HB	2.04	0.73
1:A:113:LYS:CE	1:A:115:LEU:CD1	2.60	0.73
1:A:26:TRP:CZ3	1:A:81:LEU:HG	2.23	0.73
1:A:503:PRO:O	1:A:504:THR:CB	2.35	0.73
1:B:315:SER:O	1:B:316:GLN:HB3	1.89	0.72
1:A:1:GLU:N	1:A:71:ILE:HD13	2.05	0.72
1:A:507:GLU:O	1:A:508:PHE:HB2	1.90	0.72
1:A:1:GLU:H2	1:A:2:PRO:HD2	1.51	0.72
1:A:6:MET:HG2	1:A:8:LYS:H	1.53	0.71
1:A:228:SER:HA	1:A:252:GLN:HE21	1.54	0.71
1:B:163:ARG:O	5:B:607:HOH:O	2.07	0.71
1:A:35:ASP:OD1	1:A:37:THR:HG23	1.91	0.71
1:B:217:GLY:HA3	1:B:247:GLN:NE2	2.05	0.71
1:B:229:THR:OG1	1:B:253:LEU:HA	1.90	0.70
1:A:101:GLU:OE1	1:A:108:ARG:NH1	2.24	0.70
1:B:339:LYS:HG3	1:B:346:ILE:CD1	2.21	0.70
1:A:79:LYS:N	1:A:79:LYS:CD	2.46	0.70
1:A:270:GLU:OE1	1:A:343:LYS:CE	2.39	0.70
1:A:22:PRO:C	1:A:24:ASP:H	1.94	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:O	1:A:114:SER:N	2.25	0.69
1:B:113:LYS:HG2	1:B:113:LYS:O	1.90	0.69
1:A:24:ASP:N	1:A:24:ASP:OD1	2.23	0.69
1:A:75:ILE:CD1	2:A:560:HEM:HBB1	2.22	0.69
1:B:109:LYS:HA	1:B:112:LEU:HG	1.75	0.68
1:A:256:ASN:HD22	1:A:257:SER:N	1.92	0.67
1:A:197:THR:CG2	1:A:436:LEU:HD21	2.24	0.67
1:A:155:ARG:HH21	1:B:491:PRO:HB2	1.60	0.67
1:B:196:ALA:CB	1:B:226:MET:HE2	2.25	0.67
1:A:3:LYS:O	1:A:4:LEU:HB2	1.93	0.66
1:A:158:HIS:ND1	1:A:411:GLY:O	2.27	0.66
1:A:1:GLU:H2	1:A:71:ILE:HD13	1.60	0.66
1:A:1:GLU:H1	1:A:71:ILE:CG1	2.09	0.66
1:A:102:THR:O	1:A:102:THR:CG2	2.29	0.66
1:B:248:ILE:HD11	1:B:250:TRP:NE1	2.10	0.66
1:B:257:SER:OG	1:B:324:LYS:HG2	1.95	0.66
1:A:1:GLU:HA	1:A:71:ILE:CD1	2.26	0.66
1:A:69:ASN:N	1:A:69:ASN:HD22	1.88	0.66
1:A:9:GLN:CG	1:A:11:ILE:HD13	2.26	0.66
1:B:249:GLN:H	1:B:275:LYS:HE3	1.59	0.66
1:A:16:VAL:HG11	1:A:88:MET:CE	2.26	0.66
1:A:32:TYR:CE2	1:A:80:LYS:HB3	2.28	0.66
1:A:2:PRO:C	1:A:3:LYS:CG	2.63	0.66
1:B:228:SER:HA	1:B:252:GLN:HG3	1.77	0.65
1:A:490:VAL:HG23	1:A:491:PRO:O	1.96	0.65
1:A:386:GLU:OE1	5:A:583:HOH:O	2.14	0.65
1:B:396:GLU:OE2	1:B:401:LYS:NZ	2.26	0.65
1:B:227:ILE:HG13	1:B:250:TRP:O	1.97	0.65
1:B:316:GLN:HB2	1:B:320:ARG:HA	1.78	0.65
1:A:26:TRP:CZ3	1:A:81:LEU:CG	2.79	0.65
1:A:5:ASP:O	1:A:6:MET:HB3	1.95	0.65
1:B:398:ARG:O	1:B:399:ASN:CB	2.31	0.64
1:A:338:LEU:HD13	1:A:346:ILE:HD13	1.79	0.64
1:A:1:GLU:N	1:A:71:ILE:CB	2.61	0.64
1:A:93:VAL:O	1:A:93:VAL:HG23	1.98	0.64
1:B:108:ARG:C	1:B:112:LEU:CD2	2.65	0.64
1:A:73:LYS:HE3	1:A:74:TYR:CZ	2.32	0.64
1:A:108:ARG:HH12	1:A:138:LYS:N	1.95	0.64
1:A:163:ARG:O	5:A:709:HOH:O	2.15	0.64
1:A:21:LYS:HG3	1:A:22:PRO:HD2	1.78	0.64
1:B:197:THR:HG21	1:B:436:LEU:CG	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLU:OE2	1:B:138:LYS:HD3	1.97	0.64
1:A:197:THR:HG21	1:A:436:LEU:HD21	1.78	0.64
1:B:102:THR:HA	1:B:103:LYS:HD2	1.80	0.63
1:A:9:GLN:HG3	1:A:11:ILE:HD13	1.81	0.63
1:B:102:THR:CA	1:B:103:LYS:HD2	2.27	0.63
1:B:496:TYR:C	1:B:496:TYR:HD1	1.99	0.63
1:A:331:THR:HG22	1:A:333:LYS:H	1.63	0.63
1:B:217:GLY:HA3	1:B:247:GLN:HE22	1.62	0.63
1:B:190:VAL:HG11	1:B:221:THR:HG21	1.80	0.63
1:B:387:VAL:O	1:B:391:THR:HG23	1.98	0.63
1:B:239:ILE:N	1:B:239:ILE:HD12	2.13	0.63
1:B:251:TYR:OH	5:B:594:HOH:O	1.99	0.63
1:B:343:LYS:O	1:B:343:LYS:HG2	1.99	0.63
1:A:40:LEU:CD1	1:A:47:GLN:OE1	2.46	0.63
1:A:346:ILE:HB	1:A:365:VAL:HG22	1.80	0.63
1:B:354:THR:OG1	1:B:391:THR:HG22	1.99	0.63
1:A:108:ARG:HH22	1:A:138:LYS:HG2	1.64	0.63
1:A:31:GLY:O	1:A:84:LEU:HB3	1.98	0.62
1:A:22:PRO:O	1:A:24:ASP:OD1	2.17	0.62
1:A:29:ILE:O	1:A:30:ASN:HB2	1.97	0.62
1:B:320:ARG:O	1:B:320:ARG:CG	2.43	0.62
1:B:226:MET:HG2	1:B:252:GLN:HB3	1.81	0.62
1:B:239:ILE:H	1:B:239:ILE:HD12	1.64	0.62
1:A:84:LEU:CD1	1:A:88:MET:HE2	2.29	0.62
1:A:388:LEU:HD13	1:A:424:LEU:CB	2.28	0.62
1:A:9:GLN:O	1:A:10:LYS:CG	2.48	0.62
1:A:248:ILE:HD11	1:A:250:TRP:CD1	2.33	0.62
1:A:491:PRO:CD	5:A:732:HOH:O	2.28	0.62
1:B:496:TYR:CD1	1:B:496:TYR:O	2.53	0.62
1:B:286:LEU:HD12	5:B:645:HOH:O	1.95	0.62
1:B:207:GLU:O	1:B:210:LYS:HB2	2.00	0.62
1:A:8:LYS:O	1:A:9:GLN:C	2.37	0.61
1:B:105:ASP:OD1	1:B:105:ASP:N	2.28	0.61
1:B:204:ASN:ND2	1:B:211:ASP:HB2	2.16	0.61
1:A:15:GLU:OE2	1:A:18:LYS:NZ	2.33	0.61
1:A:16:VAL:CG2	1:A:33:VAL:CG1	2.78	0.61
1:A:15:GLU:CD	1:A:18:LYS:HZ1	2.04	0.61
1:B:388:LEU:HD22	1:B:392:MET:HG2	1.81	0.61
1:B:133:SER:OG	1:B:134:GLN:NE2	2.33	0.61
1:B:331:THR:CG2	1:B:333:LYS:HB2	2.30	0.61
1:A:9:GLN:O	1:A:10:LYS:HG3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:MET:O	1:A:89:PRO:O	2.17	0.61
1:A:257:SER:OG	1:A:324:LYS:HG3	2.00	0.61
1:A:243:PRO:HD2	1:A:247:GLN:OE1	2.00	0.61
1:A:15:GLU:CD	1:A:18:LYS:NZ	2.54	0.61
1:A:4:LEU:O	1:A:6:MET:N	2.32	0.60
1:A:28:VAL:HG11	1:A:84:LEU:HD22	1.81	0.60
1:A:89:PRO:HG2	1:A:92:LEU:HD12	1.83	0.60
1:A:482:THR:HB	1:B:486:ARG:O	1.99	0.60
1:A:388:LEU:HD13	1:A:424:LEU:HB2	1.82	0.60
1:A:110:GLU:CA	1:A:113:LYS:HG2	2.31	0.60
1:A:40:LEU:HD11	1:A:47:GLN:OE1	2.01	0.60
1:A:21:LYS:O	1:A:22:PRO:O	2.19	0.60
1:A:110:GLU:C	1:A:113:LYS:HG2	2.22	0.60
1:B:108:ARG:HH22	1:B:138:LYS:HG3	1.67	0.60
1:A:239:ILE:HD13	1:A:272:LEU:HB3	1.83	0.60
1:A:24:ASP:C	1:A:37:THR:HG21	2.13	0.60
1:A:112:LEU:C	1:A:112:LEU:CD1	2.69	0.60
1:B:113:LYS:O	1:B:115:LEU:N	2.34	0.60
1:B:248:ILE:HD11	1:B:250:TRP:HE1	1.66	0.60
1:A:1:GLU:H1	1:A:71:ILE:HB	1.67	0.60
1:B:136:LEU:HB3	1:B:140:ALA:HB3	1.83	0.59
1:B:177:VAL:HG22	1:B:468:THR:HA	1.84	0.59
1:A:90:PRO:C	1:A:92:LEU:H	2.00	0.59
1:A:1:GLU:HB3	1:A:62:PHE:HE2	1.67	0.59
1:A:508:PHE:CE2	1:B:116:LEU:HD23	2.38	0.59
1:A:162:HIS:N	1:A:162:HIS:ND1	2.49	0.59
1:A:155:ARG:NE	1:B:491:PRO:HB3	2.16	0.59
1:B:243:PRO:HD2	1:B:247:GLN:HE22	1.67	0.59
1:A:166:PHE:CD1	1:A:465:LEU:HD21	2.38	0.59
1:A:495:LEU:CD1	1:B:503:PRO:HB2	2.16	0.59
1:B:281:VAL:HG22	1:B:349:LYS:O	2.03	0.58
1:A:155:ARG:HE	1:B:491:PRO:CB	2.15	0.58
1:B:339:LYS:HA	1:B:346:ILE:HD11	1.85	0.58
1:A:30:ASN:H	1:A:59:THR:HG1	1.50	0.58
1:A:168:PRO:O	1:B:353:ARG:HD2	2.03	0.58
1:A:16:VAL:CG2	1:A:33:VAL:HG11	2.32	0.58
1:A:508:PHE:HZ	1:B:135:THR:CG2	2.15	0.58
1:B:419:LEU:HD21	1:B:458:ILE:HG23	1.84	0.58
1:A:84:LEU:HD11	1:A:88:MET:CG	2.33	0.58
1:B:108:ARG:O	1:B:111:GLN:HB2	2.04	0.58
1:A:113:LYS:HE3	1:A:115:LEU:HD13	1.79	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LYS:O	1:B:260:LYS:CG	2.50	0.58
1:B:349:LYS:NZ	3:B:570:FMN:O2'	2.36	0.58
1:B:102:THR:O	1:B:103:LYS:C	2.43	0.58
1:B:286:LEU:HD13	5:B:645:HOH:O	2.00	0.57
1:A:16:VAL:HG12	1:A:88:MET:HE1	1.86	0.57
1:A:84:LEU:HD12	1:A:88:MET:HE2	1.85	0.57
1:A:108:ARG:O	1:A:112:LEU:HG	2.04	0.57
1:A:102:THR:C	1:A:104:GLU:N	2.57	0.57
1:B:196:ALA:HB2	1:B:226:MET:HE2	1.87	0.57
1:A:3:LYS:C	1:A:5:ASP:H	2.08	0.57
1:B:115:LEU:N	1:B:115:LEU:HD23	2.18	0.57
1:B:196:ALA:HB3	1:B:226:MET:HE2	1.87	0.57
1:A:499:VAL:HG22	1:B:505:LEU:HD11	1.87	0.57
1:B:256:ASN:HD22	1:B:258:ASP:H	1.53	0.57
1:B:382:ARG:HH12	1:B:390:GLU:CD	2.07	0.57
1:B:113:LYS:CG	1:B:113:LYS:O	2.52	0.57
1:A:26:TRP:CH2	1:A:81:LEU:HG	2.39	0.56
1:A:502:GLY:O	1:A:503:PRO:O	2.23	0.56
1:A:15:GLU:OE1	1:A:18:LYS:NZ	2.38	0.56
1:A:110:GLU:HA	1:A:113:LYS:HB3	1.86	0.56
1:A:13:PRO:CG	1:A:87:SER:O	2.52	0.56
1:A:496:TYR:CD1	1:A:497:ASN:N	2.73	0.56
1:A:50:ILE:HG23	2:A:560:HEM:CAC	2.34	0.56
1:A:2:PRO:HG2	1:A:3:LYS:H	1.70	0.56
1:B:186:SER:OG	1:B:248:ILE:HG21	2.04	0.56
1:B:121:ASN:HD22	1:B:121:ASN:N	2.02	0.56
1:B:497:ASN:N	1:B:497:ASN:HD22	2.03	0.56
1:A:16:VAL:CG1	1:A:88:MET:CE	2.81	0.56
1:A:256:ASN:ND2	1:A:258:ASP:H	2.02	0.56
1:A:81:LEU:HD13	1:A:81:LEU:N	2.19	0.56
1:A:89:PRO:O	1:A:90:PRO:O	2.24	0.56
1:A:230:LEU:HD22	1:A:254:TYR:CE2	2.40	0.56
1:A:23:ASP:O	1:A:24:ASP:HB3	2.05	0.56
1:B:227:ILE:O	1:B:252:GLN:N	2.31	0.56
1:B:288:GLN:HG3	1:B:293:MET:SD	2.47	0.56
1:B:213:ALA:HA	1:B:225:GLN:NE2	2.20	0.56
1:A:12:SER:OG	1:A:85:GLN:NE2	2.39	0.55
1:B:197:THR:HG23	1:B:436:LEU:HD11	1.88	0.55
1:B:105:ASP:O	1:B:106:ILE:C	2.44	0.55
1:A:494:VAL:CG2	1:A:495:LEU:N	2.70	0.55
1:A:1:GLU:H2	1:A:71:ILE:HG21	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:593:HOH:O	1:B:491:PRO:CD	2.43	0.55
1:B:136:LEU:HD13	1:B:140:ALA:HB1	1.88	0.55
1:B:196:ALA:HB3	1:B:226:MET:CE	2.36	0.55
1:A:496:TYR:CD1	1:A:496:TYR:O	2.53	0.54
1:A:337:GLU:O	1:A:341:LYS:HD2	2.06	0.54
1:B:213:ALA:CA	1:B:225:GLN:HE22	2.19	0.54
1:A:481:SER:OG	1:B:484:LYS:NZ	2.40	0.54
1:A:248:ILE:CD1	1:A:250:TRP:CD1	2.91	0.54
1:B:327:ASP:C	1:B:329:SER:H	2.10	0.54
1:A:289:ARG:NH1	1:A:292:ASP:OD1	2.41	0.54
1:B:313:GLU:N	1:B:313:GLU:OE1	2.40	0.54
1:A:159:ASN:HB3	1:B:488:VAL:HG11	1.90	0.54
1:B:442:TYR:HB2	1:B:446:GLY:HA3	1.89	0.54
1:A:1:GLU:H1	1:A:71:ILE:CB	2.20	0.54
1:A:20:ASN:N	1:A:20:ASN:HD22	1.96	0.54
1:A:361:ALA:HB2	1:A:404:LEU:HD22	1.89	0.54
1:B:339:LYS:HG3	1:B:346:ILE:HD12	1.90	0.54
1:A:494:VAL:HG23	1:A:495:LEU:N	2.23	0.54
1:B:313:GLU:OE1	1:B:313:GLU:CA	2.56	0.54
1:A:476:ASP:OD1	1:A:476:ASP:N	2.39	0.54
1:A:16:VAL:HG11	1:A:88:MET:HE1	1.88	0.54
1:A:105:ASP:N	1:A:105:ASP:OD1	2.41	0.54
1:A:179:ILE:HD11	1:A:455:ARG:HG3	1.90	0.53
1:A:114:SER:O	1:A:115:LEU:HD12	2.09	0.53
1:A:75:ILE:HD12	2:A:560:HEM:HBB1	1.89	0.53
1:A:348:ILE:HD12	1:A:365:VAL:HG11	1.89	0.53
1:B:197:THR:HG22	1:B:197:THR:O	2.08	0.53
1:A:18:LYS:HE2	1:A:19:HIS:CE1	2.43	0.53
1:A:13:PRO:HG2	1:A:87:SER:O	2.08	0.53
1:A:16:VAL:HG21	1:A:33:VAL:CG1	2.39	0.53
1:A:485:ALA:HB1	1:B:487:THR:HG22	1.90	0.53
1:A:49:VAL:HG21	2:A:560:HEM:CMD	2.39	0.53
1:A:78:GLU:CD	1:A:78:GLU:H	2.10	0.53
1:B:257:SER:OG	1:B:324:LYS:O	2.26	0.53
1:B:104:GLU:OE2	1:B:138:LYS:CD	2.56	0.52
1:A:49:VAL:O	1:A:53:ASN:OD1	2.27	0.52
1:A:73:LYS:HE3	1:A:74:TYR:OH	2.09	0.52
1:A:63:GLU:HB3	1:A:64:PRO:HD3	1.91	0.52
1:A:16:VAL:HG21	1:A:33:VAL:HG13	1.90	0.52
1:A:11:ILE:O	1:A:85:GLN:CB	2.55	0.52
1:A:155:ARG:NH2	1:B:491:PRO:HB2	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:O	1:A:440:SER:OG	2.21	0.52
1:B:449:LYS:HA	1:B:452:GLU:HG2	1.91	0.52
1:A:226:MET:CE	1:A:252:GLN:CB	2.80	0.52
1:A:124:ASN:HD22	1:A:124:ASN:C	2.12	0.52
1:B:474:LYS:H	1:B:477:LEU:HD23	1.74	0.52
1:A:508:PHE:HE2	1:B:116:LEU:HD23	1.72	0.52
1:B:102:THR:O	1:B:103:LYS:HB2	2.09	0.52
1:A:108:ARG:NH1	1:A:137:THR:HA	2.23	0.52
1:A:213:ALA:HB2	1:A:225:GLN:HE22	1.75	0.52
1:A:283:ALA:N	1:A:284:PRO:CD	2.73	0.52
1:A:113:LYS:O	1:A:114:SER:O	2.27	0.52
1:A:49:VAL:HG21	2:A:560:HEM:HMD2	1.91	0.52
1:A:11:ILE:HG22	1:A:12:SER:H	1.74	0.51
1:B:369:VAL:HG22	1:B:407:PHE:HB2	1.91	0.51
1:A:84:LEU:CD1	1:A:88:MET:CE	2.89	0.51
1:A:98:ALA:O	1:A:99:PRO:C	2.47	0.51
1:B:167:LYS:HE3	5:B:680:HOH:O	2.10	0.51
1:B:326:ILE:O	1:B:328:PRO:HD3	2.11	0.51
1:A:422:LEU:HD13	1:A:470:ILE:HD12	1.92	0.51
1:A:32:TYR:HE2	1:A:80:LYS:CB	2.20	0.51
1:A:152:VAL:HG21	1:A:380:PHE:CE1	2.46	0.51
1:B:325:PHE:HD1	1:B:325:PHE:H	1.58	0.51
1:B:214:ARG:O	1:B:218:GLN:HG2	2.11	0.51
1:A:16:VAL:HG11	1:A:88:MET:HE3	1.92	0.50
1:A:510:ASP:CA	1:B:115:LEU:HD11	2.38	0.50
1:B:190:VAL:CG1	1:B:221:THR:HG21	2.41	0.50
1:B:234:SER:O	1:B:235:PRO:C	2.49	0.50
1:A:29:ILE:O	1:A:30:ASN:CB	2.60	0.50
1:A:40:LEU:HD12	1:A:47:GLN:CG	2.41	0.50
1:B:228:SER:O	1:B:231:ALA:HB2	2.11	0.50
1:B:473:LEU:O	1:B:474:LYS:HG2	2.12	0.50
1:A:110:GLU:HA	1:A:113:LYS:HG2	1.92	0.50
1:B:113:LYS:O	1:B:115:LEU:CD2	2.54	0.50
1:B:339:LYS:CG	1:B:346:ILE:HD12	2.42	0.50
1:B:197:THR:CG2	1:B:436:LEU:HD11	2.42	0.50
1:B:108:ARG:O	1:B:111:GLN:CB	2.59	0.50
1:A:108:ARG:NH1	1:A:136:LEU:O	2.45	0.49
1:A:499:VAL:HG22	1:B:505:LEU:CD1	2.41	0.49
1:B:273:GLY:O	1:B:275:LYS:HE2	2.12	0.49
1:B:327:ASP:C	1:B:329:SER:N	2.65	0.49
1:A:40:LEU:HG	1:A:41:PRO:HD3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ALA:HA	1:A:110:GLU:OE1	2.13	0.49
1:B:337:GLU:OE1	1:B:337:GLU:HA	2.12	0.49
1:B:507:GLU:O	1:B:508:PHE:HB2	2.13	0.49
1:B:384:PRO:HG2	1:B:409:ASP:O	2.13	0.49
1:B:192:PHE:HA	1:B:429:VAL:O	2.12	0.49
1:A:34:TYR:CE1	1:A:80:LYS:HG3	2.47	0.49
1:A:75:ILE:HG22	1:A:80:LYS:HD2	1.94	0.49
1:B:197:THR:HG21	1:B:436:LEU:HG	1.95	0.49
1:B:190:VAL:HG21	1:B:223:VAL:HG22	1.94	0.49
1:A:388:LEU:HD13	1:A:424:LEU:HB3	1.93	0.49
1:B:326:ILE:O	1:B:327:ASP:C	2.45	0.49
1:A:289:ARG:NH1	1:A:292:ASP:CG	2.66	0.49
1:A:22:PRO:C	1:A:24:ASP:N	2.56	0.48
1:B:316:GLN:HB2	1:B:320:ARG:CA	2.43	0.48
1:B:339:LYS:CG	1:B:346:ILE:CD1	2.91	0.48
1:A:398:ARG:HB2	1:A:400:LEU:HG	1.93	0.48
1:B:162:HIS:HE1	5:B:635:HOH:O	1.95	0.48
1:A:290:GLU:O	1:A:294:LYS:HB2	2.14	0.48
1:B:248:ILE:CD1	1:B:250:TRP:NE1	2.75	0.48
1:A:487:THR:H	1:B:489:GLY:HA2	1.78	0.48
1:A:13:PRO:HG3	1:A:87:SER:O	2.13	0.48
1:B:102:THR:C	1:B:104:GLU:N	2.64	0.48
1:B:196:ALA:H	1:B:226:MET:HE1	1.78	0.48
1:B:204:ASN:ND2	1:B:211:ASP:CB	2.77	0.48
1:B:382:ARG:NH1	1:B:390:GLU:OE1	2.46	0.48
1:A:43:HIS:CE1	2:A:560:HEM:ND	2.81	0.48
1:A:228:SER:HA	1:A:252:GLN:NE2	2.26	0.48
1:A:69:ASN:H	1:A:69:ASN:ND2	1.94	0.48
1:A:113:LYS:HE3	1:A:115:LEU:CD1	2.41	0.48
1:B:197:THR:HG23	1:B:436:LEU:HD21	1.89	0.48
1:B:326:ILE:O	1:B:328:PRO:N	2.47	0.48
1:B:402:ASP:O	1:B:402:ASP:OD1	2.31	0.48
1:B:129:GLU:HB2	1:B:437:TYR:CD2	2.49	0.48
1:A:226:MET:HE3	1:A:349:LYS:HD2	1.96	0.47
1:A:20:ASN:HA	1:A:54:ALA:HB1	1.96	0.47
1:A:111:GLN:NE2	5:A:640:HOH:O	2.47	0.47
1:B:227:ILE:HD11	1:B:249:GLN:HG2	1.95	0.47
1:B:286:LEU:HB2	5:B:645:HOH:O	2.13	0.47
1:A:34:TYR:HA	1:A:79:LYS:O	2.14	0.47
1:A:102:THR:O	1:A:103:LYS:C	2.53	0.47
1:A:40:LEU:N	1:A:41:PRO:HD2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:LEU:HD12	1:B:461:SER:HB3	1.96	0.47
1:A:93:VAL:O	1:A:93:VAL:CG2	2.62	0.47
1:A:223:VAL:HA	1:A:224:PRO:HD3	1.74	0.47
1:B:107:ALA:O	1:B:108:ARG:C	2.51	0.47
1:B:229:THR:OG1	1:B:254:TYR:N	2.47	0.47
1:A:1:GLU:H3	1:A:2:PRO:HD3	1.63	0.47
1:A:3:LYS:HB3	1:A:3:LYS:HE3	1.69	0.47
1:A:137:THR:CG2	1:A:139:GLN:HG3	2.44	0.47
1:A:1:GLU:HA	1:A:71:ILE:HD12	1.77	0.47
1:B:115:LEU:O	1:B:116:LEU:O	2.32	0.47
1:B:316:GLN:HG3	1:B:320:ARG:HB2	1.95	0.47
1:B:388:LEU:HD22	1:B:392:MET:CG	2.44	0.47
1:B:234:SER:HB2	1:B:235:PRO:HD2	1.96	0.47
1:B:282:ASP:OD1	1:B:373:HIS:ND1	2.33	0.47
1:A:209:GLU:OE2	1:A:232:SER:HB2	2.14	0.47
1:A:192:PHE:HA	1:A:429:VAL:O	2.14	0.47
1:B:249:GLN:H	1:B:275:LYS:CE	2.27	0.47
1:B:190:VAL:CG1	1:B:221:THR:CG2	2.93	0.47
1:A:1:GLU:N	1:A:71:ILE:CG1	2.73	0.47
1:A:69:ASN:N	1:A:69:ASN:ND2	2.56	0.47
1:B:496:TYR:HD1	1:B:497:ASN:HD22	1.62	0.47
1:A:38:ARG:HH11	1:A:38:ARG:HD3	1.25	0.47
1:B:351:VAL:HG21	1:B:368:VAL:HG22	1.96	0.46
1:A:102:THR:C	1:A:104:GLU:H	2.18	0.46
1:B:326:ILE:O	1:B:328:PRO:CD	2.63	0.46
1:A:13:PRO:HA	1:A:88:MET:CE	2.45	0.46
1:A:461:SER:O	1:A:465:LEU:HB2	2.16	0.46
1:A:482:THR:CB	1:B:486:ARG:O	2.64	0.46
1:A:22:PRO:O	1:A:23:ASP:C	2.51	0.46
1:A:155:ARG:HD3	1:A:155:ARG:HH11	1.39	0.46
1:A:257:SER:CB	1:A:324:LYS:CG	2.81	0.46
1:A:27:VAL:CG1	1:A:29:ILE:HD13	2.43	0.46
1:A:40:LEU:O	1:A:47:GLN:HG2	2.16	0.46
1:A:162:HIS:CE1	5:A:701:HOH:O	2.69	0.46
1:A:13:PRO:HB3	1:A:89:PRO:HD3	1.97	0.46
1:B:248:ILE:CD1	1:B:250:TRP:HE1	2.26	0.46
1:A:197:THR:HG23	1:A:436:LEU:HD21	1.95	0.46
1:A:363:ILE:HG21	1:A:363:ILE:HD13	1.74	0.46
1:A:256:ASN:ND2	1:A:257:SER:N	2.62	0.46
1:A:18:LYS:HB3	1:A:18:LYS:HE2	1.67	0.46
1:B:392:MET:N	1:B:393:PRO:CD	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:TYR:O	1:B:376:ARG:NH2	2.39	0.46
1:A:109:LYS:O	1:A:112:LEU:CD1	2.65	0.45
1:B:197:THR:HA	3:B:570:FMN:C5A	2.46	0.45
1:B:259:ARG:HD2	1:B:259:ARG:HH11	1.14	0.45
1:A:5:ASP:O	1:A:6:MET:CB	2.62	0.45
1:A:177:VAL:HG21	1:A:463:ARG:HG2	1.99	0.45
1:A:317:GLY:O	1:A:318:ALA:HB3	2.17	0.45
1:B:115:LEU:HD22	1:B:115:LEU:HA	1.53	0.45
1:A:348:ILE:O	1:A:368:VAL:HA	2.17	0.45
1:B:204:ASN:HD21	1:B:211:ASP:CB	2.29	0.45
1:B:204:ASN:HD22	1:B:211:ASP:HB2	1.80	0.45
1:B:317:GLY:O	1:B:320:ARG:HB3	2.16	0.45
1:A:81:LEU:CD1	1:A:81:LEU:N	2.79	0.45
1:B:234:SER:H	1:B:237:GLU:HG3	1.80	0.45
1:A:495:LEU:HD23	1:A:495:LEU:C	2.36	0.45
1:B:459:GLU:CD	5:B:625:HOH:O	2.55	0.45
1:A:1:GLU:HB3	1:A:62:PHE:CE2	2.51	0.45
1:A:211:ASP:HB3	1:A:439:ASN:ND2	2.26	0.45
1:A:14:ALA:O	1:A:18:LYS:HB2	2.16	0.45
1:B:260:LYS:O	1:B:260:LYS:HG2	2.11	0.45
1:A:183:MET:CE	1:A:191:PRO:HA	2.47	0.45
1:A:98:ALA:HB1	1:A:101:GLU:HB2	1.99	0.44
2:A:560:HEM:HBB2	2:A:560:HEM:CMB	2.48	0.44
1:B:182:ASP:HA	1:B:186:SER:O	2.17	0.44
1:A:20:ASN:CA	1:A:54:ALA:HB1	2.47	0.44
1:A:24:ASP:C	1:A:37:THR:HB	2.37	0.44
1:A:28:VAL:HG23	1:A:56:LYS:O	2.15	0.44
1:A:226:MET:HE3	1:A:349:LYS:CD	2.47	0.44
1:A:24:ASP:CA	1:A:37:THR:CB	2.87	0.44
1:B:108:ARG:HB3	1:B:112:LEU:HD21	1.99	0.44
1:A:95:PRO:HB2	1:A:96:PRO:CD	2.46	0.44
1:A:78:GLU:N	1:A:78:GLU:OE2	2.37	0.44
1:A:102:THR:HB	1:A:104:GLU:CG	2.47	0.44
1:A:499:VAL:HG12	1:A:499:VAL:O	2.17	0.44
1:B:379:ASP:O	1:B:380:PHE:HB2	2.18	0.44
1:B:469:SER:O	1:B:472:GLU:HB2	2.16	0.44
1:A:506:THR:O	1:B:130:TYR:CD1	2.71	0.44
1:A:15:GLU:OE1	1:A:19:HIS:HE1	2.01	0.44
1:A:460:MET:HB3	5:B:656:HOH:O	2.17	0.44
1:A:256:ASN:O	1:A:259:ARG:HD3	2.17	0.44
1:B:289:ARG:HH12	1:B:292:ASP:CG	2.21	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HB	1:A:57:ASP:OD2	2.18	0.43
1:A:13:PRO:HB3	1:A:89:PRO:CD	2.48	0.43
1:B:146:SER:OG	1:B:291:LYS:HB2	2.18	0.43
1:A:197:THR:CG2	1:A:200:CYS:SG	3.06	0.43
1:B:111:GLN:O	1:B:115:LEU:HB3	2.18	0.43
1:A:41:PRO:HA	1:A:47:GLN:CG	2.48	0.43
1:A:344:LEU:HA	1:A:345:PRO:HD3	1.92	0.43
1:A:494:VAL:HG21	1:B:503:PRO:CD	2.13	0.43
1:B:320:ARG:HH21	1:B:320:ARG:HD3	1.50	0.43
1:A:124:ASN:O	1:A:127:ASP:HB2	2.18	0.43
1:A:26:TRP:O	1:A:55:GLY:HA2	2.18	0.43
1:B:490:VAL:O	1:B:491:PRO:C	2.56	0.43
1:B:197:THR:CG2	1:B:197:THR:O	2.67	0.43
1:A:4:LEU:HA	1:A:4:LEU:HD22	1.40	0.43
1:B:248:ILE:HG21	1:B:248:ILE:HD13	1.76	0.43
1:B:278:PHE:CE2	1:B:347:VAL:HG11	2.54	0.43
1:A:508:PHE:HZ	1:B:135:THR:HG22	1.83	0.43
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.77	0.43
1:B:447:VAL:O	1:B:451:ILE:HG13	2.19	0.42
1:B:396:GLU:OE2	1:B:401:LYS:CD	2.67	0.42
1:A:460:MET:CE	1:B:318:ALA:HA	2.48	0.42
1:B:394:ILE:O	1:B:397:GLN:HB2	2.20	0.42
1:A:226:MET:CE	1:A:252:GLN:HG3	2.49	0.42
1:B:190:VAL:CG2	1:B:223:VAL:HG22	2.49	0.42
1:B:146:SER:OG	1:B:291:LYS:HD2	2.20	0.42
1:A:47:GLN:O	1:A:51:LYS:HB2	2.19	0.42
1:B:218:GLN:OE1	1:B:448:GLU:OE1	2.38	0.42
1:B:171:LEU:HA	1:B:171:LEU:HD23	1.85	0.42
1:B:454:LEU:O	1:B:458:ILE:HG13	2.19	0.42
1:B:259:ARG:NH1	1:B:334:ASP:OD2	2.42	0.42
1:A:155:ARG:NE	1:B:491:PRO:CB	2.79	0.42
1:B:223:VAL:HG12	1:B:224:PRO:O	2.19	0.42
1:A:76:ALA:HA	1:A:77:PRO:HD3	1.94	0.42
1:A:490:VAL:O	1:A:491:PRO:C	2.57	0.42
1:B:107:ALA:O	1:B:111:GLN:HB2	2.19	0.42
1:A:482:THR:HG21	1:B:486:ARG:HB3	2.02	0.42
1:B:209:GLU:H	1:B:209:GLU:HG2	1.38	0.42
1:A:24:ASP:O	1:A:25:CYS:C	2.58	0.42
1:A:226:MET:HE1	1:A:252:GLN:HG3	2.01	0.42
1:B:259:ARG:NH2	1:B:334:ASP:OD2	2.51	0.42
1:B:127:ASP:O	1:B:131:LEU:HD22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:C	1:A:114:SER:N	2.74	0.41
1:B:108:ARG:NH1	1:B:137:THR:HA	2.35	0.41
1:B:114:SER:C	1:B:115:LEU:HD23	2.41	0.41
1:A:6:MET:CG	1:A:8:LYS:HD2	2.50	0.41
1:A:106:ILE:O	1:A:107:ALA:C	2.57	0.41
1:B:190:VAL:HG13	1:B:221:THR:CG2	2.51	0.41
1:A:226:MET:CE	1:A:252:GLN:CG	2.98	0.41
1:B:108:ARG:CZ	1:B:136:LEU:O	2.68	0.41
1:A:464:LEU:HD13	1:B:285:SER:HB3	2.01	0.41
1:A:100:GLY:O	1:A:102:THR:N	2.53	0.41
1:A:162:HIS:HE1	5:A:701:HOH:O	2.02	0.41
1:A:444:ARG:HD2	1:A:444:ARG:HH11	1.35	0.41
1:B:267:LYS:HG3	1:B:267:LYS:HZ3	1.54	0.41
1:A:24:ASP:C	1:A:37:THR:CB	2.88	0.41
1:A:34:TYR:CD1	1:A:80:LYS:HG3	2.55	0.41
1:A:29:ILE:CD1	1:A:58:VAL:HG11	2.45	0.41
1:B:120:ASP:O	1:B:121:ASN:ND2	2.48	0.41
1:B:190:VAL:HG11	1:B:221:THR:CG2	2.49	0.41
1:B:260:LYS:O	1:B:260:LYS:HG3	2.19	0.41
1:B:236:GLU:OE2	1:B:268:ASN:ND2	2.50	0.41
1:B:497:ASN:N	1:B:497:ASN:ND2	2.67	0.41
1:A:15:GLU:HA	1:A:15:GLU:OE2	2.21	0.41
1:B:213:ALA:HA	1:B:225:GLN:HE22	1.80	0.41
1:B:419:LEU:HD11	1:B:461:SER:HB2	2.03	0.41
1:A:121:ASN:HA	1:B:297:PHE:CE2	2.56	0.41
1:A:473:LEU:HA	1:A:473:LEU:HD23	1.80	0.41
1:A:194:VAL:HG22	1:A:435:PHE:CD1	2.56	0.41
1:B:197:THR:CG2	1:B:436:LEU:CD2	2.70	0.41
1:A:51:LYS:HD3	1:A:52:PHE:CE1	2.56	0.41
1:A:392:MET:HG3	1:A:424:LEU:O	2.20	0.41
1:B:255:VAL:HB	1:B:262:THR:HG21	2.02	0.41
1:A:494:VAL:CG2	1:A:495:LEU:H	2.34	0.41
2:A:560:HEM:HBB2	2:A:560:HEM:HMB2	2.03	0.41
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.92	0.41
1:B:470:ILE:HD12	1:B:473:LEU:HD12	2.03	0.41
1:A:11:ILE:O	1:A:85:GLN:N	2.43	0.41
1:A:317:GLY:O	1:A:318:ALA:CB	2.69	0.41
1:B:317:GLY:H	1:B:319:SER:HB2	1.85	0.41
1:A:348:ILE:CD1	1:A:365:VAL:HG11	2.50	0.41
1:A:333:LYS:O	1:A:337:GLU:HG2	2.21	0.41
1:B:178:ASP:O	1:B:469:SER:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:HA	1:B:297:PHE:CD2	2.56	0.41
1:A:372:ASN:O	1:A:373:HIS:CB	2.69	0.41
1:B:109:LYS:CA	1:B:109:LYS:HE3	2.51	0.40
1:B:202:LEU:HD23	1:B:202:LEU:HA	1.90	0.40
1:B:394:ILE:O	1:B:397:GLN:CB	2.70	0.40
1:A:112:LEU:HA	1:A:116:LEU:HG	2.04	0.40
1:A:337:GLU:O	1:A:341:LYS:CD	2.69	0.40
1:B:377:GLN:HB3	5:B:662:HOH:O	2.20	0.40
1:B:102:THR:O	1:B:103:LYS:CB	2.69	0.40
1:B:108:ARG:HB3	1:B:112:LEU:CD2	2.51	0.40
1:A:26:TRP:CD2	1:A:81:LEU:CD2	3.00	0.40
1:B:156:GLU:CD	1:B:163:ARG:HH22	2.25	0.40
1:B:190:VAL:HA	1:B:191:PRO:HD3	1.84	0.40

All (2) 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)
1:A:38:ARG:NH2	1:A:245:ASP:OD1[3_665]	2.09	0.11
1:A:38:ARG:CZ	1:A:245:ASP:OD1[3_665]	2.12	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	490/511 (96%)	438 (89%)	27 (6%)	25 (5%)	2	1
1	B	396/511 (78%)	353 (89%)	31 (8%)	12 (3%)	5	4
All	All	886/1022 (87%)	791 (89%)	58 (6%)	37 (4%)	3	2

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	ASP
1	A	7	ASN
1	A	10	LYS
1	A	22	PRO
1	A	23	ASP
1	A	24	ASP
1	A	25	CYS
1	A	81	LEU
1	A	90	PRO
1	A	91	GLU
1	A	103	LYS
1	A	298	SER
1	A	503	PRO
1	A	504	THR
1	A	508	PHE
1	B	101	GLU
1	B	313	GLU
1	B	314	GLU
1	B	316	GLN
1	B	508	PHE
1	B	510	ASP
1	A	2	PRO
1	A	30	ASN
1	A	85	GLN
1	A	113	LYS
1	B	503	PRO
1	A	6	MET
1	A	318	ALA
1	A	380	PHE
1	B	315	SER
1	B	481	SER
1	B	399	ASN
1	B	120	ASP
1	A	9	GLN
1	B	191	PRO
1	A	89	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/440 (96%)	330 (78%)	93 (22%)	1	1
1	B	342/440 (78%)	264 (77%)	78 (23%)	1	1
All	All	765/880 (87%)	594 (78%)	171 (22%)	1	1

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	3	LYS
1	A	4	LEU
1	A	6	MET
1	A	8	LYS
1	A	10	LYS
1	A	11	ILE
1	A	18	LYS
1	A	20	ASN
1	A	21	LYS
1	A	27	VAL
1	A	29	ILE
1	A	30	ASN
1	A	36	LEU
1	A	37	THR
1	A	38	ARG
1	A	49	VAL
1	A	50	ILE
1	A	52	PHE
1	A	57	ASP
1	A	58	VAL
1	A	63	GLU
1	A	69	ASN
1	A	72	ASP
1	A	79	LYS
1	A	80	LYS
1	A	81	LEU
1	A	84	LEU
1	A	88	MET
1	A	101	GLU
1	A	103	LYS
1	A	106	ILE
1	A	108	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	109	LYS
1	A	111	GLN
1	A	112	LEU
1	A	113	LYS
1	A	124	ASN
1	A	125	LEU
1	A	131	LEU
1	A	137	THR
1	A	139	GLN
1	A	152	VAL
1	A	162	HIS
1	A	169	LYS
1	A	170	ILE
1	A	175	ARG
1	A	184	LEU
1	A	190	VAL
1	A	197	THR
1	A	212	VAL
1	A	230	LEU
1	A	232	SER
1	A	236	GLU
1	A	240	GLU
1	A	244	SER
1	A	246	LYS
1	A	248	ILE
1	A	252	GLN
1	A	256	ASN
1	A	265	LEU
1	A	271	LYS
1	A	292	ASP
1	A	297	PHE
1	A	320	ARG
1	A	329	SER
1	A	330	LEU
1	A	338	LEU
1	A	339	LYS
1	A	343	LYS
1	A	353	ARG
1	A	365	VAL
1	A	368	VAL
1	A	372	ASN
1	A	378	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	388	LEU
1	A	390	GLU
1	A	397	GLN
1	A	398	ARG
1	A	399	ASN
1	A	400	LEU
1	A	403	LYS
1	A	408	VAL
1	A	429	VAL
1	A	462	MET
1	A	465	LEU
1	A	472	GLU
1	A	477	LEU
1	A	483	LEU
1	A	492	ASN
1	A	496	TYR
1	A	504	THR
1	A	509	GLU
1	B	102	THR
1	B	103	LYS
1	B	105	ASP
1	B	108	ARG
1	B	109	LYS
1	B	111	GLN
1	B	112	LEU
1	B	115	LEU
1	B	120	ASP
1	B	125	LEU
1	B	131	LEU
1	B	133	SER
1	B	134	GLN
1	B	139	GLN
1	B	152	VAL
1	B	176	LYS
1	B	184	LEU
1	B	186	SER
1	B	195	SER
1	B	197	THR
1	B	209	GLU
1	B	218	GLN
1	B	220	VAL
1	B	222	LYS

Continued from previous page...

Mol	Chain	Res	Type
1	B	225	GLN
1	B	230	LEU
1	B	236	GLU
1	B	237	GLU
1	B	245	ASP
1	B	248	ILE
1	B	249	GLN
1	B	252	GLN
1	B	256	ASN
1	B	257	SER
1	B	260	LYS
1	B	263	ASP
1	B	268	ASN
1	B	275	LYS
1	B	294	LYS
1	B	295	LEU
1	B	296	LYS
1	B	312	VAL
1	B	313	GLU
1	B	320	ARG
1	B	323	SER
1	B	324	LYS
1	B	325	PHE
1	B	330	LEU
1	B	331	THR
1	B	343	LYS
1	B	353	ARG
1	B	368	VAL
1	B	370	LEU
1	B	373	HIS
1	B	378	LEU
1	B	388	LEU
1	B	391	THR
1	B	397	GLN
1	B	398	ARG
1	B	403	LYS
1	B	404	LEU
1	B	408	VAL
1	B	429	VAL
1	B	448	GLU
1	B	462	MET
1	B	463	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	464	LEU
1	B	477	LEU
1	B	481	SER
1	B	483	LEU
1	B	484	LYS
1	B	492	ASN
1	B	496	TYR
1	B	498	GLU
1	B	504	THR
1	B	506	THR
1	B	508	PHE
1	B	509	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	20	ASN
1	A	53	ASN
1	A	69	ASN
1	A	85	GLN
1	A	124	ASN
1	A	139	GLN
1	A	157	ASN
1	A	159	ASN
1	A	218	GLN
1	A	225	GLN
1	A	249	GLN
1	A	252	GLN
1	A	256	ASN
1	A	372	ASN
1	A	377	GLN
1	A	439	ASN
1	B	121	ASN
1	B	134	GLN
1	B	139	GLN
1	B	204	ASN
1	B	225	GLN
1	B	247	GLN
1	B	249	GLN
1	B	252	GLN
1	B	256	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	377	GLN
1	B	492	ASN
1	B	497	ASN

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)

4 ligands are modelled in this entry.

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	$\#|Z| > 2$
2	HEM	A	560	1	24,50,50	2.20	7 (29%)	16,82,82	3.20	7 (43%)
3	FMN	A	570	-	32,33,33	1.12	2 (6%)	34,50,50	4.23	15 (44%)
3	FMN	B	570	-	32,33,33	1.46	4 (12%)	34,50,50	3.85	19 (55%)
4	PYR	B	580	-	2,5,5	5.49	2 (100%)	2,6,6	5.77	2 (100%)

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
2	HEM	A	560	1	-	0/6/54/54	0/0/8/8
3	FMN	A	570	-	1/1/4/4	0/18/18/18	0/3/3/3
3	FMN	B	570	-	-	0/18/18/18	0/3/3/3
4	PYR	B	580	-	-	0/0/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	560	HEM	C3B-C2B	-5.72	1.33	1.40
2	A	560	HEM	C3C-C2C	-4.13	1.35	1.40
3	A	570	FMN	C10-N1	-2.96	1.30	1.35
3	B	570	FMN	C10-N1	-2.78	1.30	1.35
3	B	570	FMN	P-O5'	-2.22	1.53	1.59
2	A	560	HEM	C1B-NB	2.25	1.39	1.36
2	A	560	HEM	CMD-C2D	2.27	1.56	1.51
2	A	560	HEM	C3B-CAB	2.75	1.53	1.47
3	B	570	FMN	C5A-N5	2.83	1.39	1.35
3	A	570	FMN	C4-C4A	3.17	1.47	1.41
2	A	560	HEM	CAD-C3D	3.74	1.57	1.52
2	A	560	HEM	C3C-CAC	3.92	1.55	1.47
3	B	570	FMN	C4-C4A	4.36	1.50	1.41
4	B	580	PYR	O3-C2	5.05	1.39	1.22
4	B	580	PYR	C3-C2	5.89	1.67	1.49

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	FMN	C4A-C10-N10	-9.30	113.76	120.52
3	A	570	FMN	C4A-C10-N10	-7.85	114.81	120.52
3	A	570	FMN	C4-C4A-C10	-7.68	115.03	119.94
3	A	570	FMN	N3-C2-N1	-7.65	114.81	127.69
3	B	570	FMN	C4-C4A-C10	-7.57	115.10	119.94
4	B	580	PYR	O3-C2-C3	-7.38	102.50	120.14
3	A	570	FMN	C4A-C4-N3	-6.91	114.49	123.52
3	B	570	FMN	N3-C2-N1	-5.58	118.29	127.69
3	B	570	FMN	C4A-C4-N3	-5.47	116.38	123.52
2	A	560	HEM	C3B-CAB-CBB	-5.18	115.98	126.40
2	A	560	HEM	C3C-CAC-CBC	-4.85	116.64	126.40
3	A	570	FMN	O3'-C3'-C2'	-3.76	98.97	108.73
2	A	560	HEM	CBD-CAD-C3D	-3.70	105.97	112.47
2	A	560	HEM	CMD-C2D-C1D	-3.66	122.08	128.31
3	B	570	FMN	O3P-P-O1P	-3.54	99.07	110.63
3	B	570	FMN	O3'-C3'-C2'	-2.87	101.27	108.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	FMN	O3P-P-O2P	-2.55	98.08	107.44
3	B	570	FMN	O2P-P-O1P	-2.14	103.63	110.63
3	B	570	FMN	C9A-C5A-N5	-2.07	118.81	122.18
3	A	570	FMN	C7-C6-C5A	2.02	124.21	120.90
3	A	570	FMN	C4-C4A-N5	2.04	121.18	118.70
3	B	570	FMN	O3'-C3'-C4'	2.29	114.66	108.73
2	A	560	HEM	CAD-CBD-CGD	2.48	117.61	112.78
3	B	570	FMN	O2'-C2'-C3'	2.50	115.38	108.96
3	A	570	FMN	C4A-N5-C5A	3.08	120.35	116.72
3	A	570	FMN	O2'-C2'-C3'	3.26	117.34	108.96
3	B	570	FMN	C4A-N5-C5A	3.27	120.58	116.72
3	B	570	FMN	O4'-C4'-C5'	3.40	117.51	110.09
3	A	570	FMN	C1'-C2'-C3'	3.42	119.59	109.82
4	B	580	PYR	C3-C2-C1	3.47	130.54	120.19
3	B	570	FMN	O2'-C2'-C1'	3.48	118.53	109.93
3	B	570	FMN	O4'-C4'-C3'	3.53	118.03	108.96
3	A	570	FMN	C6-C5A-N5	3.70	123.53	118.92
3	B	570	FMN	O5'-P-O1P	3.79	116.62	107.08
3	A	570	FMN	O4'-C4'-C5'	3.79	118.36	110.09
3	A	570	FMN	O3'-C3'-C4'	3.82	118.64	108.73
3	B	570	FMN	C1'-N10-C9A	3.87	123.31	118.83
2	A	560	HEM	CMB-C2B-C3B	4.08	133.08	125.09
3	A	570	FMN	O2'-C2'-C1'	4.73	121.62	109.93
3	B	570	FMN	O2P-P-O5'	5.73	123.44	106.72
2	A	560	HEM	CAA-CBA-CGA	7.01	126.42	112.78
3	B	570	FMN	C4-N3-C2	11.01	124.34	115.16
3	A	570	FMN	C4-N3-C2	15.57	128.15	115.16

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	570	FMN	C2'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	560	HEM	9	0
3	B	570	FMN	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.