



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:43 PM UTC

PDB ID : 1IVR / pdb_00001ivr
Title : STRUCTURE OF ASPARTATE AMINOTRANSFERASE
Authors : Graf Von Stosch, A.
Deposited on : 1996-10-11
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

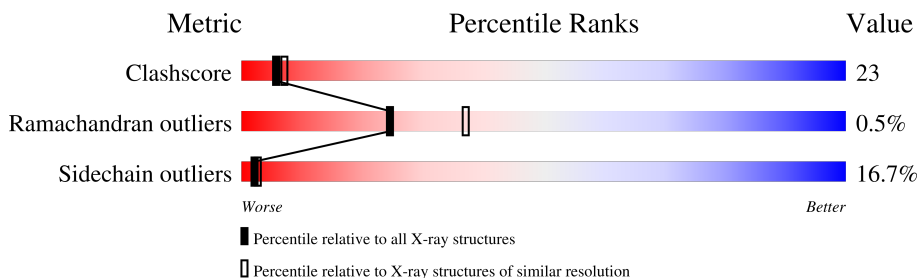
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

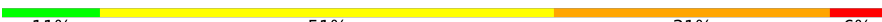
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	 11% 51% 31% 6%

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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.

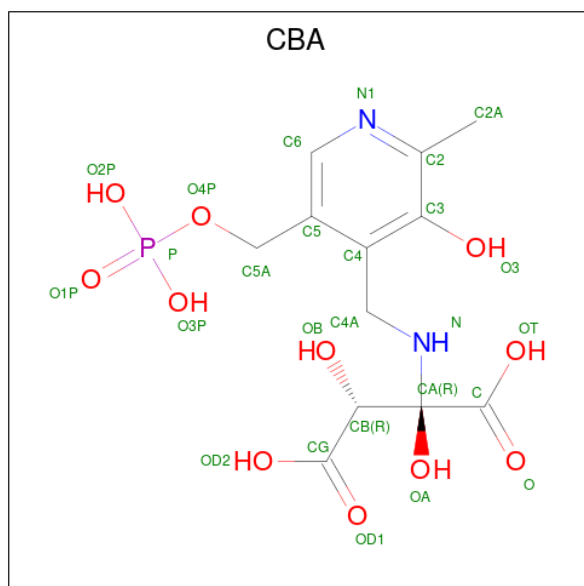
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3161	2004	558	581	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	PRO	SER	conflict	UNP P00508

- Molecule 2 is N-PYRIDOXYL-2,3-DIHYDROXYASPARTIC ACID-5-MONOPHOSPHATE (CCD ID: CBA) (formula: $C_{12}H_{17}N_2O_{11}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	12	2	11	1		

- Molecule 3 is water.

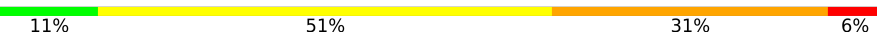
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	307	Total 307	O 307	0	0

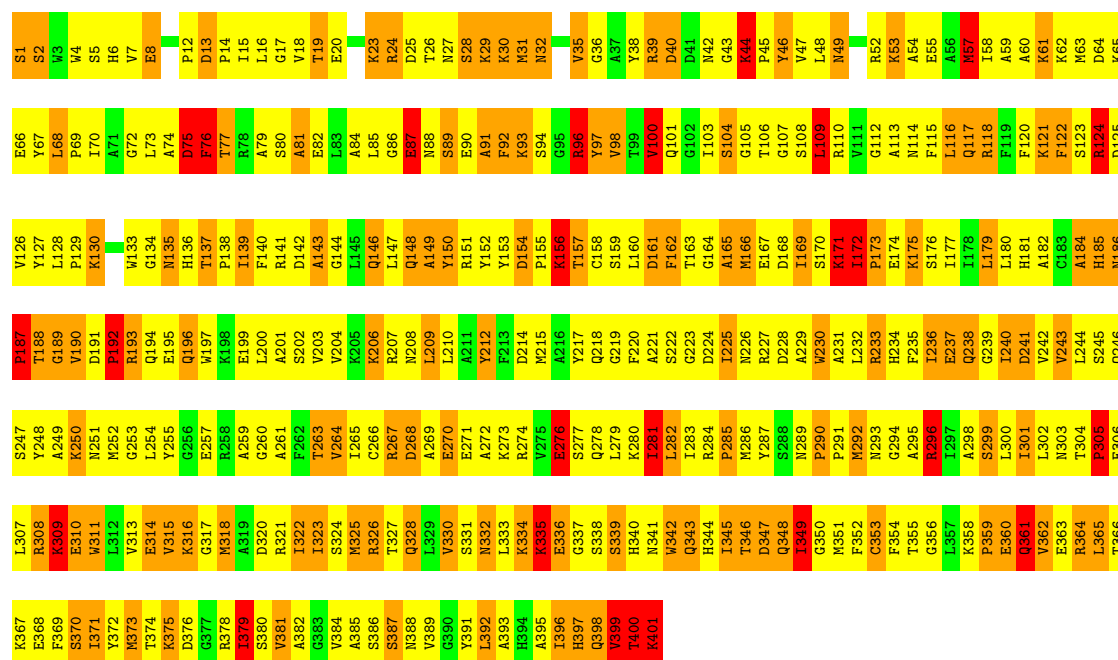
3 Residue-property plots

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

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	69.70Å 91.40Å 128.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, PROLSQ	Depositor
R, R_{free}	0.153 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3494	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: CBA

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	1.70	21/3231 (0.6%)	3.85	763/4360 (17.5%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	ILE	CA-CB	7.87	1.62	1.55
1	A	12	PRO	C-O	7.00	1.31	1.23
1	A	107	GLY	C-O	6.50	1.31	1.23
1	A	371	ILE	CA-CB	6.04	1.60	1.53
1	A	112	GLY	C-O	6.00	1.31	1.23
1	A	167	GLU	N-CA	5.84	1.53	1.46
1	A	13	ASP	N-CA	5.81	1.53	1.45
1	A	291	PRO	C-O	5.72	1.31	1.24
1	A	115	PHE	C-O	5.53	1.30	1.24
1	A	135	ASN	C-O	5.50	1.31	1.24
1	A	124	ARG	CD-NE	-5.47	1.38	1.46
1	A	221	ALA	N-CA	-5.39	1.39	1.46
1	A	392	LEU	CA-CB	5.35	1.61	1.53
1	A	187	PRO	C-N	-5.23	1.26	1.34
1	A	177	ILE	CA-CB	5.20	1.60	1.54
1	A	107	GLY	CA-C	5.17	1.57	1.52
1	A	177	ILE	C-N	-5.16	1.26	1.33
1	A	217	TYR	CA-CB	5.15	1.60	1.53
1	A	400	THR	CA-CB	5.15	1.61	1.53
1	A	137	THR	CA-CB	5.04	1.59	1.53
1	A	341	ASN	C-N	-5.03	1.27	1.33

All (763) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	CD-NE-CZ	28.18	163.85	124.40
1	A	268	ASP	CA-CB-CG	26.45	139.05	112.60
1	A	274	ARG	CD-NE-CZ	22.63	156.08	124.40
1	A	276	GLU	CA-CB-CG	17.80	149.69	114.10
1	A	270	GLU	CA-C-O	-16.72	103.48	120.70
1	A	148	GLN	OE1-CD-NE2	-16.37	106.23	122.60
1	A	228	ASP	CA-CB-CG	16.12	128.72	112.60
1	A	13	ASP	CA-C-O	16.11	136.93	120.17
1	A	124	ARG	CD-NE-CZ	15.56	146.19	124.40
1	A	367	LYS	CA-C-O	-15.00	105.25	120.70
1	A	136	HIS	CA-C-O	-14.80	104.86	120.55
1	A	149	ALA	O-C-N	14.55	140.15	123.27
1	A	107	GLY	CA-C-O	-14.52	105.79	120.75
1	A	172	ILE	O-C-N	14.48	136.78	121.14
1	A	296	ARG	NE-CZ-NH2	-13.44	107.11	119.20
1	A	289	ASN	OD1-CG-ND2	13.42	136.02	122.60
1	A	194	GLN	CA-C-N	13.35	137.80	120.44
1	A	194	GLN	C-N-CA	13.35	137.80	120.44
1	A	322	ILE	O-C-N	13.23	134.70	121.87
1	A	331	SER	CA-C-O	-13.18	106.45	120.42
1	A	309	LYS	CA-CB-CG	13.05	140.19	114.10
1	A	70	ILE	CA-C-O	-12.93	106.73	120.57
1	A	91	ALA	CA-C-O	12.73	134.19	120.82
1	A	237	GLU	CB-CG-CD	12.57	133.98	112.60
1	A	197	TRP	CA-C-O	-12.39	107.41	120.55
1	A	249	ALA	CA-C-O	12.28	133.72	120.82
1	A	265	ILE	N-CA-CB	12.24	124.95	111.00
1	A	194	GLN	OE1-CD-NE2	12.18	134.78	122.60
1	A	389	VAL	CB-CA-C	12.15	127.52	111.97
1	A	334	LYS	CA-C-N	12.03	136.40	120.28
1	A	334	LYS	C-N-CA	12.03	136.40	120.28
1	A	392	LEU	CA-C-O	12.03	133.77	120.90
1	A	31	MET	CA-C-O	-11.80	107.22	120.32
1	A	236	ILE	CA-C-O	-11.70	108.45	120.85
1	A	270	GLU	CB-CG-CD	11.65	132.41	112.60
1	A	124	ARG	NE-CZ-NH2	-11.60	108.76	119.20
1	A	167	GLU	N-CA-CB	11.57	126.85	110.07
1	A	23	LYS	CA-CB-CG	11.33	136.77	114.10
1	A	307	LEU	N-CA-C	-11.27	96.78	112.45
1	A	260	GLY	CA-C-O	-11.23	110.70	121.60
1	A	300	LEU	O-C-N	-11.22	110.22	122.12
1	A	223	GLY	CA-C-N	11.22	138.59	122.77
1	A	223	GLY	C-N-CA	11.22	138.59	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	SER	O-C-N	11.20	133.61	122.07
1	A	194	GLN	CG-CD-NE2	-11.20	99.60	116.40
1	A	354	PHE	CA-C-N	11.19	135.27	120.28
1	A	354	PHE	C-N-CA	11.19	135.27	120.28
1	A	296	ARG	CD-NE-CZ	11.17	140.04	124.40
1	A	259	ALA	CA-C-O	-11.14	108.33	120.36
1	A	336	GLU	CG-CD-OE2	11.06	143.84	118.40
1	A	173	PRO	CA-C-N	11.03	137.03	120.82
1	A	173	PRO	C-N-CA	11.03	137.03	120.82
1	A	77	THR	CB-CA-C	11.01	128.43	110.81
1	A	284	ARG	NE-CZ-NH2	10.97	129.07	119.20
1	A	388	ASN	OD1-CG-ND2	10.90	133.50	122.60
1	A	321	ARG	CD-NE-CZ	10.77	139.47	124.40
1	A	232	LEU	O-C-N	10.69	133.64	122.09
1	A	110	ARG	NE-CZ-NH2	-10.69	109.58	119.20
1	A	296	ARG	NE-CZ-NH1	10.62	132.12	121.50
1	A	341	ASN	OD1-CG-ND2	10.61	133.21	122.60
1	A	250	LYS	O-C-N	-10.61	110.12	122.32
1	A	372	TYR	O-C-N	-10.61	111.13	123.22
1	A	335	LYS	CA-C-O	-10.59	109.32	120.55
1	A	163	THR	CA-CB-OG1	-10.58	93.73	109.60
1	A	105	GLY	O-C-N	10.57	132.33	122.18
1	A	393	ALA	N-CA-CB	10.53	125.28	110.01
1	A	310	GLU	O-C-N	-10.52	111.23	122.07
1	A	105	GLY	CA-C-O	-10.50	109.66	121.00
1	A	157	THR	CA-CB-OG1	-10.32	94.13	109.60
1	A	248	TYR	O-C-N	10.28	134.49	122.25
1	A	148	GLN	CG-CD-NE2	10.27	131.81	116.40
1	A	232	LEU	CA-C-O	-10.16	110.24	120.70
1	A	106	THR	O-C-N	10.13	132.63	122.09
1	A	362	VAL	CA-C-N	10.10	133.57	120.44
1	A	362	VAL	C-N-CA	10.10	133.57	120.44
1	A	28	SER	CA-C-N	10.10	139.21	122.54
1	A	28	SER	C-N-CA	10.10	139.21	122.54
1	A	242	VAL	CA-CB-CG1	10.10	127.56	110.40
1	A	172	ILE	CA-C-O	-10.09	110.54	119.62
1	A	355	THR	CA-C-O	-10.03	109.92	120.55
1	A	261	ALA	CA-C-O	-10.00	109.78	120.99
1	A	13	ASP	O-C-N	-9.96	111.04	121.30
1	A	271	GLU	CB-CG-CD	9.94	129.50	112.60
1	A	293	ASN	CA-C-N	9.91	130.94	119.94
1	A	293	ASN	C-N-CA	9.91	130.94	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ARG	NE-CZ-NH1	-9.91	111.59	121.50
1	A	122	PHE	CA-C-O	-9.86	107.35	119.28
1	A	149	ALA	CA-C-O	-9.84	109.65	121.06
1	A	342	TRP	O-C-N	9.84	134.10	122.19
1	A	49	ASN	OD1-CG-ND2	9.70	132.30	122.60
1	A	20	GLU	CA-CB-CG	9.68	133.47	114.10
1	A	162	PHE	CA-C-O	-9.68	110.65	120.82
1	A	15	ILE	CA-C-N	9.68	133.24	120.28
1	A	15	ILE	C-N-CA	9.68	133.24	120.28
1	A	40	ASP	O-C-N	-9.64	109.12	121.74
1	A	35	VAL	CA-C-O	9.61	131.48	121.59
1	A	100	VAL	N-CA-CB	-9.60	97.50	111.52
1	A	210	LEU	N-CA-CB	9.59	125.50	109.87
1	A	143	ALA	CA-C-N	9.49	134.81	122.00
1	A	143	ALA	C-N-CA	9.49	134.81	122.00
1	A	393	ALA	CA-C-O	-9.48	110.86	120.82
1	A	314	GLU	CA-C-O	-9.43	109.45	120.10
1	A	347	ASP	CA-C-O	-9.41	110.44	120.42
1	A	66	GLU	O-C-N	9.39	133.94	122.86
1	A	136	HIS	N-CA-CB	9.36	123.87	110.12
1	A	185	HIS	CA-C-N	9.34	138.81	122.28
1	A	185	HIS	C-N-CA	9.34	138.81	122.28
1	A	81	ALA	N-CA-C	-9.31	99.66	111.02
1	A	336	GLU	CA-C-O	9.30	130.82	119.38
1	A	280	LYS	O-C-N	9.30	132.13	122.09
1	A	270	GLU	N-CA-CB	9.28	123.53	110.07
1	A	176	SER	CA-C-N	9.26	134.68	123.19
1	A	176	SER	C-N-CA	9.26	134.68	123.19
1	A	326	ARG	NE-CZ-NH2	9.26	127.54	119.20
1	A	300	LEU	CA-C-N	9.25	132.40	120.56
1	A	300	LEU	C-N-CA	9.25	132.40	120.56
1	A	337	GLY	O-C-N	9.20	134.66	122.70
1	A	245	SER	O-C-N	-9.20	112.55	123.31
1	A	164	GLY	O-C-N	9.19	132.30	122.28
1	A	347	ASP	CA-C-N	9.16	134.58	120.75
1	A	347	ASP	C-N-CA	9.16	134.58	120.75
1	A	339	SER	CB-CA-C	-9.14	93.75	109.65
1	A	188	THR	N-CA-CB	-9.12	96.14	110.28
1	A	225	ILE	N-CA-C	9.05	119.04	110.53
1	A	268	ASP	N-CA-CB	-9.03	96.23	111.31
1	A	289	ASN	CB-CA-C	9.02	123.94	109.97
1	A	292	MET	N-CA-C	9.00	122.26	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	GLU	CA-C-O	-8.99	110.89	120.42
1	A	139	ILE	N-CA-CB	8.97	121.05	110.55
1	A	236	ILE	O-C-N	8.96	131.06	121.83
1	A	48	LEU	CA-C-O	8.88	130.96	121.19
1	A	58	ILE	CA-C-O	8.87	130.25	120.85
1	A	74	ALA	N-CA-C	8.85	122.04	111.33
1	A	313	VAL	CB-CA-C	8.85	123.62	112.02
1	A	172	ILE	N-CA-C	-8.83	100.81	109.02
1	A	276	GLU	CG-CD-OE1	-8.82	98.11	118.40
1	A	27	ASN	OD1-CG-ND2	8.80	131.40	122.60
1	A	85	LEU	N-CA-C	8.80	123.32	112.23
1	A	96	ARG	CB-CG-CD	8.78	131.49	111.30
1	A	274	ARG	CA-C-O	-8.74	109.48	119.79
1	A	339	SER	O-C-N	8.69	133.80	122.42
1	A	387	SER	CA-C-O	-8.64	108.90	119.18
1	A	378	ARG	CA-C-O	-8.62	110.90	120.81
1	A	328	GLN	CG-CD-NE2	-8.57	103.54	116.40
1	A	393	ALA	O-C-N	8.57	130.89	122.07
1	A	168	ASP	CA-C-O	-8.56	111.83	120.82
1	A	142	ASP	CA-CB-CG	8.56	121.16	112.60
1	A	385	ALA	CA-C-N	8.55	132.10	120.38
1	A	385	ALA	C-N-CA	8.55	132.10	120.38
1	A	332	ASN	O-C-N	8.55	133.79	122.33
1	A	280	LYS	CG-CD-CE	8.55	130.96	111.30
1	A	97	TYR	CA-C-O	-8.52	111.47	121.44
1	A	191	ASP	CA-CB-CG	8.52	121.12	112.60
1	A	218	GLN	OE1-CD-NE2	-8.48	114.12	122.60
1	A	185	HIS	ND1-CE1-NE2	-8.46	99.94	108.40
1	A	168	ASP	O-C-N	8.46	130.78	122.07
1	A	144	GLY	CA-C-O	-8.45	109.22	118.86
1	A	75	ASP	CA-C-N	-8.44	106.14	120.58
1	A	75	ASP	C-N-CA	-8.44	106.14	120.58
1	A	294	GLY	CA-C-N	8.39	131.53	120.28
1	A	294	GLY	C-N-CA	8.39	131.53	120.28
1	A	249	ALA	O-C-N	-8.39	113.43	122.07
1	A	283	ILE	CA-C-O	-8.39	111.74	120.71
1	A	180	LEU	CA-C-O	-8.36	110.56	120.60
1	A	270	GLU	O-C-N	8.36	131.12	122.09
1	A	40	ASP	CA-CB-CG	-8.36	104.24	112.60
1	A	96	ARG	NE-CZ-NH1	8.35	129.85	121.50
1	A	323	ILE	CA-C-O	8.35	130.02	121.17
1	A	378	ARG	CD-NE-CZ	8.35	136.08	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	PRO	CA-C-O	-8.34	107.08	119.34
1	A	174	GLU	CB-CG-CD	8.34	126.78	112.60
1	A	206	LYS	N-CA-CB	-8.33	97.87	110.12
1	A	361	GLN	CA-C-O	-8.31	111.61	120.42
1	A	317	GLY	CA-C-N	8.29	131.72	120.44
1	A	317	GLY	C-N-CA	8.29	131.72	120.44
1	A	116	LEU	O-C-N	-8.29	112.70	122.15
1	A	55	GLU	CB-CA-C	-8.28	97.05	110.79
1	A	351	MET	CG-SD-CE	8.28	119.11	100.90
1	A	169	ILE	N-CA-C	8.27	119.05	110.62
1	A	272	ALA	N-CA-C	-8.23	102.26	111.07
1	A	188	THR	N-CA-C	8.23	121.36	111.82
1	A	304	THR	CA-C-O	8.22	128.15	120.09
1	A	107	GLY	O-C-N	8.22	130.08	122.19
1	A	392	LEU	O-C-N	-8.22	113.54	122.09
1	A	76	PHE	N-CA-C	-8.21	101.59	111.69
1	A	187	PRO	CA-C-N	8.19	132.75	120.31
1	A	187	PRO	C-N-CA	8.19	132.75	120.31
1	A	141	ARG	CA-C-O	-8.17	111.76	120.42
1	A	70	ILE	O-C-N	8.16	130.11	121.87
1	A	103	ILE	CA-C-O	8.16	130.97	120.78
1	A	274	ARG	NE-CZ-NH2	-8.14	111.88	119.20
1	A	164	GLY	CA-C-O	-8.11	111.38	120.30
1	A	296	ARG	CA-CB-CG	8.10	130.29	114.10
1	A	98	VAL	N-CA-CB	8.08	124.56	111.23
1	A	202	SER	CA-C-O	-8.08	112.34	120.82
1	A	66	GLU	CA-C-O	-8.07	112.76	121.56
1	A	282	LEU	CB-CA-C	8.06	124.55	110.85
1	A	25	ASP	CB-CA-C	8.05	123.42	109.65
1	A	386	SER	O-C-N	8.04	130.64	122.12
1	A	279	LEU	CA-C-O	8.04	129.28	119.79
1	A	180	LEU	O-C-N	8.03	133.05	123.33
1	A	186	ASN	OD1-CG-ND2	-8.03	114.57	122.60
1	A	279	LEU	CA-C-N	8.02	131.35	120.44
1	A	279	LEU	C-N-CA	8.02	131.35	120.44
1	A	181	HIS	CA-CB-CG	8.02	121.81	113.80
1	A	311	TRP	CZ3-CH2-CZ2	-8.00	111.10	121.50
1	A	281	ILE	CA-C-N	7.98	131.62	120.29
1	A	281	ILE	C-N-CA	7.98	131.62	120.29
1	A	110	ARG	CA-C-O	-7.97	112.49	120.70
1	A	141	ARG	CD-NE-CZ	7.96	135.55	124.40
1	A	322	ILE	CA-C-O	-7.96	112.67	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	LYS	CG-CD-CE	7.96	129.61	111.30
1	A	389	VAL	N-CA-C	-7.95	102.79	110.42
1	A	153	TYR	CA-CB-CG	7.94	128.19	113.90
1	A	332	ASN	CA-C-O	-7.91	110.45	119.79
1	A	341	ASN	CA-C-O	-7.89	112.14	120.58
1	A	75	ASP	CA-CB-CG	-7.87	104.73	112.60
1	A	68	LEU	CA-C-O	-7.87	112.39	120.96
1	A	364	ARG	NH1-CZ-NH2	7.85	129.51	119.30
1	A	386	SER	CA-C-O	-7.84	112.16	120.63
1	A	175	LYS	CA-C-O	-7.84	111.40	119.78
1	A	330	VAL	CA-C-O	7.83	128.95	120.57
1	A	38	TYR	O-C-N	7.82	132.19	123.04
1	A	185	HIS	CB-CG-CD2	7.82	141.36	131.20
1	A	254	LEU	N-CA-C	-7.81	103.82	112.72
1	A	304	THR	CA-CB-CG2	7.81	123.77	110.50
1	A	209	LEU	O-C-N	7.81	132.08	123.10
1	A	182	ALA	O-C-N	-7.80	113.74	122.08
1	A	308	ARG	CB-CG-CD	-7.79	93.38	111.30
1	A	279	LEU	O-C-N	-7.78	111.90	122.33
1	A	392	LEU	N-CA-CB	-7.78	98.35	109.94
1	A	208	ASN	N-CA-CB	-7.78	100.09	111.91
1	A	285	PRO	CA-C-N	7.78	136.40	121.54
1	A	285	PRO	C-N-CA	7.78	136.40	121.54
1	A	110	ARG	NH1-CZ-NH2	7.77	129.41	119.30
1	A	126	VAL	N-CA-CB	7.77	121.74	111.64
1	A	290	PRO	N-CA-C	7.76	120.17	110.70
1	A	384	VAL	CB-CA-C	7.75	122.58	110.81
1	A	90	GLU	CA-C-N	7.74	130.51	120.44
1	A	90	GLU	C-N-CA	7.74	130.51	120.44
1	A	356	GLY	O-C-N	7.72	131.78	122.60
1	A	209	LEU	CA-C-O	-7.68	112.21	121.28
1	A	335	LYS	CG-CD-CE	7.67	128.95	111.30
1	A	307	LEU	CA-C-N	-7.65	110.03	120.28
1	A	307	LEU	C-N-CA	-7.65	110.03	120.28
1	A	108	SER	CA-C-O	7.65	128.53	120.42
1	A	166	MET	N-CA-C	-7.64	103.42	112.89
1	A	96	ARG	CB-CA-C	-7.63	101.76	111.22
1	A	166	MET	CB-CG-SD	-7.61	89.87	112.70
1	A	171	LYS	CA-C-O	-7.61	110.27	119.32
1	A	84	ALA	CA-C-N	7.59	133.58	120.68
1	A	84	ALA	C-N-CA	7.59	133.58	120.68
1	A	86	GLY	N-CA-C	-7.58	103.31	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ARG	NE-CZ-NH1	7.58	129.08	121.50
1	A	176	SER	O-C-N	-7.58	112.15	122.23
1	A	217	TYR	CA-C-N	7.55	135.95	121.54
1	A	217	TYR	C-N-CA	7.55	135.95	121.54
1	A	45	PRO	O-C-N	7.53	131.67	123.01
1	A	217	TYR	CA-C-O	-7.50	110.87	119.95
1	A	360	GLU	CB-CG-CD	7.50	125.35	112.60
1	A	326	ARG	CA-C-N	7.50	135.86	121.54
1	A	326	ARG	C-N-CA	7.50	135.86	121.54
1	A	165	ALA	N-CA-CB	7.49	120.94	110.07
1	A	381	VAL	CA-C-N	7.46	130.27	120.28
1	A	381	VAL	C-N-CA	7.46	130.27	120.28
1	A	118	ARG	CD-NE-CZ	7.46	134.84	124.40
1	A	146	GLN	OE1-CD-NE2	7.43	130.03	122.60
1	A	12	PRO	CA-C-N	-7.42	110.08	120.39
1	A	12	PRO	C-N-CA	-7.42	110.08	120.39
1	A	370	SER	O-C-N	7.42	132.35	122.41
1	A	69	PRO	N-CA-CB	7.40	110.35	103.39
1	A	20	GLU	CG-CD-OE2	7.40	135.42	118.40
1	A	25	ASP	CA-C-O	-7.40	112.88	121.16
1	A	363	GLU	CA-C-O	-7.40	113.05	120.82
1	A	114	ASN	CA-CB-CG	7.39	119.99	112.60
1	A	92	PHE	CA-CB-CG	-7.37	106.43	113.80
1	A	224	ASP	CB-CG-OD1	7.37	135.35	118.40
1	A	307	LEU	CB-CA-C	7.36	124.03	110.11
1	A	201	ALA	CA-C-N	7.34	129.98	120.44
1	A	201	ALA	C-N-CA	7.34	129.98	120.44
1	A	337	GLY	CA-C-O	-7.33	107.82	120.57
1	A	380	SER	CA-C-O	7.29	128.72	120.84
1	A	349	ILE	CA-C-O	-7.28	114.03	121.67
1	A	373	MET	N-CA-C	-7.24	98.17	108.96
1	A	339	SER	CA-CB-OG	-7.23	96.64	111.10
1	A	166	MET	CA-C-N	-7.21	110.64	120.44
1	A	166	MET	C-N-CA	-7.21	110.64	120.44
1	A	233	ARG	CA-C-N	-7.20	109.37	120.31
1	A	233	ARG	C-N-CA	-7.20	109.37	120.31
1	A	327	THR	CA-CB-CG2	7.19	122.73	110.50
1	A	272	ALA	N-CA-CB	7.19	120.44	110.01
1	A	92	PHE	O-C-N	-7.15	114.60	122.03
1	A	130	LYS	CA-CB-CG	-7.15	99.81	114.10
1	A	236	ILE	CB-CG1-CD1	-7.14	98.80	113.80
1	A	182	ALA	CA-C-N	7.11	135.28	121.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ALA	C-N-CA	7.11	135.28	121.63
1	A	273	LYS	CA-C-O	-7.10	113.02	120.55
1	A	268	ASP	CA-C-O	-7.09	113.53	121.40
1	A	117	GLN	OE1-CD-NE2	-7.09	115.51	122.60
1	A	302	LEU	CA-C-O	7.08	128.48	120.90
1	A	355	THR	N-CA-C	7.08	119.00	111.28
1	A	188	THR	CA-C-O	7.06	128.09	119.97
1	A	150	TYR	N-CA-C	-7.05	98.36	109.50
1	A	65	LYS	CB-CA-C	-7.05	100.19	111.18
1	A	315	VAL	CA-C-O	7.05	128.32	120.85
1	A	285	PRO	N-CA-CB	7.03	110.83	102.60
1	A	55	GLU	CG-CD-OE2	-7.02	102.25	118.40
1	A	388	ASN	CB-CG-ND2	-7.01	105.89	116.40
1	A	63	MET	CA-C-O	7.00	129.52	121.47
1	A	137	THR	CA-C-O	6.97	125.71	119.08
1	A	308	ARG	CB-CA-C	6.94	122.31	110.79
1	A	379	ILE	CA-CB-CG2	6.94	122.30	110.50
1	A	311	TRP	CE3-CZ3-CH2	6.93	130.11	121.10
1	A	49	ASN	CA-CB-CG	-6.92	105.68	112.60
1	A	251	ASN	CB-CA-C	6.92	123.96	110.67
1	A	143	ALA	CA-C-O	6.92	127.89	119.38
1	A	159	SER	N-CA-CB	6.90	122.14	111.24
1	A	282	LEU	N-CA-CB	-6.89	99.96	110.16
1	A	171	LYS	O-C-N	6.89	130.57	122.24
1	A	115	PHE	CA-CB-CG	-6.88	106.92	113.80
1	A	55	GLU	CB-CG-CD	6.88	124.30	112.60
1	A	194	GLN	N-CA-CB	-6.88	98.87	110.49
1	A	290	PRO	N-CA-CB	-6.86	96.42	103.08
1	A	195	GLU	N-CA-CB	6.86	119.96	110.01
1	A	154	ASP	O-C-N	6.86	129.43	121.47
1	A	195	GLU	N-CA-C	-6.85	103.74	111.07
1	A	396	ILE	CA-CB-CG1	6.84	122.02	110.40
1	A	17	GLY	N-CA-C	-6.82	105.25	113.99
1	A	398	GLN	O-C-N	-6.82	115.04	122.07
1	A	242	VAL	O-C-N	6.82	129.03	122.69
1	A	243	VAL	N-CA-C	-6.82	98.36	108.99
1	A	156	LYS	N-CA-CB	6.81	120.84	110.28
1	A	235	PHE	CA-C-O	6.81	127.97	120.82
1	A	235	PHE	N-CA-C	6.81	118.36	111.07
1	A	364	ARG	CB-CA-C	-6.81	96.50	110.38
1	A	181	HIS	CA-C-N	6.80	130.24	120.79
1	A	181	HIS	C-N-CA	6.80	130.24	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	ILE	N-CA-CB	6.80	118.97	110.47
1	A	268	ASP	O-C-N	6.79	131.81	122.78
1	A	143	ALA	O-C-N	-6.79	113.33	122.43
1	A	19	THR	CA-CB-OG1	-6.78	99.43	109.60
1	A	388	ASN	CA-CB-CG	-6.77	105.83	112.60
1	A	314	GLU	CG-CD-OE2	6.76	133.96	118.40
1	A	77	THR	N-CA-CB	-6.76	99.87	109.94
1	A	73	LEU	CA-C-O	-6.75	112.75	120.58
1	A	177	ILE	CA-CB-CG2	6.74	121.96	110.50
1	A	5	SER	CA-C-N	6.73	131.97	120.72
1	A	5	SER	C-N-CA	6.73	131.97	120.72
1	A	299	SER	CA-CB-OG	6.73	124.57	111.10
1	A	356	GLY	CA-C-O	-6.73	111.53	119.07
1	A	303	ASN	CB-CG-ND2	-6.72	106.33	116.40
1	A	323	ILE	N-CA-C	6.70	116.85	110.42
1	A	257	GLU	CG-CD-OE2	-6.70	103.00	118.40
1	A	284	ARG	CA-C-N	6.70	127.66	120.83
1	A	284	ARG	C-N-CA	6.70	127.66	120.83
1	A	314	GLU	CA-C-N	6.69	129.92	120.42
1	A	314	GLU	C-N-CA	6.69	129.92	120.42
1	A	392	LEU	CB-CA-C	6.66	121.47	110.81
1	A	25	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	308	ARG	CG-CD-NE	-6.66	97.36	112.00
1	A	193	ARG	CA-C-O	-6.65	113.82	121.47
1	A	156	LYS	O-C-N	6.65	130.44	122.27
1	A	96	ARG	CA-CB-CG	6.64	127.39	114.10
1	A	233	ARG	CB-CG-CD	-6.63	96.06	111.30
1	A	359	PRO	N-CA-C	6.63	122.45	113.84
1	A	87	GLU	O-C-N	-6.62	114.12	122.27
1	A	321	ARG	CB-CG-CD	6.62	126.53	111.30
1	A	73	LEU	N-CA-CB	-6.62	99.52	109.71
1	A	125	ASP	OD1-CG-OD2	-6.61	107.05	122.90
1	A	343	GLN	OE1-CD-NE2	6.61	129.21	122.60
1	A	293	ASN	N-CA-C	6.60	118.14	111.07
1	A	231	ALA	CA-C-O	-6.59	113.90	120.82
1	A	349	ILE	CB-CG1-CD1	6.59	127.64	113.80
1	A	229	ALA	N-CA-CB	-6.59	100.94	110.56
1	A	149	ALA	CA-C-N	-6.59	112.35	122.62
1	A	149	ALA	C-N-CA	-6.59	112.35	122.62
1	A	141	ARG	NE-CZ-NH1	6.58	128.08	121.50
1	A	331	SER	CA-CB-OG	6.58	124.27	111.10
1	A	379	ILE	N-CA-CB	6.58	123.49	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	LEU	N-CA-C	-6.57	99.19	109.25
1	A	376	ASP	N-CA-CB	6.57	120.49	110.44
1	A	17	GLY	CA-C-O	-6.56	111.90	119.65
1	A	46	TYR	CB-CA-C	6.56	121.05	110.16
1	A	239	GLY	O-C-N	6.55	129.89	122.55
1	A	331	SER	O-C-N	6.55	129.62	122.15
1	A	49	ASN	CA-C-O	-6.55	113.89	120.90
1	A	115	PHE	CB-CA-C	6.54	121.23	110.90
1	A	374	THR	O-C-N	-6.53	115.59	122.96
1	A	246	GLN	CA-C-N	6.52	132.72	122.94
1	A	246	GLN	C-N-CA	6.52	132.72	122.94
1	A	308	ARG	O-C-N	-6.51	115.22	122.12
1	A	87	GLU	CG-CD-OE2	6.51	133.37	118.40
1	A	218	GLN	O-C-N	6.50	131.24	122.59
1	A	315	VAL	CA-C-N	6.50	129.52	120.29
1	A	315	VAL	C-N-CA	6.50	129.52	120.29
1	A	115	PHE	CA-C-N	-6.49	111.07	120.29
1	A	115	PHE	C-N-CA	-6.49	111.07	120.29
1	A	222	SER	CA-C-O	6.48	126.14	118.69
1	A	26	THR	CA-C-N	6.48	130.61	121.02
1	A	26	THR	C-N-CA	6.48	130.61	121.02
1	A	110	ARG	CB-CG-CD	-6.47	96.41	111.30
1	A	186	ASN	CB-CG-ND2	6.47	126.11	116.40
1	A	372	TYR	CA-C-N	6.46	132.47	121.87
1	A	372	TYR	C-N-CA	6.46	132.47	121.87
1	A	96	ARG	O-C-N	-6.45	112.43	121.72
1	A	245	SER	CA-CB-OG	-6.44	98.21	111.10
1	A	340	HIS	CA-CB-CG	-6.44	107.36	113.80
1	A	325	MET	CA-CB-CG	6.44	126.98	114.10
1	A	154	ASP	CA-CB-CG	-6.41	106.19	112.60
1	A	302	LEU	O-C-N	-6.41	115.42	122.09
1	A	313	VAL	N-CA-C	-6.41	104.51	110.53
1	A	193	ARG	CD-NE-CZ	-6.39	115.45	124.40
1	A	318	MET	CA-C-O	-6.39	114.11	120.70
1	A	197	TRP	N-CA-CB	6.39	119.51	110.12
1	A	38	TYR	N-CA-C	6.38	119.91	109.76
1	A	245	SER	CA-C-N	6.38	132.51	122.94
1	A	245	SER	C-N-CA	6.38	132.51	122.94
1	A	158	CYS	N-CA-CB	6.38	121.27	110.49
1	A	296	ARG	CG-CD-NE	6.38	126.03	112.00
1	A	82	GLU	CG-CD-OE2	-6.37	103.74	118.40
1	A	214	ASP	CB-CA-C	6.37	120.64	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASN	CA-C-O	-6.37	113.38	120.70
1	A	39	ARG	CA-C-O	-6.36	113.92	121.11
1	A	361	GLN	N-CA-C	-6.36	104.42	111.36
1	A	337	GLY	CA-C-N	-6.35	110.97	120.94
1	A	337	GLY	C-N-CA	-6.35	110.97	120.94
1	A	294	GLY	O-C-N	6.35	128.27	122.18
1	A	346	THR	CA-CB-OG1	-6.35	100.08	109.60
1	A	336	GLU	CG-CD-OE1	-6.34	103.82	118.40
1	A	227	ARG	CA-C-O	6.33	127.25	120.10
1	A	248	TYR	CA-C-O	-6.33	112.12	119.59
1	A	379	ILE	CB-CG1-CD1	-6.33	100.51	113.80
1	A	91	ALA	O-C-N	-6.33	115.55	122.07
1	A	136	HIS	O-C-N	6.33	128.82	122.12
1	A	231	ALA	O-C-N	6.31	128.57	122.07
1	A	271	GLU	CA-CB-CG	6.31	126.73	114.10
1	A	106	THR	CA-CB-OG1	-6.31	100.13	109.60
1	A	180	LEU	N-CA-C	-6.31	98.33	109.06
1	A	376	ASP	OD1-CG-OD2	6.31	138.04	122.90
1	A	130	LYS	CG-CD-CE	-6.30	96.81	111.30
1	A	314	GLU	CG-CD-OE1	-6.29	103.93	118.40
1	A	89	SER	CA-C-O	6.28	127.81	120.96
1	A	328	GLN	CA-C-O	-6.28	113.16	120.20
1	A	235	PHE	O-C-N	6.27	128.52	122.07
1	A	277	SER	CA-C-O	6.26	127.39	120.82
1	A	268	ASP	N-CA-C	-6.26	100.04	108.86
1	A	125	ASP	O-C-N	6.25	130.35	123.22
1	A	156	LYS	CB-CG-CD	-6.25	96.92	111.30
1	A	359	PRO	N-CD-CG	-6.25	93.83	103.20
1	A	400	THR	OG1-CB-CG2	6.25	121.79	109.30
1	A	156	LYS	CA-CB-CG	-6.22	101.66	114.10
1	A	276	GLU	CA-C-N	6.21	128.52	120.44
1	A	276	GLU	C-N-CA	6.21	128.52	120.44
1	A	200	LEU	N-CA-C	-6.20	104.52	111.28
1	A	230	TRP	CB-CA-C	-6.19	101.07	110.92
1	A	269	ALA	CA-C-N	6.19	128.85	120.44
1	A	269	ALA	C-N-CA	6.19	128.85	120.44
1	A	401	LYS	CB-CA-C	-6.18	98.35	110.10
1	A	129	PRO	CA-C-N	6.18	133.47	122.35
1	A	129	PRO	C-N-CA	6.18	133.47	122.35
1	A	103	ILE	CA-CB-CG1	-6.17	99.92	110.40
1	A	376	ASP	CA-C-N	6.16	132.69	121.85
1	A	376	ASP	C-N-CA	6.16	132.69	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	LEU	N-CA-C	-6.16	102.11	110.36
1	A	305	PRO	CA-C-N	6.16	131.91	121.14
1	A	305	PRO	C-N-CA	6.16	131.91	121.14
1	A	323	ILE	CB-CG1-CD1	-6.16	100.87	113.80
1	A	240	ILE	CA-CB-CG2	6.14	120.93	110.50
1	A	376	ASP	CB-CG-OD2	-6.13	104.30	118.40
1	A	197	TRP	O-C-N	6.12	128.60	122.12
1	A	224	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	32	ASN	CA-CB-CG	-6.10	106.50	112.60
1	A	109	LEU	CB-CA-C	6.09	120.56	110.81
1	A	124	ARG	CA-C-O	-6.09	111.99	119.18
1	A	75	ASP	O-C-N	6.09	129.76	122.27
1	A	161	ASP	CA-C-N	6.08	128.34	120.44
1	A	161	ASP	C-N-CA	6.08	128.34	120.44
1	A	352	PHE	N-CA-C	6.07	118.44	109.69
1	A	28	SER	O-C-N	-6.07	114.09	122.46
1	A	395	ALA	CB-CA-C	6.07	120.48	110.90
1	A	208	ASN	CB-CA-C	6.05	119.97	111.86
1	A	264	VAL	CA-CB-CG1	6.04	120.67	110.40
1	A	308	ARG	CA-C-N	6.04	128.29	120.44
1	A	308	ARG	C-N-CA	6.04	128.29	120.44
1	A	293	ASN	CB-CA-C	6.01	120.31	110.88
1	A	254	LEU	CA-C-O	-6.00	112.63	119.78
1	A	100	VAL	CA-C-O	-6.00	114.00	120.36
1	A	220	PHE	O-C-N	6.00	130.28	122.42
1	A	74	ALA	CA-C-N	5.99	129.42	120.31
1	A	74	ALA	C-N-CA	5.99	129.42	120.31
1	A	202	SER	CA-CB-OG	-5.98	99.13	111.10
1	A	271	GLU	CA-C-N	5.98	128.22	120.44
1	A	271	GLU	C-N-CA	5.98	128.22	120.44
1	A	150	TYR	CB-CA-C	5.98	121.88	109.38
1	A	330	VAL	CA-C-N	5.98	128.78	120.29
1	A	330	VAL	C-N-CA	5.98	128.78	120.29
1	A	137	THR	CA-CB-OG1	-5.97	100.64	109.60
1	A	97	TYR	CA-C-N	5.97	132.72	121.97
1	A	97	TYR	C-N-CA	5.97	132.72	121.97
1	A	106	THR	CA-C-O	-5.97	114.51	120.90
1	A	332	ASN	N-CA-C	-5.97	104.71	112.23
1	A	348	GLN	CA-C-O	-5.97	115.23	121.55
1	A	355	THR	CA-CB-OG1	-5.96	100.66	109.60
1	A	17	GLY	CA-C-N	5.95	130.06	120.30
1	A	17	GLY	C-N-CA	5.95	130.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	LYS	CA-C-O	-5.95	113.13	119.97
1	A	282	LEU	CA-C-N	5.94	130.06	120.55
1	A	282	LEU	C-N-CA	5.94	130.06	120.55
1	A	27	ASN	CA-CB-CG	5.94	118.54	112.60
1	A	355	THR	O-C-N	5.94	128.42	122.12
1	A	45	PRO	CB-CA-C	5.94	119.12	111.64
1	A	274	ARG	N-CA-CB	5.92	119.42	110.30
1	A	265	ILE	CA-CB-CG2	5.91	120.55	110.50
1	A	379	ILE	N-CA-C	-5.91	99.20	108.95
1	A	375	LYS	N-CA-CB	5.91	120.81	110.42
1	A	166	MET	N-CA-CB	5.89	120.01	110.40
1	A	265	ILE	CA-C-O	5.88	127.53	120.65
1	A	135	ASN	CB-CA-C	5.88	122.60	110.31
1	A	267	ARG	NE-CZ-NH2	-5.87	113.91	119.20
1	A	238	GLN	N-CA-C	-5.87	106.08	113.18
1	A	75	ASP	OD1-CG-OD2	5.86	136.97	122.90
1	A	42	ASN	N-CA-C	-5.86	104.63	113.89
1	A	155	PRO	N-CA-C	-5.86	105.89	113.57
1	A	201	ALA	N-CA-CB	5.86	118.67	109.94
1	A	253	GLY	CA-C-N	5.83	132.12	122.73
1	A	253	GLY	C-N-CA	5.83	132.12	122.73
1	A	215	MET	CB-CA-C	-5.82	103.76	112.09
1	A	118	ARG	CA-C-O	-5.82	114.71	120.70
1	A	62	LYS	CA-C-O	-5.81	114.76	122.03
1	A	242	VAL	N-CA-CB	-5.81	105.71	112.34
1	A	352	PHE	CA-C-O	5.81	128.63	121.60
1	A	263	THR	N-CA-C	5.81	118.87	109.40
1	A	142	ASP	CA-C-O	5.80	126.64	119.97
1	A	389	VAL	CA-C-N	5.79	126.37	119.94
1	A	389	VAL	C-N-CA	5.79	126.37	119.94
1	A	139	ILE	CB-CA-C	-5.79	104.56	111.97
1	A	7	VAL	CA-C-O	5.79	127.98	120.69
1	A	196	GLN	OE1-CD-NE2	5.78	128.38	122.60
1	A	266	CYS	CA-C-O	5.78	129.53	121.73
1	A	157	THR	CA-C-N	5.77	132.56	121.54
1	A	157	THR	C-N-CA	5.77	132.56	121.54
1	A	39	ARG	O-C-N	5.76	130.68	123.19
1	A	47	VAL	N-CA-CB	5.75	118.60	111.41
1	A	167	GLU	CB-CG-CD	5.75	122.37	112.60
1	A	310	GLU	CA-C-O	5.74	126.85	120.82
1	A	399	VAL	N-CA-CB	-5.74	97.68	111.23
1	A	350	GLY	N-CA-C	-5.74	104.66	112.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	HIS	N-CA-C	-5.73	101.82	110.24
1	A	316	LYS	CB-CG-CD	-5.73	98.12	111.30
1	A	150	TYR	CA-C-O	-5.70	114.44	121.11
1	A	5	SER	O-C-N	-5.69	115.27	122.27
1	A	338	SER	N-CA-CB	5.69	118.36	110.17
1	A	42	ASN	O-C-N	5.68	128.43	122.23
1	A	148	GLN	CA-C-N	-5.66	112.94	122.29
1	A	148	GLN	C-N-CA	-5.66	112.94	122.29
1	A	4	TRP	N-CA-C	5.65	118.96	112.57
1	A	189	GLY	CA-C-N	5.65	130.62	123.10
1	A	189	GLY	C-N-CA	5.65	130.62	123.10
1	A	44	LYS	N-CA-CB	-5.65	100.78	110.72
1	A	192	PRO	O-C-N	-5.65	115.81	122.99
1	A	291	PRO	O-C-N	-5.65	115.01	122.64
1	A	27	ASN	N-CA-CB	5.64	118.43	109.51
1	A	125	ASP	CB-CG-OD2	5.64	131.38	118.40
1	A	361	GLN	N-CA-CB	5.64	118.51	110.16
1	A	113	ALA	CA-C-O	5.64	126.53	120.55
1	A	172	ILE	CB-CG1-CD1	-5.64	101.96	113.80
1	A	63	MET	N-CA-C	5.64	118.82	110.48
1	A	212	TYR	CB-CG-CD2	-5.64	112.35	120.80
1	A	204	VAL	CA-CB-CG1	5.63	119.98	110.40
1	A	2	SER	CA-C-O	-5.63	114.56	121.88
1	A	368	GLU	CB-CA-C	-5.62	98.91	110.38
1	A	166	MET	CG-SD-CE	-5.61	88.56	100.90
1	A	53	LYS	N-CA-CB	5.61	118.97	110.28
1	A	45	PRO	N-CA-CB	5.61	108.32	103.27
1	A	1	SER	O-C-N	5.60	131.96	123.00
1	A	264	VAL	CA-C-O	-5.60	114.51	120.39
1	A	293	ASN	CB-CG-ND2	5.60	124.80	116.40
1	A	332	ASN	CA-C-N	-5.59	113.17	120.44
1	A	332	ASN	C-N-CA	-5.59	113.17	120.44
1	A	30	LYS	N-CA-CB	-5.59	102.13	110.17
1	A	110	ARG	O-C-N	5.59	128.12	122.09
1	A	287	TYR	N-CA-C	-5.58	104.30	113.50
1	A	109	LEU	CA-CB-CG	5.57	135.80	116.30
1	A	326	ARG	NH1-CZ-NH2	-5.57	112.06	119.30
1	A	54	ALA	CA-C-N	5.57	127.74	120.28
1	A	54	ALA	C-N-CA	5.57	127.74	120.28
1	A	247	SER	N-CA-CB	5.57	120.52	110.83
1	A	398	GLN	CA-C-O	5.57	126.67	120.82
1	A	84	ALA	O-C-N	-5.56	116.09	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	HIS	CA-CB-CG	5.54	119.34	113.80
1	A	289	ASN	CB-CG-OD1	-5.54	109.72	120.80
1	A	243	VAL	CA-C-N	-5.54	112.17	121.75
1	A	243	VAL	C-N-CA	-5.54	112.17	121.75
1	A	224	ASP	O-C-N	5.53	129.74	123.27
1	A	120	PHE	N-CA-CB	5.52	118.03	110.57
1	A	208	ASN	CA-CB-CG	-5.52	107.08	112.60
1	A	117	GLN	CA-C-N	5.51	127.94	120.44
1	A	117	GLN	C-N-CA	5.51	127.94	120.44
1	A	366	THR	CA-C-N	5.51	127.94	120.44
1	A	366	THR	C-N-CA	5.51	127.94	120.44
1	A	299	SER	CB-CA-C	5.51	119.45	110.96
1	A	340	HIS	CA-C-N	5.50	129.74	122.42
1	A	340	HIS	C-N-CA	5.50	129.74	122.42
1	A	114	ASN	CA-C-N	5.50	127.92	120.44
1	A	114	ASN	C-N-CA	5.50	127.92	120.44
1	A	282	LEU	O-C-N	-5.50	115.89	122.15
1	A	378	ARG	CA-C-N	-5.50	114.00	122.68
1	A	378	ARG	C-N-CA	-5.50	114.00	122.68
1	A	187	PRO	N-CA-CB	-5.49	96.56	102.60
1	A	345	ILE	O-C-N	5.49	127.89	121.96
1	A	151	ARG	NH1-CZ-NH2	-5.49	112.17	119.30
1	A	259	ALA	O-C-N	5.49	129.83	123.30
1	A	299	SER	CA-C-N	5.48	127.89	120.38
1	A	299	SER	C-N-CA	5.48	127.89	120.38
1	A	174	GLU	CA-CB-CG	5.47	125.05	114.10
1	A	238	GLN	CA-C-O	5.47	126.12	119.11
1	A	271	GLU	CG-CD-OE1	5.47	130.98	118.40
1	A	336	GLU	CA-C-N	5.47	132.13	121.41
1	A	336	GLU	C-N-CA	5.47	132.13	121.41
1	A	369	PHE	CA-C-O	-5.46	112.89	118.90
1	A	24	ARG	CB-CA-C	-5.46	99.03	110.17
1	A	278	GLN	OE1-CD-NE2	5.45	128.05	122.60
1	A	301	ILE	CA-C-N	5.45	127.90	120.54
1	A	301	ILE	C-N-CA	5.45	127.90	120.54
1	A	241	ASP	CB-CG-OD2	-5.45	105.87	118.40
1	A	309	LYS	CG-CD-CE	5.45	123.83	111.30
1	A	126	VAL	O-C-N	5.45	128.97	123.20
1	A	298	ALA	O-C-N	5.44	127.68	122.07
1	A	306	GLU	CB-CA-C	-5.43	98.64	109.99
1	A	364	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	A	115	PHE	N-CA-C	-5.43	105.28	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	GLU	CG-CD-OE2	5.42	130.88	118.40
1	A	60	ALA	O-C-N	5.42	127.87	122.12
1	A	92	PHE	CA-C-O	5.42	126.69	121.00
1	A	187	PRO	N-CA-C	5.42	126.19	112.10
1	A	330	VAL	O-C-N	-5.42	116.40	121.87
1	A	249	ALA	N-CA-C	5.41	116.86	111.07
1	A	219	GLY	CA-C-O	-5.41	113.00	119.01
1	A	65	LYS	O-C-N	5.41	129.44	122.19
1	A	289	ASN	CA-C-N	5.41	125.95	120.38
1	A	289	ASN	C-N-CA	5.41	125.95	120.38
1	A	343	GLN	CA-CB-CG	-5.41	103.29	114.10
1	A	106	THR	N-CA-CB	5.40	117.99	109.94
1	A	134	GLY	O-C-N	-5.40	116.63	122.19
1	A	326	ARG	N-CA-C	-5.40	105.08	110.97
1	A	39	ARG	CG-CD-NE	5.40	123.88	112.00
1	A	27	ASN	O-C-N	5.39	130.18	123.01
1	A	398	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	42	ASN	OD1-CG-ND2	5.39	127.99	122.60
1	A	274	ARG	O-C-N	5.39	129.55	122.33
1	A	177	ILE	CA-C-O	-5.38	114.78	120.48
1	A	24	ARG	N-CA-C	5.38	119.47	113.01
1	A	66	GLU	CG-CD-OE1	-5.37	106.06	118.40
1	A	77	THR	CA-C-N	5.37	127.91	120.29
1	A	77	THR	C-N-CA	5.37	127.91	120.29
1	A	364	ARG	NE-CZ-NH2	-5.36	114.37	119.20
1	A	399	VAL	CA-C-N	5.36	131.58	122.36
1	A	399	VAL	C-N-CA	5.36	131.58	122.36
1	A	148	GLN	O-C-N	5.36	129.91	122.78
1	A	191	ASP	CA-C-O	-5.36	113.95	120.54
1	A	184	ALA	CA-C-O	5.36	128.72	122.03
1	A	189	GLY	O-C-N	-5.36	116.20	122.31
1	A	397	HIS	CA-CB-CG	-5.36	108.44	113.80
1	A	267	ARG	N-CA-C	5.35	118.28	111.69
1	A	30	LYS	CB-CA-C	5.35	119.39	109.54
1	A	298	ALA	N-CA-CB	5.35	117.77	110.01
1	A	320	ASP	CA-C-O	5.35	126.44	120.82
1	A	264	VAL	CA-C-N	5.34	129.05	122.37
1	A	264	VAL	C-N-CA	5.34	129.05	122.37
1	A	230	TRP	CA-C-N	5.34	127.39	120.44
1	A	230	TRP	C-N-CA	5.34	127.39	120.44
1	A	18	VAL	CA-C-O	-5.34	114.70	120.47
1	A	188	THR	CA-CB-CG2	5.34	119.58	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ALA	O-C-N	5.34	127.58	122.03
1	A	257	GLU	N-CA-C	-5.34	106.61	113.23
1	A	141	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	A	313	VAL	CA-CB-CG1	5.33	119.47	110.40
1	A	69	PRO	N-CA-C	-5.33	103.09	111.34
1	A	98	VAL	CA-C-O	5.32	127.43	120.78
1	A	343	GLN	CB-CA-C	5.32	121.56	110.32
1	A	140	PHE	CA-C-O	-5.32	114.34	120.24
1	A	8	GLU	OE1-CD-OE2	5.31	135.64	122.90
1	A	281	ILE	CA-C-O	5.31	126.47	120.95
1	A	57	MET	CA-C-O	-5.31	113.53	119.79
1	A	117	GLN	CG-CD-NE2	5.30	124.35	116.40
1	A	140	PHE	O-C-N	5.30	129.12	122.23
1	A	299	SER	O-C-N	-5.29	116.53	122.03
1	A	121	LYS	N-CA-C	5.29	119.35	113.01
1	A	301	ILE	CB-CG1-CD1	-5.29	102.70	113.80
1	A	49	ASN	CB-CG-OD1	-5.28	110.23	120.80
1	A	384	VAL	N-CA-C	-5.28	100.88	108.53
1	A	191	ASP	O-C-N	5.27	127.61	121.39
1	A	185	HIS	CE1-NE2-CD2	5.27	114.27	109.00
1	A	343	GLN	N-CA-C	5.27	118.81	112.38
1	A	349	ILE	O-C-N	5.27	128.89	123.04
1	A	276	GLU	CG-CD-OE2	5.27	130.51	118.40
1	A	118	ARG	N-CA-C	5.26	116.82	111.14
1	A	104	SER	CA-C-O	5.25	128.02	120.51
1	A	112	GLY	CA-C-N	5.25	127.32	120.28
1	A	112	GLY	C-N-CA	5.25	127.32	120.28
1	A	64	ASP	N-CA-CB	-5.25	103.12	110.25
1	A	79	ALA	N-CA-CB	5.24	118.41	110.28
1	A	398	GLN	CB-CA-C	5.24	119.11	110.88
1	A	65	LYS	N-CA-CB	-5.24	103.94	111.54
1	A	67	TYR	CA-CB-CG	5.24	123.33	113.90
1	A	70	ILE	CA-C-N	-5.24	112.90	122.38
1	A	70	ILE	C-N-CA	-5.24	112.90	122.38
1	A	333	LEU	CA-C-O	-5.23	115.33	120.82
1	A	248	TYR	N-CA-C	-5.23	106.13	112.88
1	A	284	ARG	NH1-CZ-NH2	-5.23	112.50	119.30
1	A	321	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	A	157	THR	N-CA-C	5.22	119.74	112.90
1	A	24	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	A	310	GLU	CA-CB-CG	-5.21	103.68	114.10
1	A	124	ARG	O-C-N	5.21	128.34	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	LEU	CA-C-O	5.19	125.92	120.42
1	A	233	ARG	N-CA-CB	-5.19	102.24	110.28
1	A	192	PRO	CB-CA-C	-5.19	104.75	111.39
1	A	29	LYS	CA-CB-CG	-5.18	103.73	114.10
1	A	207	ARG	CD-NE-CZ	-5.18	117.14	124.40
1	A	124	ARG	N-CA-CB	5.18	118.52	110.80
1	A	232	LEU	N-CA-C	-5.18	105.55	111.14
1	A	32	ASN	CA-C-N	5.18	131.06	122.73
1	A	32	ASN	C-N-CA	5.18	131.06	122.73
1	A	382	ALA	N-CA-C	-5.18	105.64	111.28
1	A	170	SER	CA-C-O	5.17	125.77	119.05
1	A	106	THR	CA-C-N	5.17	125.72	119.98
1	A	106	THR	C-N-CA	5.17	125.72	119.98
1	A	15	ILE	CB-CG1-CD1	5.17	124.65	113.80
1	A	242	VAL	CG1-CB-CG2	-5.16	99.45	110.80
1	A	322	ILE	N-CA-C	-5.16	105.36	110.62
1	A	60	ALA	CA-C-O	-5.15	115.09	120.55
1	A	217	TYR	N-CA-C	5.15	119.11	112.41
1	A	348	GLN	OE1-CD-NE2	5.15	127.75	122.60
1	A	384	VAL	CA-CB-CG2	5.15	119.16	110.40
1	A	114	ASN	CB-CG-ND2	-5.15	108.68	116.40
1	A	146	GLN	CB-CG-CD	-5.15	103.85	112.60
1	A	388	ASN	N-CA-C	-5.15	105.35	113.02
1	A	4	TRP	N-CA-CB	-5.14	102.79	110.91
1	A	393	ALA	CB-CA-C	-5.14	102.81	110.88
1	A	293	ASN	CA-C-O	-5.14	115.43	120.82
1	A	182	ALA	CB-CA-C	5.13	119.08	110.92
1	A	157	THR	CA-C-O	-5.11	113.62	119.60
1	A	368	GLU	OE1-CD-OE2	5.11	135.17	122.90
1	A	124	ARG	NH1-CZ-NH2	5.09	125.92	119.30
1	A	202	SER	CB-CA-C	-5.09	102.89	110.88
1	A	137	THR	N-CA-C	5.09	119.42	112.55
1	A	36	GLY	CA-C-O	-5.08	111.73	120.57
1	A	65	LYS	CA-CB-CG	-5.08	103.94	114.10
1	A	353	CYS	CA-C-N	5.07	129.11	122.06
1	A	353	CYS	C-N-CA	5.07	129.11	122.06
1	A	146	GLN	CA-C-O	-5.06	115.31	121.28
1	A	268	ASP	CB-CA-C	-5.04	99.54	111.65
1	A	341	ASN	CB-CG-ND2	-5.04	108.83	116.40
1	A	375	LYS	N-CA-C	-5.04	107.19	113.19
1	A	61	LYS	N-CA-CB	-5.04	102.03	110.39
1	A	285	PRO	CA-N-CD	-5.03	104.95	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CA-C-O	-5.03	114.86	120.54
1	A	368	GLU	CA-CB-CG	-5.02	104.06	114.10
1	A	186	ASN	CA-CB-CG	5.01	117.61	112.60
1	A	224	ASP	OD1-CG-OD2	-5.01	110.88	122.90
1	A	86	GLY	CA-C-O	-5.01	117.89	122.24
1	A	75	ASP	CB-CG-OD2	-5.00	106.90	118.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3161	0	3157	147	2
2	A	26	0	13	6	0
3	A	307	0	0	27	6
All	All	3494	0	3170	148	6

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 23.

All (148) 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:19:THR:O	1:A:23:LYS:HG2	1.75	0.86
1:A:396:ILE:O	1:A:400:THR:HB	1.77	0.85
1:A:31:MET:HE3	1:A:371:ILE:HG12	1.61	0.82
1:A:276:GLU:HG3	3:A:678:HOH:O	1.84	0.78
1:A:165:ALA:O	1:A:169:ILE:HG13	1.86	0.76
1:A:31:MET:HE1	1:A:392:LEU:HB2	1.67	0.75
1:A:325:MET:HE2	1:A:328:GLN:NE2	2.04	0.72
1:A:93:LYS:HE2	3:A:552:HOH:O	1.89	0.71
1:A:325:MET:HE3	3:A:727:HOH:O	1.90	0.71
1:A:188:THR:HG23	1:A:190:VAL:HG23	1.73	0.71
1:A:31:MET:HE2	1:A:391:TYR:HD2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:TRP:O	1:A:315:VAL:HG23	1.92	0.69
1:A:157:THR:HG21	3:A:429:HOH:O	1.91	0.69
1:A:361:GLN:HG3	3:A:686:HOH:O	1.92	0.69
1:A:53:LYS:HE3	1:A:310:GLU:OE1	1.92	0.69
1:A:398:GLN:NE2	1:A:401:LYS:HE2	2.10	0.67
1:A:185:HIS:ND1	1:A:188:THR:HB	2.10	0.67
1:A:188:THR:HG22	1:A:190:VAL:H	1.60	0.66
1:A:325:MET:CE	1:A:328:GLN:HE22	2.08	0.66
1:A:87:GLU:O	1:A:93:LYS:HD3	1.96	0.65
1:A:398:GLN:HE22	1:A:401:LYS:HE2	1.62	0.65
1:A:169:ILE:HA	1:A:172:ILE:HD12	1.82	0.62
1:A:75:ASP:OD1	1:A:75:ASP:N	2.33	0.61
1:A:53:LYS:NZ	3:A:698:HOH:O	2.24	0.61
1:A:57:MET:O	1:A:61:LYS:HB2	2.01	0.61
1:A:365:LEU:HD23	1:A:373:MET:HE1	1.81	0.61
1:A:124:ARG:HA	1:A:124:ARG:HE	1.66	0.61
1:A:154:ASP:OD2	1:A:157:THR:HB	2.00	0.60
1:A:335:LYS:HE2	3:A:506:HOH:O	2.02	0.60
1:A:199:GLU:HG3	3:A:578:HOH:O	2.00	0.60
1:A:325:MET:HE2	1:A:328:GLN:HE22	1.66	0.60
1:A:94:SER:OG	1:A:96:ARG:HG3	2.02	0.59
1:A:250:LYS:CE	2:A:402:CBA:H4A2	2.32	0.59
1:A:225:ILE:HG13	1:A:226:ASN:N	2.17	0.59
1:A:334:LYS:HG3	3:A:543:HOH:O	2.02	0.58
1:A:172:ILE:HG22	1:A:209:LEU:HD22	1.85	0.58
1:A:252:MET:HE2	1:A:301:ILE:HG21	1.86	0.57
1:A:2:SER:HA	3:A:706:HOH:O	2.05	0.57
1:A:137:THR:HB	1:A:138:PRO:HD3	1.85	0.57
1:A:397:HIS:O	1:A:401:LYS:N	2.35	0.57
1:A:43:GLY:HA2	3:A:697:HOH:O	2.05	0.56
1:A:358:LYS:HE3	1:A:361:GLN:OE1	2.06	0.56
1:A:91:ALA:HA	1:A:96:ARG:HD3	1.87	0.56
1:A:250:LYS:HE3	2:A:402:CBA:H4A2	1.88	0.56
1:A:237:GLU:OE1	3:A:617:HOH:O	2.18	0.56
1:A:175:LYS:HB2	3:A:619:HOH:O	2.06	0.55
1:A:325:MET:CE	1:A:328:GLN:NE2	2.69	0.55
1:A:365:LEU:HD23	1:A:373:MET:CE	2.37	0.55
1:A:23:LYS:HB2	3:A:526:HOH:O	2.06	0.55
1:A:31:MET:HE2	1:A:391:TYR:CD2	2.39	0.55
1:A:282:LEU:O	1:A:286:MET:HE3	2.07	0.54
1:A:225:ILE:HG13	1:A:226:ASN:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:NZ	3:A:760:HOH:O	2.40	0.54
1:A:361:GLN:HB3	1:A:399:VAL:CG1	2.37	0.54
1:A:128:LEU:HD11	1:A:147:LEU:HD22	1.90	0.53
1:A:233:ARG:O	3:A:752:HOH:O	2.18	0.53
1:A:184:ALA:O	1:A:185:HIS:C	2.48	0.53
1:A:130:LYS:HG3	1:A:150:TYR:O	2.09	0.52
1:A:186:ASN:ND2	2:A:402:CBA:O3	2.39	0.52
1:A:330:VAL:HG21	1:A:346:THR:HG23	1.91	0.52
1:A:234:HIS:HE1	3:A:549:HOH:O	1.92	0.52
1:A:328:GLN:O	1:A:332:ASN:OD1	2.27	0.52
1:A:318:MET:O	1:A:322:ILE:HG13	2.09	0.52
1:A:53:LYS:O	1:A:57:MET:HG3	2.11	0.51
1:A:72:GLY:HA3	1:A:101:GLN:HB2	1.93	0.51
1:A:172:ILE:HG22	1:A:209:LEU:CD2	2.41	0.51
1:A:353:CYS:HB3	1:A:379:ILE:CD1	2.41	0.50
1:A:124:ARG:HE	1:A:124:ARG:CA	2.20	0.50
1:A:127:TYR:CE2	1:A:172:ILE:HG12	2.46	0.50
1:A:117:GLN:HG3	1:A:143:ALA:O	2.11	0.50
1:A:98:VAL:O	1:A:263:THR:HA	2.11	0.49
1:A:135:ASN:O	1:A:139:ILE:HG13	2.12	0.49
1:A:31:MET:CE	1:A:371:ILE:HG12	2.37	0.49
1:A:76:PHE:HB2	1:A:299:SER:HB2	1.93	0.49
1:A:179:LEU:HA	1:A:212:TYR:O	2.13	0.49
1:A:154:ASP:OD2	1:A:157:THR:CB	2.61	0.49
1:A:332:ASN:O	1:A:336:GLU:HG2	2.13	0.49
1:A:30:LYS:CB	1:A:370:SER:HB3	2.43	0.48
1:A:358:LYS:HB3	1:A:359:PRO:CD	2.43	0.48
1:A:365:LEU:HD22	1:A:399:VAL:HG11	1.93	0.48
1:A:8:GLU:HB3	3:A:565:HOH:O	2.12	0.48
1:A:40:ASP:HB3	1:A:46:TYR:HB2	1.95	0.48
1:A:243:VAL:HG12	1:A:264:VAL:HG13	1.95	0.48
1:A:133:TRP:CH2	2:A:402:CBA:H5A1	2.49	0.48
1:A:96:ARG:NH2	1:A:241:ASP:OD1	2.46	0.47
1:A:189:GLY:O	1:A:349:ILE:HG13	2.14	0.47
1:A:230:TRP:O	1:A:234:HIS:N	2.43	0.47
1:A:361:GLN:HB3	1:A:399:VAL:HG13	1.96	0.47
1:A:13:ASP:O	1:A:14:PRO:C	2.57	0.47
1:A:250:LYS:HE2	2:A:402:CBA:H4A2	1.97	0.47
1:A:362:VAL:HG11	1:A:375:LYS:HA	1.96	0.47
1:A:30:LYS:HA	1:A:370:SER:O	2.15	0.46
1:A:392:LEU:O	1:A:396:ILE:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:O	1:A:196:GLN:N	2.49	0.46
1:A:305:PRO:O	1:A:309:LYS:HG3	2.15	0.46
1:A:24:ARG:NH2	3:A:448:HOH:O	2.49	0.46
1:A:401:LYS:HG2	1:A:401:LYS:OXT	2.15	0.46
1:A:124:ARG:HB3	3:A:597:HOH:O	2.14	0.46
1:A:39:ARG:HB2	3:A:697:HOH:O	2.15	0.46
1:A:32:ASN:C	1:A:32:ASN:HD22	2.22	0.45
1:A:109:LEU:HA	1:A:212:TYR:OH	2.16	0.45
1:A:81:ALA:CB	1:A:97:TYR:CE2	3.00	0.45
1:A:162:PHE:CE1	1:A:196:GLN:HB3	2.52	0.45
1:A:32:ASN:C	1:A:32:ASN:ND2	2.75	0.44
1:A:166:MET:HE1	1:A:199:GLU:HG3	1.98	0.44
1:A:116:LEU:O	1:A:117:GLN:C	2.56	0.44
1:A:28:SER:HB3	3:A:421:HOH:O	2.17	0.44
1:A:154:ASP:HB2	1:A:161:ASP:HB2	1.99	0.44
1:A:238:GLN:NE2	3:A:584:HOH:O	2.41	0.44
1:A:326:ARG:HD3	1:A:345:ILE:O	2.18	0.44
1:A:172:ILE:CG2	1:A:209:LEU:HD22	2.46	0.44
1:A:100:VAL:HG12	1:A:100:VAL:O	2.17	0.44
1:A:118:ARG:HB2	3:A:703:HOH:O	2.17	0.44
1:A:365:LEU:CD2	1:A:373:MET:HE1	2.48	0.44
1:A:89:SER:HB3	1:A:92:PHE:HB3	2.00	0.43
1:A:286:MET:O	3:A:544:HOH:O	2.21	0.43
1:A:360:GLU:O	1:A:364:ARG:HG3	2.18	0.43
1:A:152:TYR:OH	1:A:192:PRO:HD3	2.18	0.43
1:A:188:THR:O	1:A:348:GLN:HG2	2.18	0.43
1:A:281:ILE:O	1:A:285:PRO:HD3	2.19	0.43
2:A:402:CBA:C4A	2:A:402:CBA:HOB	2.31	0.43
1:A:40:ASP:OD1	1:A:40:ASP:C	2.62	0.43
1:A:186:ASN:HA	1:A:187:PRO:HA	1.80	0.42
1:A:101:GLN:NE2	1:A:295:ALA:HB2	2.34	0.42
1:A:203:VAL:HG22	3:A:559:HOH:O	2.18	0.42
1:A:236:ILE:HA	1:A:240:ILE:O	2.19	0.42
1:A:137:THR:HB	1:A:138:PRO:CD	2.50	0.42
1:A:342:TRP:HB3	1:A:345:ILE:HD12	2.01	0.42
1:A:31:MET:HE3	1:A:371:ILE:CG1	2.40	0.42
1:A:185:HIS:CE1	1:A:188:THR:HB	2.55	0.42
1:A:137:THR:CB	1:A:138:PRO:CD	2.98	0.42
1:A:358:LYS:CB	1:A:359:PRO:CD	2.98	0.41
1:A:391:TYR:O	1:A:392:LEU:C	2.58	0.41
1:A:80:SER:O	1:A:81:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HB2	1:A:171:LYS:NZ	2.35	0.41
1:A:49:ASN:HB2	1:A:314:GLU:CD	2.46	0.41
1:A:392:LEU:HA	1:A:392:LEU:HD12	1.74	0.41
1:A:344:HIS:HA	1:A:347:ASP:HB2	2.03	0.41
1:A:137:THR:CB	1:A:138:PRO:HD3	2.51	0.41
1:A:172:ILE:HA	1:A:173:PRO:HD3	1.94	0.41
1:A:31:MET:HE1	1:A:392:LEU:CB	2.44	0.41
1:A:53:LYS:CE	1:A:310:GLU:OE1	2.65	0.40
1:A:122:PHE:O	1:A:123:SER:HB2	2.21	0.40
1:A:292:MET:HE2	1:A:296:ARG:CZ	2.52	0.40
1:A:98:VAL:HG21	1:A:276:GLU:HB2	2.02	0.40
1:A:52:ARG:HD3	1:A:52:ARG:HA	1.91	0.40
1:A:130:LYS:CG	1:A:149:ALA:HB1	2.51	0.40
1:A:364:ARG:NH2	3:A:719:HOH:O	2.54	0.40

All (6) 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:A:673:HOH:O	3:A:673:HOH:O[3_655]	0.87	1.33
3:A:485:HOH:O	3:A:485:HOH:O[3_655]	1.33	0.87
3:A:428:HOH:O	3:A:428:HOH:O[3_655]	1.42	0.78
3:A:404:HOH:O	3:A:404:HOH:O[3_655]	1.81	0.39
1:A:241:ASP:OD2	3:A:758:HOH:O[3_655]	2.07	0.13
1:A:156:LYS:O	3:A:668:HOH:O[8_556]	2.09	0.11

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	399/401 (100%)	372 (93%)	25 (6%)	2 (0%)	24 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	TYR
1	A	305	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	335/335 (100%)	279 (83%)	56 (17%)	2 3

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	16	LEU
1	A	29	LYS
1	A	35	VAL
1	A	44	LYS
1	A	57	MET
1	A	68	LEU
1	A	75	ASP
1	A	76	PHE
1	A	77	THR
1	A	87	GLU
1	A	88	ASN
1	A	93	LYS
1	A	96	ARG
1	A	100	VAL
1	A	104	SER
1	A	109	LEU
1	A	121	LYS
1	A	124	ARG
1	A	146	GLN
1	A	148	GLN
1	A	156	LYS
1	A	160	LEU

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Mol	Chain	Res	Type
1	A	171	LYS
1	A	172	ILE
1	A	179	LEU
1	A	187	PRO
1	A	190	VAL
1	A	192	PRO
1	A	206	LYS
1	A	244	LEU
1	A	267	ARG
1	A	268	ASP
1	A	270	GLU
1	A	276	GLU
1	A	281	ILE
1	A	290	PRO
1	A	296	ARG
1	A	305	PRO
1	A	308	ARG
1	A	309	LYS
1	A	316	LYS
1	A	323	ILE
1	A	324	SER
1	A	335	LYS
1	A	339	SER
1	A	343	GLN
1	A	349	ILE
1	A	361	GLN
1	A	365	LEU
1	A	379	ILE
1	A	381	VAL
1	A	387	SER
1	A	399	VAL
1	A	400	THR
1	A	401	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	117	GLN
1	A	208	ASN
1	A	226	ASN
1	A	234	HIS

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Mol	Chain	Res	Type
1	A	328	GLN
1	A	398	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	CBA	A	402	-	23,26,26	1.91	9 (39%)	30,39,39	3.43	16 (53%)

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	CBA	A	402	-	-	10/19/28/28	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	CBA	C6-N1	3.92	1.42	1.34
2	A	402	CBA	C2-N1	3.21	1.39	1.33
2	A	402	CBA	P-O1P	3.14	1.60	1.50
2	A	402	CBA	C6-C5	2.54	1.42	1.37
2	A	402	CBA	OD1-CG	2.42	1.29	1.22
2	A	402	CBA	O4P-C5A	-2.36	1.36	1.44
2	A	402	CBA	P-O2P	-2.24	1.46	1.54
2	A	402	CBA	CA-C	-2.24	1.51	1.55
2	A	402	CBA	OB-CB	2.11	1.46	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	CBA	OT-C-CA	7.29	122.79	112.20
2	A	402	CBA	OA-CA-CB	-7.02	96.25	108.92
2	A	402	CBA	C2A-C2-C3	-5.82	113.98	120.80
2	A	402	CBA	O4P-C5A-C5	5.56	119.78	109.36
2	A	402	CBA	C2A-C2-N1	4.97	127.00	117.64
2	A	402	CBA	OD1-CG-CB	-4.74	103.14	122.45
2	A	402	CBA	O4P-P-O1P	4.72	119.19	106.44
2	A	402	CBA	O3-C3-C2	-4.71	107.81	117.58
2	A	402	CBA	OB-CB-CG	4.06	117.58	109.12
2	A	402	CBA	OD2-CG-CB	3.30	125.84	112.80
2	A	402	CBA	C4-C3-C2	3.29	124.88	119.91
2	A	402	CBA	O3-C3-C4	3.15	127.31	118.18
2	A	402	CBA	OD2-CG-OD1	3.06	131.01	124.08
2	A	402	CBA	C4A-C4-C5	2.40	122.36	119.75
2	A	402	CBA	O3P-P-O1P	-2.27	101.98	110.83
2	A	402	CBA	C3-C4-C5	-2.13	116.80	118.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	CBA	C4-C5-C5A-O4P
2	A	402	CBA	C6-C5-C5A-O4P
2	A	402	CBA	C5A-O4P-P-O1P
2	A	402	CBA	C5A-O4P-P-O2P
2	A	402	CBA	C5A-O4P-P-O3P
2	A	402	CBA	O-C-CA-OA
2	A	402	CBA	OT-C-CA-OA
2	A	402	CBA	C5-C4-C4A-N

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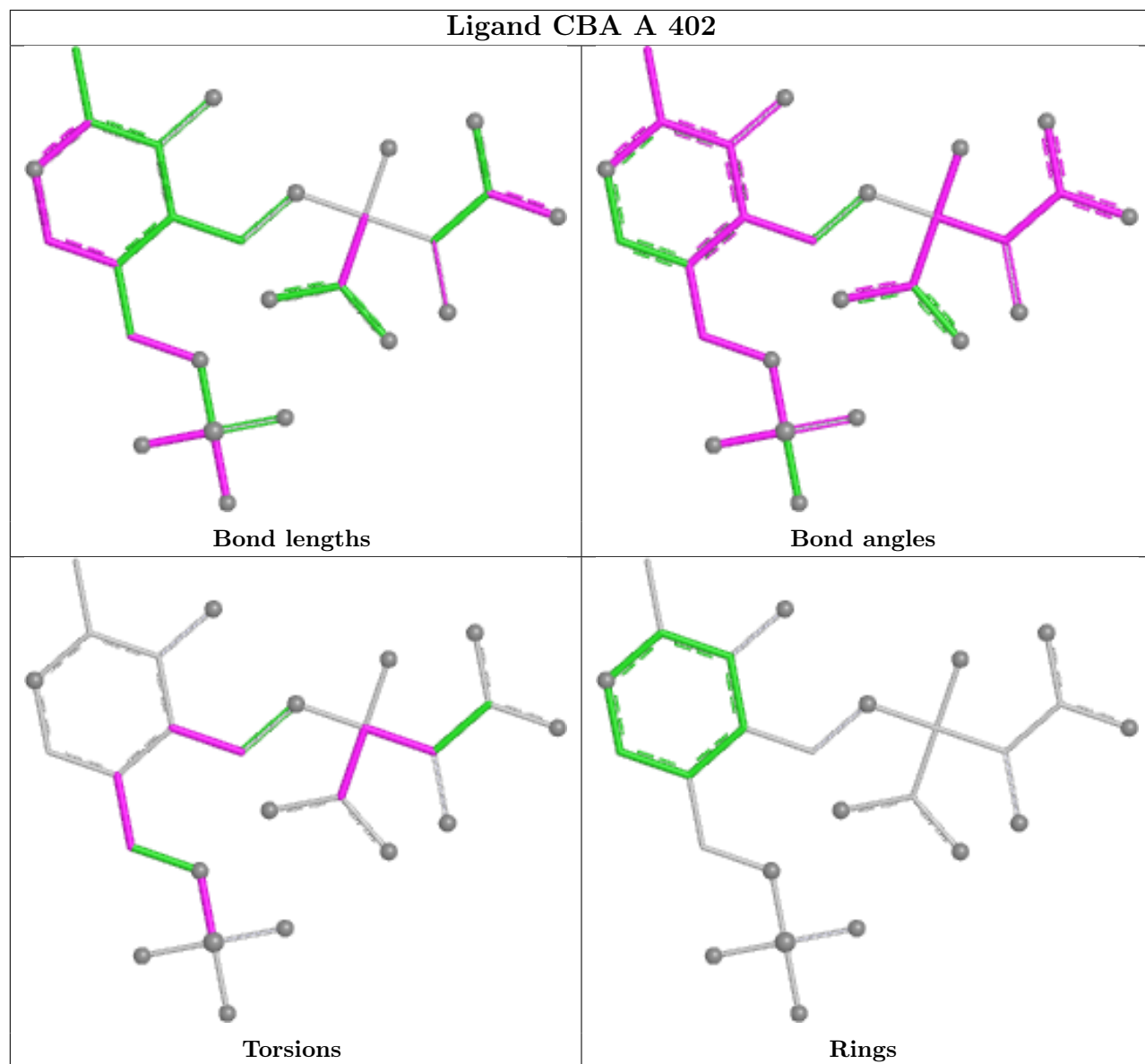
Mol	Chain	Res	Type	Atoms
2	A	402	CBA	C3-C4-C4A-N
2	A	402	CBA	OA-CA-CB-OB

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	CBA	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.