



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:47 AM UTC

PDB ID : 1WAT / pdb_00001wat
Title : THE THREE-DIMENSIONAL STRUCTURE OF THE LIGAND-BINDING
DOMAIN OF A WILD-TYPE BACTERIAL CHEMOTAXIS RECEPTOR
Authors : Kim, S.-H.
Deposited on : 1993-03-09
Resolution : 3.00 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
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

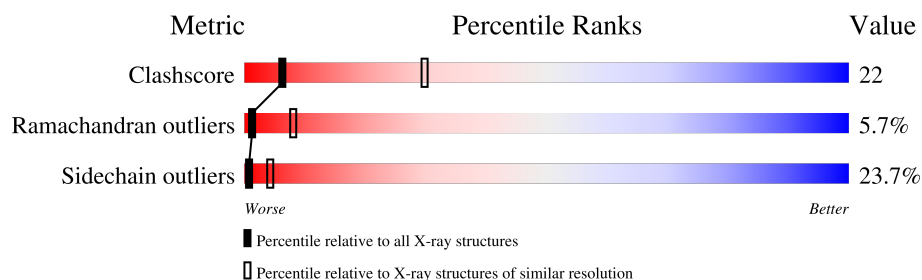
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

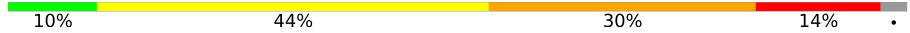
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	146	
1	B	146	

2 Entry composition [i](#)

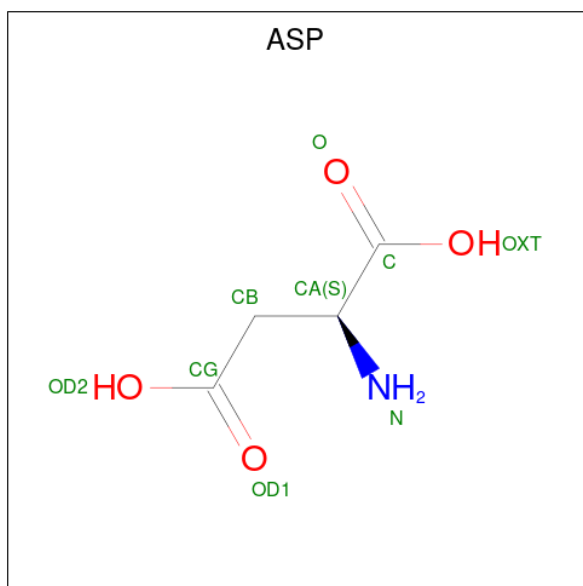
There are 2 unique types of molecules in this entry. The entry contains 2238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ASPARTATE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1110	684	197	221	8			
1	B	143	Total	C	N	O	S	0	0	0
			1119	689	199	223	8			

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



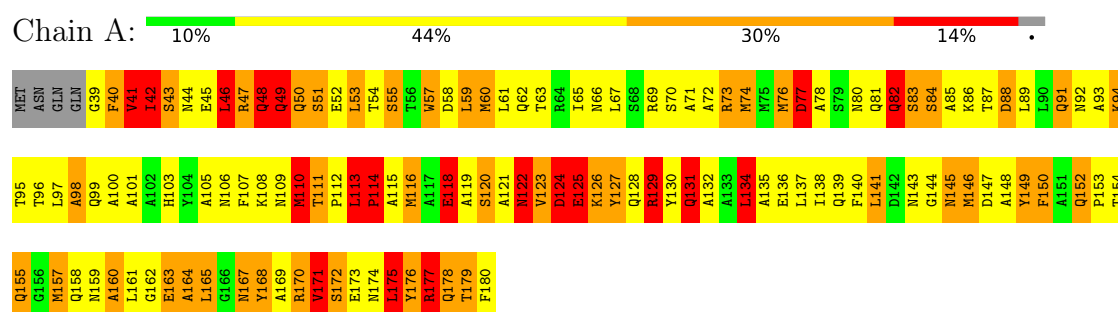
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			9	4	1	4		

3 Residue-property plots

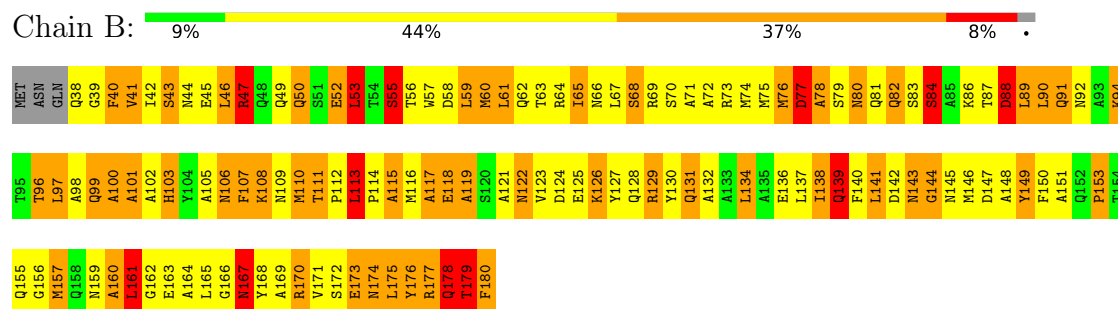
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ASPARTATE RECEPTOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	132.67Å 132.67Å 55.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2238	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	3.14	128/1126 (11.4%)	3.09	159/1520 (10.5%)
1	B	3.19	123/1135 (10.8%)	3.01	153/1532 (10.0%)
All	All	3.16	251/2261 (11.1%)	3.05	312/3052 (10.2%)

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	5
1	B	0	4
All	All	0	9

All (251) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	GLY	N-CA	12.60	1.61	1.45
1	B	143	ASN	C-N	12.37	1.51	1.33
1	B	149	TYR	CA-C	-12.19	1.36	1.52
1	A	103	HIS	CG-CD2	11.28	1.48	1.35
1	B	102	ALA	C-N	-11.04	1.18	1.33
1	A	63	THR	CA-CB	10.93	1.71	1.53
1	B	170	ARG	CD-NE	10.69	1.61	1.46
1	B	167	ASN	CA-CB	10.13	1.69	1.53
1	B	84	SER	C-O	-10.00	1.11	1.24
1	B	150	PHE	C-O	-9.88	1.11	1.24
1	B	80	ASN	CA-CB	9.81	1.67	1.53
1	A	150	PHE	C-O	9.80	1.35	1.24
1	A	86	LYS	N-CA	-9.32	1.34	1.46
1	A	82	GLN	CA-CB	9.18	1.69	1.53
1	B	112	PRO	C-O	9.17	1.34	1.23
1	A	40	PHE	CA-CB	9.11	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	THR	N-CA	9.06	1.57	1.46
1	B	109	ASN	C-N	9.01	1.46	1.33
1	A	171	VAL	N-CA	-8.97	1.35	1.46
1	A	157	MET	N-CA	8.95	1.57	1.46
1	A	72	ALA	CA-CB	-8.88	1.38	1.53
1	A	89	LEU	C-N	8.86	1.46	1.33
1	B	126	LYS	CA-CB	8.77	1.68	1.53
1	B	177	ARG	NE-CZ	8.69	1.42	1.33
1	A	66	ASN	C-N	8.68	1.45	1.33
1	A	98	ALA	N-CA	-8.57	1.36	1.46
1	B	57	TRP	CA-CB	-8.55	1.40	1.53
1	A	103	HIS	CD2-NE2	-8.54	1.28	1.37
1	A	74	MET	C-N	8.50	1.46	1.33
1	A	154	THR	N-CA	-8.45	1.35	1.46
1	B	172	SER	CA-C	8.32	1.63	1.52
1	A	96	THR	CA-CB	8.26	1.67	1.53
1	B	164	ALA	CA-CB	-8.23	1.40	1.53
1	A	45	GLU	CA-CB	-8.16	1.41	1.52
1	B	44	ASN	CA-C	8.09	1.63	1.52
1	B	47	ARG	CA-C	-8.04	1.41	1.52
1	A	94	LYS	C-O	8.03	1.33	1.24
1	B	52	GLU	CA-CB	-8.03	1.40	1.53
1	B	103	HIS	CA-CB	-8.02	1.39	1.53
1	B	92	ASN	CA-CB	-8.02	1.40	1.53
1	B	103	HIS	CD2-NE2	-7.98	1.29	1.37
1	A	130	TYR	CB-CG	7.97	1.69	1.51
1	A	115	ALA	N-CA	7.95	1.56	1.46
1	A	83	SER	C-O	-7.92	1.14	1.24
1	A	66	ASN	CA-C	-7.91	1.42	1.52
1	B	77	ASP	C-O	7.91	1.32	1.23
1	A	159	ASN	CA-CB	-7.90	1.41	1.53
1	B	94	LYS	N-CA	-7.90	1.36	1.46
1	B	121	ALA	C-N	-7.82	1.24	1.33
1	A	178	GLN	C-N	-7.81	1.23	1.33
1	A	158	GLN	CA-CB	-7.81	1.41	1.53
1	B	131	GLN	C-O	7.76	1.33	1.24
1	B	55	SER	CA-C	-7.61	1.42	1.52
1	A	132	ALA	C-N	7.60	1.43	1.33
1	A	47	ARG	N-CA	7.59	1.55	1.46
1	A	113	LEU	CA-CB	7.59	1.65	1.53
1	B	103	HIS	ND1-CE1	-7.57	1.25	1.32
1	B	98	ALA	C-O	7.57	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	ALA	C-N	-7.54	1.24	1.33
1	A	91	GLN	C-N	-7.54	1.22	1.33
1	A	141	LEU	N-CA	-7.53	1.37	1.46
1	B	174	ASN	C-O	-7.51	1.14	1.24
1	A	91	GLN	CG-CD	7.47	1.70	1.52
1	A	171	VAL	C-O	7.46	1.32	1.24
1	B	118	GLU	CA-CB	7.46	1.65	1.53
1	A	129	ARG	C-N	7.45	1.44	1.33
1	A	57	TRP	CZ2-CH2	-7.45	1.23	1.37
1	B	50	GLN	CA-CB	-7.45	1.41	1.53
1	A	172	SER	CA-C	7.42	1.62	1.52
1	B	105	ALA	C-O	-7.40	1.14	1.24
1	B	125	GLU	CD-OE2	-7.39	1.11	1.25
1	B	118	GLU	CA-C	7.33	1.62	1.52
1	A	73	ARG	C-N	-7.29	1.24	1.33
1	A	110	MET	CA-CB	-7.29	1.41	1.53
1	B	171	VAL	C-O	-7.28	1.15	1.24
1	A	162	GLY	C-O	-7.25	1.14	1.23
1	A	83	SER	N-CA	7.25	1.55	1.46
1	B	76	MET	C-N	7.17	1.42	1.33
1	A	85	ALA	N-CA	7.16	1.55	1.46
1	A	77	ASP	CG-OD2	-7.14	1.11	1.25
1	A	157	MET	CA-C	7.06	1.61	1.52
1	B	71	ALA	CA-C	-7.05	1.42	1.52
1	B	64	ARG	C-N	7.04	1.42	1.33
1	A	123	VAL	N-CA	7.01	1.54	1.46
1	B	175	LEU	C-O	6.99	1.32	1.23
1	B	45	GLU	CA-CB	-6.99	1.42	1.53
1	A	116	MET	CA-CB	6.96	1.65	1.53
1	B	173	GLU	N-CA	6.94	1.54	1.46
1	A	74	MET	CA-CB	6.94	1.65	1.53
1	A	179	THR	C-N	6.90	1.43	1.33
1	A	59	LEU	CA-CB	-6.87	1.42	1.53
1	A	119	ALA	N-CA	6.87	1.54	1.46
1	B	56	THR	C-N	6.85	1.42	1.33
1	A	50	GLN	N-CA	6.79	1.55	1.46
1	A	153	PRO	CA-C	6.79	1.59	1.53
1	A	109	ASN	N-CA	6.79	1.54	1.46
1	B	39	GLY	CA-C	6.78	1.61	1.51
1	B	58	ASP	CA-C	6.77	1.61	1.52
1	B	177	ARG	CZ-NH2	-6.75	1.24	1.33
1	A	145	ASN	CG-OD1	-6.74	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	ASP	N-CA	6.72	1.54	1.46
1	A	67	LEU	CA-C	6.71	1.61	1.52
1	A	73	ARG	CD-NE	-6.69	1.36	1.46
1	B	75	MET	C-N	-6.67	1.25	1.33
1	B	159	ASN	C-N	6.65	1.42	1.33
1	B	170	ARG	CZ-NH1	6.65	1.42	1.32
1	A	85	ALA	CA-C	6.59	1.61	1.52
1	A	170	ARG	CD-NE	6.59	1.55	1.46
1	A	66	ASN	CA-CB	6.59	1.63	1.53
1	A	160	ALA	CA-CB	-6.57	1.43	1.53
1	A	97	LEU	C-N	6.49	1.42	1.33
1	A	114	PRO	C-N	6.49	1.42	1.33
1	A	144	GLY	C-O	-6.48	1.16	1.24
1	A	145	ASN	CA-C	-6.48	1.44	1.52
1	A	70	SER	CB-OG	-6.47	1.29	1.42
1	B	43	SER	C-N	6.45	1.42	1.33
1	B	172	SER	C-N	-6.45	1.26	1.33
1	B	109	ASN	CA-CB	6.45	1.62	1.53
1	B	91	GLN	CG-CD	6.44	1.68	1.52
1	B	103	HIS	N-CA	6.43	1.54	1.46
1	A	165	LEU	C-O	6.41	1.32	1.24
1	A	145	ASN	CG-ND2	6.39	1.46	1.33
1	B	148	ALA	N-CA	-6.38	1.38	1.46
1	A	69	ARG	NE-CZ	-6.37	1.26	1.33
1	B	124	ASP	C-O	-6.32	1.16	1.24
1	A	107	PHE	C-N	6.31	1.42	1.33
1	A	84	SER	N-CA	-6.30	1.38	1.46
1	A	51	SER	CA-CB	6.29	1.64	1.53
1	A	77	ASP	CA-CB	6.29	1.64	1.53
1	B	43	SER	CA-C	6.29	1.61	1.52
1	B	145	ASN	CG-ND2	6.29	1.46	1.33
1	A	97	LEU	N-CA	-6.28	1.37	1.46
1	B	122	ASN	C-N	6.27	1.41	1.33
1	A	164	ALA	C-O	-6.26	1.16	1.24
1	A	46	LEU	C-O	-6.24	1.16	1.24
1	A	65	ILE	C-N	6.21	1.42	1.33
1	B	73	ARG	C-N	-6.20	1.25	1.33
1	A	147	ASP	C-N	6.20	1.43	1.33
1	A	57	TRP	CZ3-CH2	6.20	1.55	1.40
1	A	42	ILE	C-O	-6.18	1.16	1.24
1	A	63	THR	C-N	6.13	1.42	1.33
1	A	129	ARG	N-CA	-6.12	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	PHE	N-CA	6.11	1.53	1.46
1	B	123	VAL	C-N	6.11	1.42	1.34
1	A	136	GLU	CD-OE2	-6.04	1.13	1.25
1	A	61	LEU	N-CA	6.03	1.53	1.46
1	B	60	MET	C-N	6.03	1.41	1.33
1	B	119	ALA	CA-CB	-6.02	1.43	1.53
1	A	58	ASP	CG-OD1	-6.01	1.14	1.25
1	B	173	GLU	CD-OE1	6.01	1.36	1.25
1	B	141	LEU	C-O	-6.01	1.17	1.24
1	A	143	ASN	C-N	-5.98	1.25	1.33
1	B	57	TRP	C-N	5.93	1.41	1.33
1	B	90	LEU	CB-CG	5.93	1.65	1.53
1	B	125	GLU	CA-CB	-5.93	1.43	1.53
1	B	167	ASN	CA-C	5.93	1.60	1.52
1	B	155	GLN	C-O	5.93	1.31	1.24
1	B	69	ARG	CA-C	-5.91	1.44	1.52
1	A	86	LYS	CA-C	5.89	1.61	1.52
1	A	172	SER	N-CA	-5.88	1.38	1.46
1	B	52	GLU	CD-OE2	-5.87	1.14	1.25
1	A	108	LYS	N-CA	-5.87	1.38	1.46
1	B	57	TRP	CD2-CE2	-5.85	1.31	1.41
1	A	80	ASN	C-O	5.85	1.31	1.24
1	A	120	SER	CA-CB	-5.84	1.43	1.53
1	B	138	ILE	CA-CB	5.83	1.61	1.54
1	A	125	GLU	N-CA	-5.82	1.39	1.46
1	A	125	GLU	CA-CB	5.82	1.62	1.53
1	B	134	LEU	CA-CB	-5.81	1.44	1.53
1	B	129	ARG	NE-CZ	5.81	1.39	1.33
1	B	49	GLN	CA-CB	-5.80	1.44	1.53
1	A	177	ARG	NE-CZ	5.79	1.39	1.33
1	B	61	LEU	CA-CB	-5.79	1.44	1.53
1	A	116	MET	N-CA	-5.71	1.38	1.46
1	B	118	GLU	N-CA	-5.70	1.39	1.46
1	B	40	PHE	CB-CG	5.68	1.63	1.50
1	B	60	MET	CA-C	-5.67	1.45	1.52
1	A	171	VAL	CA-CB	5.66	1.62	1.54
1	B	74	MET	C-O	5.65	1.31	1.23
1	A	177	ARG	N-CA	-5.65	1.39	1.46
1	B	136	GLU	C-N	5.65	1.41	1.34
1	B	110	MET	N-CA	-5.62	1.39	1.45
1	A	129	ARG	CA-CB	5.61	1.62	1.53
1	B	147	ASP	C-N	5.61	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	HIS	C-N	-5.61	1.26	1.33
1	B	113	LEU	C-N	5.61	1.41	1.34
1	B	168	TYR	CA-C	5.58	1.59	1.52
1	B	72	ALA	C-O	-5.55	1.17	1.24
1	A	84	SER	C-N	5.54	1.41	1.33
1	A	80	ASN	CA-C	5.54	1.59	1.52
1	B	96	THR	C-N	5.53	1.41	1.33
1	B	68	SER	N-CA	5.52	1.53	1.46
1	A	168	TYR	CA-CB	5.52	1.62	1.53
1	A	139	GLN	CA-CB	5.52	1.62	1.53
1	A	59	LEU	CA-C	-5.51	1.45	1.52
1	B	52	GLU	N-CA	5.51	1.53	1.46
1	B	165	LEU	C-O	-5.51	1.17	1.24
1	B	42	ILE	C-N	-5.51	1.26	1.33
1	A	118	GLU	CD-OE2	-5.50	1.14	1.25
1	A	42	ILE	CB-CG2	5.50	1.70	1.52
1	A	158	GLN	N-CA	5.49	1.52	1.46
1	A	145	ASN	CA-CB	5.48	1.59	1.52
1	B	87	THR	C-O	5.46	1.30	1.23
1	B	173	GLU	C-O	5.46	1.30	1.24
1	B	78	ALA	C-N	5.46	1.41	1.33
1	A	60	MET	C-N	5.44	1.41	1.34
1	A	163	GLU	CD-OE2	-5.44	1.15	1.25
1	B	160	ALA	N-CA	-5.42	1.40	1.46
1	A	122	ASN	C-N	-5.42	1.27	1.33
1	B	127	TYR	C-N	5.42	1.40	1.33
1	B	65	ILE	N-CA	-5.40	1.39	1.46
1	A	128	GLN	N-CA	5.40	1.52	1.46
1	B	106	ASN	CA-CB	-5.38	1.45	1.53
1	B	170	ARG	NE-CZ	-5.37	1.27	1.33
1	B	168	TYR	CG-CD1	-5.37	1.28	1.39
1	B	56	THR	C-O	-5.36	1.17	1.24
1	A	59	LEU	N-CA	-5.36	1.39	1.46
1	B	89	LEU	C-N	5.36	1.41	1.33
1	B	75	MET	CA-C	-5.34	1.46	1.52
1	B	136	GLU	CD-OE1	-5.34	1.15	1.25
1	B	180	PHE	N-CA	-5.34	1.36	1.46
1	A	55	SER	C-O	-5.31	1.17	1.24
1	A	124	ASP	CA-C	5.30	1.59	1.52
1	B	50	GLN	N-CA	5.27	1.53	1.46
1	A	71	ALA	CA-C	5.26	1.59	1.52
1	A	149	TYR	CA-C	-5.26	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	THR	C-O	-5.25	1.17	1.24
1	A	82	GLN	N-CA	5.24	1.52	1.46
1	B	149	TYR	C-O	5.23	1.30	1.24
1	B	122	ASN	C-O	-5.23	1.18	1.24
1	B	77	ASP	CA-C	-5.20	1.46	1.53
1	B	88	ASP	CG-OD1	-5.19	1.15	1.25
1	A	87	THR	C-N	5.18	1.40	1.33
1	B	169	ALA	N-CA	-5.17	1.40	1.46
1	A	43	SER	C-N	5.12	1.40	1.33
1	B	58	ASP	CG-OD1	-5.11	1.15	1.25
1	B	163	GLU	C-N	5.10	1.40	1.33
1	B	83	SER	C-N	5.08	1.40	1.33
1	A	171	VAL	C-N	-5.08	1.26	1.33
1	A	94	LYS	CA-C	5.07	1.59	1.52
1	A	140	PHE	CA-C	-5.07	1.46	1.52
1	A	150	PHE	N-CA	-5.07	1.40	1.46
1	B	94	LYS	CE-NZ	-5.06	1.34	1.49
1	A	97	LEU	CA-C	5.06	1.59	1.52
1	A	124	ASP	CA-CB	5.06	1.61	1.53
1	B	96	THR	CA-C	5.05	1.59	1.52
1	B	166	GLY	CA-C	5.05	1.57	1.52
1	A	99	GLN	C-O	-5.04	1.18	1.24
1	B	38	GLN	N-CA	5.02	1.55	1.46
1	B	171	VAL	N-CA	5.02	1.52	1.46
1	A	179	THR	CA-CB	5.00	1.62	1.53

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ASN	OD1-CG-ND2	-13.23	109.37	122.60
1	A	167	ASN	CA-CB-CG	12.87	125.47	112.60
1	B	62	GLN	CA-C-O	-12.58	107.44	120.90
1	A	77	ASP	CA-CB-CG	12.54	125.14	112.60
1	A	80	ASN	CA-CB-CG	12.52	125.12	112.60
1	A	47	ARG	N-CA-C	-12.50	95.11	111.24
1	A	128	GLN	OE1-CD-NE2	-12.46	110.14	122.60
1	A	106	ASN	OD1-CG-ND2	-12.25	110.35	122.60
1	B	179	THR	N-CA-C	-11.71	90.15	109.24
1	B	143	ASN	CA-C-O	11.70	134.11	119.95
1	A	44	ASN	OD1-CG-ND2	-11.45	111.15	122.60
1	A	140	PHE	CA-CB-CG	11.20	125.00	113.80
1	A	109	ASN	CA-CB-CG	10.93	123.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ASP	CA-CB-CG	10.91	123.51	112.60
1	A	174	ASN	OD1-CG-ND2	-10.89	111.71	122.60
1	A	91	GLN	N-CA-C	-10.54	99.87	111.36
1	A	125	GLU	N-CA-C	10.53	122.83	111.36
1	B	143	ASN	OD1-CG-ND2	-10.24	112.36	122.60
1	A	66	ASN	OD1-CG-ND2	-10.11	112.49	122.60
1	B	167	ASN	CA-C-O	-10.00	109.82	120.42
1	B	143	ASN	O-C-N	-9.74	109.56	122.22
1	A	69	ARG	NE-CZ-NH2	9.64	127.88	119.20
1	A	157	MET	O-C-N	9.62	132.32	122.12
1	A	152	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	B	109	ASN	OD1-CG-ND2	-9.39	113.21	122.60
1	A	138	ILE	CA-C-O	-9.30	110.39	121.18
1	A	100	ALA	N-CA-C	-9.18	100.97	110.97
1	B	143	ASN	CA-CB-CG	9.09	121.69	112.60
1	B	174	ASN	OD1-CG-ND2	-9.08	113.52	122.60
1	A	62	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	B	161	LEU	CA-C-O	8.92	130.00	120.55
1	A	57	TRP	CH2-CZ2-CE2	8.85	129.01	117.50
1	B	98	ALA	CA-C-O	-8.76	111.26	120.55
1	B	113	LEU	N-CA-C	-8.74	98.64	109.65
1	A	171	VAL	CA-CB-CG2	-8.71	95.59	110.40
1	B	167	ASN	CA-CB-CG	8.68	121.28	112.60
1	B	132	ALA	CA-C-O	-8.68	111.61	120.90
1	A	176	TYR	CA-C-O	8.67	131.93	122.13
1	A	53	LEU	N-CA-C	-8.62	101.96	111.36
1	B	150	PHE	CA-C-O	8.58	129.87	119.49
1	B	116	MET	N-CA-C	8.51	120.55	111.28
1	B	102	ALA	CA-C-O	-8.44	111.47	120.42
1	A	129	ARG	O-C-N	-8.35	113.47	122.07
1	B	123	VAL	O-C-N	-8.35	113.59	121.94
1	A	103	HIS	CB-CG-ND1	8.33	135.20	122.70
1	B	168	TYR	O-C-N	8.28	130.59	122.07
1	A	40	PHE	N-CA-C	-8.21	99.03	110.35
1	B	103	HIS	CA-CB-CG	-8.15	105.65	113.80
1	B	50	GLN	N-CA-C	-8.13	101.99	112.23
1	A	163	GLU	CB-CG-CD	8.08	126.34	112.60
1	A	69	ARG	N-CA-C	-7.98	100.55	112.04
1	A	171	VAL	N-CA-CB	-7.96	98.10	111.23
1	A	40	PHE	CA-CB-CG	7.87	121.67	113.80
1	A	106	ASN	CB-CG-ND2	7.86	128.20	116.40
1	A	127	TYR	O-C-N	7.80	130.20	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	LEU	N-CA-C	-7.75	102.91	111.36
1	B	109	ASN	CB-CG-ND2	7.74	128.01	116.40
1	A	143	ASN	CA-CB-CG	-7.72	104.88	112.60
1	A	44	ASN	CB-CG-ND2	7.67	127.91	116.40
1	B	50	GLN	CA-C-O	-7.66	110.75	119.79
1	B	106	ASN	N-CA-CB	7.65	121.31	110.07
1	B	46	LEU	CA-C-O	-7.62	112.38	120.92
1	B	82	GLN	O-C-N	7.62	132.11	123.27
1	B	100	ALA	N-CA-C	-7.61	102.58	111.03
1	B	106	ASN	N-CA-C	-7.61	101.43	111.24
1	B	92	ASN	N-CA-C	-7.60	102.93	111.14
1	A	87	THR	CB-CA-C	7.58	122.98	110.92
1	B	66	ASN	CB-CG-ND2	7.58	127.77	116.40
1	A	50	GLN	CB-CG-CD	7.54	125.42	112.60
1	B	67	LEU	CA-C-O	-7.51	113.17	120.90
1	A	124	ASP	CA-CB-CG	7.47	120.08	112.60
1	A	116	MET	CA-C-O	7.47	128.53	119.49
1	A	134	LEU	O-C-N	7.47	130.04	122.12
1	A	87	THR	CA-C-O	7.40	129.21	121.07
1	B	88	ASP	N-CA-CB	7.37	121.19	110.20
1	A	44	ASN	N-CA-C	-7.31	103.25	111.14
1	B	47	ARG	N-CA-C	7.26	120.24	111.82
1	A	116	MET	N-CA-C	7.24	121.21	112.38
1	A	114	PRO	N-CA-C	7.21	127.33	112.47
1	A	103	HIS	ND1-CG-CD2	-7.21	98.89	106.10
1	B	177	ARG	NE-CZ-NH2	7.18	125.66	119.20
1	A	145	ASN	CA-CB-CG	-7.17	105.43	112.60
1	A	173	GLU	CA-C-O	-7.13	113.23	121.07
1	A	125	GLU	CA-C-O	7.10	127.95	120.42
1	B	52	GLU	CB-CG-CD	7.07	124.61	112.60
1	B	179	THR	CA-C-O	7.04	128.10	120.43
1	B	166	GLY	O-C-N	-6.99	115.48	122.19
1	B	171	VAL	CA-C-O	6.96	128.19	120.95
1	B	42	ILE	CA-C-O	-6.93	113.35	121.05
1	B	98	ALA	N-CA-C	-6.92	103.74	111.28
1	A	147	ASP	CB-CA-C	-6.90	97.86	110.63
1	A	78	ALA	CA-C-O	6.88	127.82	119.49
1	A	42	ILE	CA-CB-CG2	-6.84	98.86	110.50
1	B	63	THR	CA-C-O	-6.84	113.58	120.90
1	B	139	GLN	CA-CB-CG	-6.84	100.42	114.10
1	A	168	TYR	O-C-N	6.80	129.35	122.08
1	B	56	THR	CA-CB-OG1	-6.79	99.41	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	TYR	CG-CD1-CE1	-6.79	111.01	121.20
1	B	176	TYR	N-CA-C	6.79	121.27	112.92
1	A	167	ASN	N-CA-C	-6.78	102.27	112.04
1	B	106	ASN	CA-C-O	-6.77	113.69	120.80
1	A	43	SER	CA-CB-OG	6.76	124.63	111.10
1	A	170	ARG	NE-CZ-NH2	-6.75	113.13	119.20
1	A	88	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	132	ALA	O-C-N	6.72	129.08	122.09
1	B	62	GLN	OE1-CD-NE2	-6.72	115.88	122.60
1	B	91	GLN	OE1-CD-NE2	6.71	129.31	122.60
1	A	150	PHE	CA-C-O	-6.67	113.35	120.42
1	A	131	GLN	CA-C-O	6.64	128.00	120.90
1	B	44	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	A	98	ALA	N-CA-C	6.63	118.17	111.07
1	B	71	ALA	CA-C-O	6.59	128.31	120.92
1	B	121	ALA	N-CA-C	-6.55	104.06	111.14
1	A	144	GLY	CA-C-O	6.55	126.44	119.04
1	B	80	ASN	N-CA-C	-6.55	101.31	110.35
1	A	73	ARG	N-CA-C	-6.51	104.37	112.90
1	B	178	GLN	O-C-N	6.50	131.39	122.41
1	B	68	SER	CA-CB-OG	6.49	124.08	111.10
1	B	144	GLY	O-C-N	-6.49	114.27	122.70
1	B	168	TYR	CA-C-O	-6.48	114.01	120.82
1	B	47	ARG	O-C-N	-6.48	114.30	122.27
1	A	66	ASN	CB-CG-ND2	6.47	126.11	116.40
1	A	76	MET	O-C-N	6.47	131.55	122.36
1	B	88	ASP	N-CA-C	-6.47	103.74	111.69
1	B	57	TRP	O-C-N	-6.45	115.32	122.03
1	B	86	LYS	O-C-N	6.44	130.89	123.29
1	B	141	LEU	N-CA-C	6.43	117.95	111.07
1	A	111	THR	N-CA-C	-6.43	95.60	109.81
1	A	41	VAL	N-CA-CB	-6.42	100.64	111.23
1	B	84	SER	CA-C-O	6.42	129.69	120.51
1	A	155	GLN	N-CA-C	-6.41	104.34	111.71
1	A	52	GLU	N-CA-C	-6.38	105.32	113.23
1	A	176	TYR	CA-CB-CG	-6.32	102.53	113.90
1	B	159	ASN	CA-C-O	6.31	127.23	120.10
1	B	106	ASN	O-C-N	6.29	129.41	122.11
1	B	153	PRO	N-CA-CB	-6.29	97.84	102.25
1	B	84	SER	N-CA-C	-6.29	97.41	110.80
1	B	71	ALA	CA-C-N	6.28	128.60	120.44
1	B	71	ALA	C-N-CA	6.28	128.60	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	GLN	CA-C-O	-6.26	114.18	121.07
1	B	45	GLU	CA-C-O	-6.24	114.45	121.00
1	A	50	GLN	CA-C-O	-6.22	112.81	119.97
1	B	105	ALA	CA-C-O	6.21	127.02	119.31
1	A	158	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	B	107	PHE	O-C-N	-6.20	115.64	122.09
1	A	80	ASN	CA-C-N	6.19	133.37	121.54
1	A	80	ASN	C-N-CA	6.19	133.37	121.54
1	B	162	GLY	O-C-N	6.18	128.12	122.18
1	A	167	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	B	131	GLN	O-C-N	-6.15	114.73	122.17
1	B	118	GLU	CB-CA-C	-6.14	100.41	110.85
1	B	170	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	B	57	TRP	CG-CD2-CE3	6.11	140.01	133.90
1	A	48	GLN	N-CA-C	-6.11	97.72	108.23
1	A	48	GLN	CA-C-O	-6.10	114.39	120.98
1	B	67	LEU	N-CA-C	-6.10	104.26	111.03
1	A	170	ARG	CA-C-O	6.08	127.39	121.00
1	A	93	ALA	N-CA-C	-6.08	104.22	111.69
1	B	125	GLU	CA-C-O	6.02	129.12	120.51
1	A	42	ILE	CA-C-O	6.01	128.30	120.78
1	B	72	ALA	O-C-N	6.00	128.25	122.07
1	B	149	TYR	O-C-N	-5.99	115.86	122.09
1	B	117	ALA	O-C-N	-5.98	114.63	122.59
1	A	50	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	B	110	MET	CA-CB-CG	-5.98	102.14	114.10
1	B	172	SER	N-CA-C	-5.97	104.46	110.97
1	B	45	GLU	N-CA-C	-5.97	104.47	110.97
1	B	86	LYS	CA-C-N	-5.96	113.56	123.33
1	B	86	LYS	C-N-CA	-5.96	113.56	123.33
1	A	129	ARG	CA-CB-CG	5.95	126.00	114.10
1	B	109	ASN	CA-C-O	5.94	127.14	119.95
1	B	74	MET	N-CA-C	-5.90	106.62	113.88
1	A	87	THR	N-CA-CB	-5.89	100.87	109.82
1	A	171	VAL	CA-C-O	5.87	128.12	120.78
1	B	53	LEU	N-CA-C	5.87	118.47	111.71
1	A	83	SER	CA-C-N	5.87	128.42	120.38
1	A	83	SER	C-N-CA	5.87	128.42	120.38
1	A	105	ALA	CA-C-O	-5.86	113.47	120.10
1	A	61	LEU	CA-C-N	5.84	128.03	120.44
1	A	61	LEU	C-N-CA	5.84	128.03	120.44
1	B	128	GLN	OE1-CD-NE2	-5.83	116.77	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	PRO	CB-CA-C	5.83	120.53	112.89
1	B	115	ALA	CA-C-O	5.82	127.44	120.92
1	B	88	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	92	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	B	44	ASN	N-CA-C	-5.81	106.32	113.41
1	B	81	GLN	CG-CD-NE2	5.81	125.11	116.40
1	B	66	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	167	ASN	CA-C-N	5.80	128.85	120.79
1	A	167	ASN	C-N-CA	5.80	128.85	120.79
1	B	111	THR	CA-C-N	5.80	125.99	119.90
1	B	111	THR	C-N-CA	5.80	125.99	119.90
1	A	129	ARG	CA-C-O	5.79	126.89	120.82
1	B	103	HIS	N-CA-CB	5.78	119.99	110.39
1	B	56	THR	CA-CB-CG2	5.77	120.31	110.50
1	A	82	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	A	171	VAL	O-C-N	-5.76	115.37	122.57
1	B	129	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	A	175	LEU	CA-C-N	-5.73	114.33	122.41
1	A	175	LEU	C-N-CA	-5.73	114.33	122.41
1	A	45	GLU	CA-C-N	5.72	132.47	121.54
1	A	45	GLU	C-N-CA	5.72	132.47	121.54
1	A	177	ARG	N-CA-C	-5.72	98.62	110.80
1	A	78	ALA	N-CA-C	5.70	119.33	112.38
1	A	72	ALA	CA-C-O	5.67	126.49	119.97
1	A	163	GLU	O-C-N	5.65	128.11	122.12
1	A	152	GLN	CB-CG-CD	5.64	122.18	112.60
1	B	57	TRP	CA-C-O	5.63	126.92	121.00
1	B	99	GLN	CA-CB-CG	5.63	125.36	114.10
1	A	39	GLY	N-CA-C	-5.62	96.99	113.30
1	B	101	ALA	N-CA-C	5.61	118.92	111.75
1	B	70	SER	N-CA-C	-5.60	104.02	111.24
1	A	128	GLN	CA-C-N	5.59	127.71	120.44
1	A	128	GLN	C-N-CA	5.59	127.71	120.44
1	B	60	MET	CA-C-N	5.59	128.05	120.44
1	B	60	MET	C-N-CA	5.59	128.05	120.44
1	B	57	TRP	CE2-CD2-CG	-5.59	100.49	107.20
1	B	129	ARG	O-C-N	-5.59	116.31	122.07
1	B	100	ALA	O-C-N	-5.58	116.00	122.03
1	A	69	ARG	NH1-CZ-NH2	-5.58	112.05	119.30
1	A	109	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	B	77	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	159	ASN	O-C-N	5.55	127.86	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ASP	CA-C-O	-5.53	114.10	120.24
1	A	157	MET	CA-C-O	-5.53	114.69	120.55
1	A	143	ASN	OD1-CG-ND2	5.53	128.13	122.60
1	A	93	ALA	CA-C-O	5.52	126.37	120.24
1	B	90	LEU	CA-C-O	5.50	126.25	120.42
1	A	103	HIS	CE1-NE2-CD2	5.49	114.49	109.00
1	A	165	LEU	N-CA-C	-5.49	105.32	112.23
1	A	91	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	B	115	ALA	CA-C-N	5.47	127.61	120.28
1	B	115	ALA	C-N-CA	5.47	127.61	120.28
1	B	96	THR	CA-C-O	-5.46	113.70	119.97
1	A	98	ALA	O-C-N	5.45	127.69	122.07
1	A	85	ALA	CA-C-N	5.45	128.99	120.82
1	A	85	ALA	C-N-CA	5.45	128.99	120.82
1	B	146	MET	N-CA-C	5.44	117.21	111.28
1	A	122	ASN	CA-C-N	5.42	127.89	120.46
1	A	122	ASN	C-N-CA	5.42	127.89	120.46
1	B	162	GLY	CA-C-O	-5.42	115.14	121.00
1	A	93	ALA	O-C-N	-5.41	115.19	122.23
1	B	114	PRO	O-C-N	-5.41	116.05	122.17
1	A	147	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	161	LEU	O-C-N	-5.40	116.39	122.12
1	A	178	GLN	O-C-N	5.40	129.66	122.43
1	B	157	MET	CA-C-N	5.40	127.45	120.44
1	B	157	MET	C-N-CA	5.40	127.45	120.44
1	B	140	PHE	O-C-N	-5.39	116.48	122.09
1	A	65	ILE	CA-C-O	5.39	126.56	120.85
1	A	95	THR	O-C-N	-5.36	116.04	122.15
1	A	113	LEU	CA-C-N	5.36	126.54	119.84
1	A	113	LEU	C-N-CA	5.36	126.54	119.84
1	A	131	GLN	CA-C-N	5.34	127.39	120.44
1	A	131	GLN	C-N-CA	5.34	127.39	120.44
1	B	121	ALA	CA-C-O	5.34	126.20	120.70
1	A	126	LYS	CG-CD-CE	5.33	123.56	111.30
1	B	130	TYR	O-C-N	-5.32	115.73	122.27
1	B	179	THR	CA-C-N	5.30	131.24	121.70
1	B	179	THR	C-N-CA	5.30	131.24	121.70
1	B	170	ARG	N-CA-CB	-5.29	102.32	110.16
1	B	45	GLU	CA-C-N	5.28	128.74	120.82
1	B	45	GLU	C-N-CA	5.28	128.74	120.82
1	A	48	GLN	CA-C-N	5.28	131.63	121.54
1	A	48	GLN	C-N-CA	5.28	131.63	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	SER	O-C-N	5.26	128.20	122.20
1	A	170	ARG	CD-NE-CZ	-5.26	117.04	124.40
1	A	49	GLN	N-CA-C	-5.25	99.61	110.80
1	A	155	GLN	O-C-N	-5.22	116.11	122.22
1	A	171	VAL	CA-CB-CG1	5.22	119.28	110.40
1	A	176	TYR	CD1-CG-CD2	5.22	125.94	118.10
1	A	155	GLN	N-CA-CB	5.22	118.26	110.22
1	B	94	LYS	CA-C-N	5.22	128.05	120.79
1	B	94	LYS	C-N-CA	5.22	128.05	120.79
1	A	114	PRO	CA-N-CD	-5.21	104.70	112.00
1	A	119	ALA	N-CA-C	-5.21	105.29	110.97
1	A	138	ILE	CB-CA-C	5.21	118.59	111.87
1	B	81	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	147	ASP	N-CA-CB	5.20	118.22	110.22
1	B	162	GLY	N-CA-C	-5.19	106.48	112.50
1	A	141	LEU	O-C-N	5.18	127.41	122.07
1	B	122	ASN	CB-CG-ND2	5.17	124.15	116.40
1	A	86	LYS	O-C-N	5.16	128.05	122.11
1	A	174	ASN	CA-C-O	5.16	125.71	119.11
1	B	42	ILE	O-C-N	5.15	127.25	121.90
1	B	40	PHE	CA-C-N	5.15	131.23	121.97
1	B	40	PHE	C-N-CA	5.15	131.23	121.97
1	B	77	ASP	CA-C-N	5.14	131.35	121.54
1	B	77	ASP	C-N-CA	5.14	131.35	121.54
1	B	80	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	B	62	GLN	O-C-N	5.13	127.42	122.09
1	B	156	GLY	O-C-N	-5.12	117.27	122.19
1	A	103	HIS	N-CA-C	-5.12	105.70	111.28
1	A	70	SER	N-CA-C	5.12	117.25	111.11
1	B	90	LEU	CB-CA-C	5.12	119.55	110.85
1	A	86	LYS	CA-CB-CG	5.11	124.31	114.10
1	A	81	GLN	N-CA-C	-5.10	99.94	110.80
1	A	146	MET	CA-C-N	5.09	127.62	120.28
1	A	146	MET	C-N-CA	5.09	127.62	120.28
1	A	135	ALA	CB-CA-C	-5.08	102.21	110.85
1	B	148	ALA	O-C-N	-5.06	115.55	122.33
1	B	57	TRP	CG-CD1-NE1	-5.05	103.63	110.20
1	A	89	LEU	O-C-N	-5.05	116.32	122.22
1	A	178	GLN	CA-C-O	5.04	125.58	119.38
1	B	123	VAL	CA-C-O	5.04	126.51	121.27
1	A	179	THR	N-CA-C	-5.03	101.65	109.14
1	A	168	TYR	CA-C-O	-5.02	115.55	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	THR	CA-C-N	5.02	129.16	120.58
1	B	87	THR	C-N-CA	5.02	129.16	120.58
1	A	77	ASP	N-CA-C	5.01	121.47	110.80
1	B	155	GLN	CB-CA-C	-5.01	101.37	110.63
1	A	80	ASN	OD1-CG-ND2	-5.00	117.60	122.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	THR	Peptide
1	A	113	LEU	Peptide
1	A	124	ASP	Mainchain
1	A	155	GLN	Mainchain
1	A	169	ALA	Mainchain
1	B	144	GLY	Mainchain
1	B	151	ALA	Mainchain
1	B	167	ASN	Mainchain
1	B	179	THR	Peptide

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	1110	0	1072	56	0
1	B	1119	0	1080	51	0
2	B	9	0	6	0	0
All	All	2238	0	2158	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (98) 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:40:PHE:HE1	1:B:180:PHE:CD2	1.27	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:PHE:CE1	1:B:180:PHE:CD2	2.20	1.29
1:A:40:PHE:CE1	1:B:180:PHE:CG	2.47	1.02
1:A:40:PHE:HE1	1:B:180:PHE:CG	1.80	0.98
1:A:40:PHE:CE1	1:B:180:PHE:HB2	2.06	0.91
1:A:40:PHE:CE1	1:B:180:PHE:CB	2.58	0.87
1:A:40:PHE:HE1	1:B:180:PHE:HD2	1.23	0.84
1:A:47:ARG:HD2	1:A:51:SER:HB3	1.61	0.83
1:B:179:THR:C	1:B:180:PHE:O	2.18	0.81
1:B:177:ARG:NE	1:B:179:THR:OG1	2.14	0.81
1:B:115:ALA:HB1	1:B:175:LEU:HD13	1.66	0.78
1:B:179:THR:HG22	1:B:180:PHE:HB3	1.66	0.76
1:A:73:ARG:HA	1:A:76:MET:SD	2.28	0.74
1:A:74:MET:SD	1:A:146:MET:HE1	2.31	0.71
1:A:40:PHE:CZ	1:B:180:PHE:HB2	2.28	0.69
1:A:123:VAL:HA	1:A:164:ALA:HB1	1.76	0.68
1:A:40:PHE:CE1	1:B:180:PHE:HD2	1.97	0.67
1:B:52:GLU:HG3	1:B:110:MET:HE1	1.77	0.65
1:A:129:ARG:HD3	1:A:157:MET:HA	1.79	0.64
1:B:76:MET:HB3	1:B:80:ASN:HB3	1.81	0.63
1:B:179:THR:O	1:B:180:PHE:O	2.16	0.62
1:A:49:GLN:HG2	1:A:110:MET:HG2	1.81	0.62
1:A:50:GLN:O	1:A:53:LEU:HB3	2.00	0.62
1:A:82:GLN:O	1:A:82:GLN:HG3	1.99	0.61
1:B:76:MET:SD	1:B:84:SER:HB3	2.40	0.61
1:A:47:ARG:HD2	1:A:51:SER:CB	2.32	0.60
1:A:134:LEU:O	1:A:137:LEU:HB2	2.02	0.60
1:A:57:TRP:HZ3	1:A:161:LEU:HB3	1.66	0.60
1:B:90:LEU:O	1:B:94:LYS:HG3	2.01	0.59
1:A:41:VAL:HG22	1:A:42:ILE:H	1.67	0.59
1:B:60:MET:HE1	1:B:161:LEU:CD1	2.33	0.59
1:A:43:SER:H	1:A:46:LEU:HB2	1.67	0.58
1:A:127:TYR:CZ	1:A:131:GLN:HG3	2.40	0.57
1:B:47:ARG:NH2	1:B:50:GLN:HB3	2.20	0.57
1:B:108:LYS:HA	1:B:108:LYS:HE2	1.87	0.56
1:A:91:GLN:HA	1:A:94:LYS:HD2	1.88	0.56
1:B:179:THR:CG2	1:B:180:PHE:HB3	2.33	0.56
1:A:49:GLN:HA	1:A:110:MET:SD	2.46	0.56
1:A:118:GLU:HA	1:A:121:ALA:HB2	1.87	0.56
1:B:60:MET:HE1	1:B:161:LEU:HD11	1.89	0.55
1:B:118:GLU:HG3	1:B:119:ALA:N	2.22	0.55
1:B:113:LEU:HD12	1:B:176:TYR:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLN:O	1:A:49:GLN:HB2	2.07	0.54
1:A:176:TYR:HA	1:A:179:THR:O	2.07	0.54
1:B:103:HIS:HA	1:B:106:ASN:OD1	2.08	0.53
1:A:41:VAL:HG13	1:A:42:ILE:HG13	1.91	0.53
1:A:46:LEU:HA	1:A:49:GLN:HB3	1.91	0.52
1:A:123:VAL:HG22	1:A:164:ALA:O	2.09	0.52
1:B:170:ARG:HD3	1:B:174:ASN:ND2	2.25	0.52
1:B:115:ALA:HB1	1:B:175:LEU:CD1	2.39	0.51
1:B:107:PHE:HA	1:B:110:MET:HE3	1.93	0.50
1:A:129:ARG:HG2	1:A:157:MET:HG3	1.93	0.49
1:B:157:MET:O	1:B:160:ALA:HB3	2.12	0.49
1:B:177:ARG:NE	1:B:179:THR:HG1	2.09	0.49
1:B:178:GLN:OE1	1:B:179:THR:O	2.31	0.49
1:B:122:ASN:O	1:B:126:LYS:HG2	2.12	0.49
1:B:55:SER:O	1:B:59:LEU:HB2	2.13	0.48
1:B:178:GLN:OE1	1:B:179:THR:C	2.56	0.48
1:A:50:GLN:HA	1:A:53:LEU:HB3	1.96	0.48
1:A:126:LYS:HD3	1:A:160:ALA:HB1	1.96	0.48
1:B:137:LEU:HD22	1:B:149:TYR:CD2	2.49	0.48
1:A:46:LEU:HA	1:A:49:GLN:CB	2.45	0.47
1:A:175:LEU:HD22	1:A:176:TYR:CZ	2.49	0.47
1:A:116:MET:SD	1:A:171:VAL:O	2.73	0.46
1:A:126:LYS:O	1:A:129:ARG:HB3	2.15	0.46
1:A:74:MET:SD	1:A:141:LEU:HD22	2.56	0.46
1:B:60:MET:HG3	1:B:100:ALA:HB1	1.98	0.45
1:B:99:GLN:O	1:B:103:HIS:ND1	2.47	0.45
1:A:145:ASN:OD1	1:A:148:ALA:HB3	2.17	0.44
1:A:134:LEU:HD12	1:A:137:LEU:HD12	1.98	0.44
1:A:177:ARG:NH2	1:A:180:PHE:HZ	2.16	0.44
1:B:178:GLN:HE22	1:B:180:PHE:H	1.65	0.44
1:A:171:VAL:HG22	1:A:175:LEU:HD12	1.98	0.44
1:A:48:GLN:NE2	1:A:110:MET:HE1	2.32	0.44
1:A:41:VAL:HG13	1:A:42:ILE:N	2.33	0.43
1:B:115:ALA:HB3	1:B:176:TYR:OH	2.18	0.43
1:A:57:TRP:HE3	1:A:161:LEU:HD23	1.83	0.43
1:A:149:TYR:HD2	1:A:150:PHE:CD2	2.36	0.43
1:A:175:LEU:HA	1:A:178:GLN:HG2	2.00	0.43
1:A:43:SER:N	1:A:46:LEU:HB2	2.32	0.43
1:B:88:ASP:O	1:B:91:GLN:N	2.52	0.42
1:B:53:LEU:HD12	1:B:53:LEU:HA	1.72	0.42
1:B:101:ALA:HB2	1:B:131:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ALA:O	1:A:101:ALA:HB3	2.19	0.42
1:B:118:GLU:HG3	1:B:119:ALA:H	1.84	0.42
1:B:178:GLN:NE2	1:B:180:PHE:H	2.18	0.42
1:B:76:MET:SD	1:B:84:SER:CB	3.08	0.41
1:B:52:GLU:CG	1:B:110:MET:HE1	2.46	0.41
1:A:118:GLU:HA	1:A:121:ALA:CB	2.51	0.41
1:A:120:SER:HA	1:A:123:VAL:HG23	2.03	0.41
1:B:97:LEU:HD12	1:B:138:ILE:HD12	2.02	0.41
1:A:121:ALA:HA	1:A:124:ASP:OD2	2.21	0.40
1:B:52:GLU:HG3	1:B:110:MET:CE	2.48	0.40
1:A:122:ASN:HA	1:A:125:GLU:CG	2.51	0.40
1:B:77:ASP:O	1:B:79:SER:N	2.53	0.40
1:A:167:ASN:OD1	1:A:168:TYR:N	2.54	0.40
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.85	0.40
1:B:139:GLN:HA	1:B:142:ASP:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/146 (96%)	114 (81%)	16 (11%)	10 (7%)		
1	B	141/146 (97%)	120 (85%)	15 (11%)	6 (4%)		
All	All	281/292 (96%)	234 (83%)	31 (11%)	16 (6%)		

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	49	GLN
1	A	114	PRO

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Mol	Chain	Res	Type
1	B	41	VAL
1	A	41	VAL
1	A	77	ASP
1	A	110	MET
1	B	78	ALA
1	B	84	SER
1	B	89	LEU
1	B	117	ALA
1	A	113	LEU
1	A	177	ARG
1	B	40	PHE
1	A	112	PRO
1	A	42	ILE

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	115/119 (97%)	88 (76%)	27 (24%)	1	4
1	B	116/119 (98%)	88 (76%)	28 (24%)	1	4
All	All	231/238 (97%)	176 (76%)	55 (24%)	1	4

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	46	LEU
1	A	48	GLN
1	A	54	THR
1	A	55	SER
1	A	59	LEU
1	A	60	MET
1	A	77	ASP
1	A	82	GLN
1	A	83	SER

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Mol	Chain	Res	Type
1	A	84	SER
1	A	88	ASP
1	A	113	LEU
1	A	114	PRO
1	A	118	GLU
1	A	122	ASN
1	A	125	GLU
1	A	129	ARG
1	A	131	GLN
1	A	134	LEU
1	A	152	GLN
1	A	163	GLU
1	A	165	LEU
1	A	170	ARG
1	A	171	VAL
1	A	172	SER
1	A	175	LEU
1	B	41	VAL
1	B	43	SER
1	B	46	LEU
1	B	47	ARG
1	B	53	LEU
1	B	55	SER
1	B	59	LEU
1	B	61	LEU
1	B	65	ILE
1	B	68	SER
1	B	77	ASP
1	B	82	GLN
1	B	88	ASP
1	B	96	THR
1	B	97	LEU
1	B	108	LYS
1	B	111	THR
1	B	113	LEU
1	B	129	ARG
1	B	134	LEU
1	B	139	GLN
1	B	141	LEU
1	B	143	ASN
1	B	153	PRO
1	B	161	LEU

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Mol	Chain	Res	Type
1	B	167	ASN
1	B	173	GLU
1	B	178	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	49	GLN
1	A	143	ASN
1	A	155	GLN
1	A	158	GLN
1	B	38	GLN
1	B	50	GLN
1	B	92	ASN
1	B	122	ASN
1	B	131	GLN
1	B	145	ASN
1	B	152	GLN
1	B	174	ASN
1	B	178	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ASP	B	1	-	7,8,8	1.56	2 (28%)	6,10,10	1.29	1 (16%)

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	ASP	B	1	-	-	3/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	ASP	OD2-CG	-2.53	1.22	1.30
2	B	1	ASP	OXT-C	-2.06	1.24	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ASP	OD2-CG-CB	2.29	121.13	114.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	ASP	O-C-CA-N
2	B	1	ASP	OXT-C-CA-N
2	B	1	ASP	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	102:ALA	C	103:HIS	N	1.18

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.