



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 06:50 AM EST

PDB ID : 1WAT
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

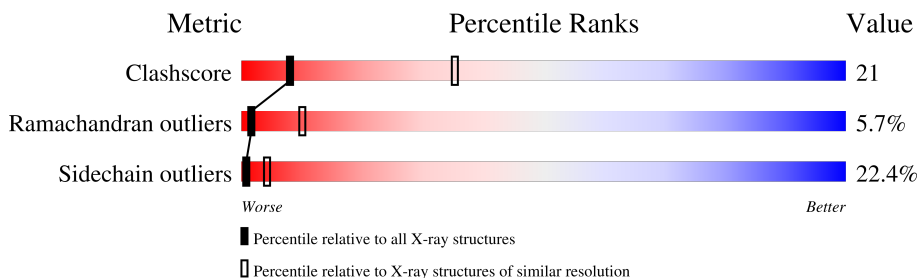
1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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	 28% 36% 23% 10% •
1	B	146	 29% 38% 25% 5% •

2 Entry composition [i](#)

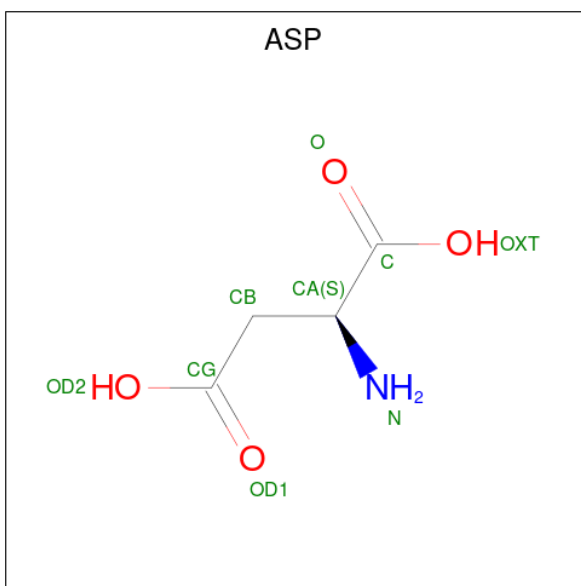
There are 2 unique types of molecules in this entry. The entry contains 2238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	142	Total 1110	C 684	N 197	O 221	S 8	0	0	0
1	B	143	Total 1119	C 689	N 199	O 223	S 8	0	0	0

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: C₄H₇NO₄).



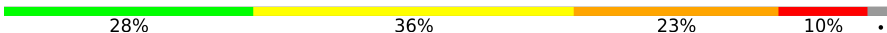
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	Total 9	C 4	N 1	O 4	0	0

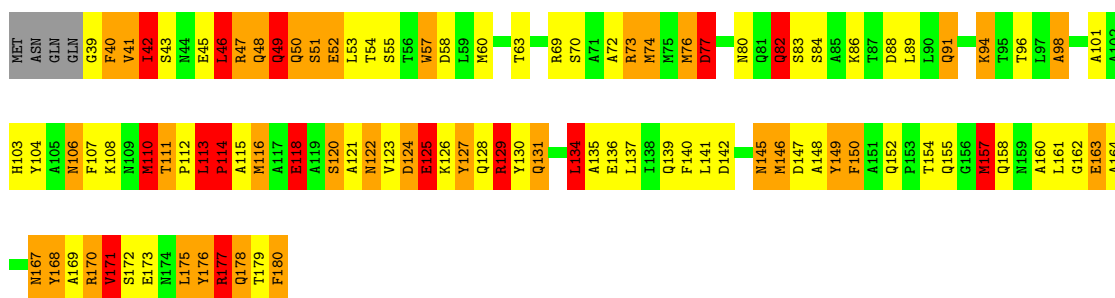
3 Residue-property plots [i](#)

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.

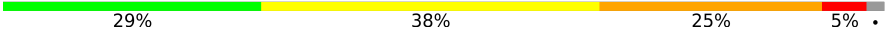
Note EDS was not executed.

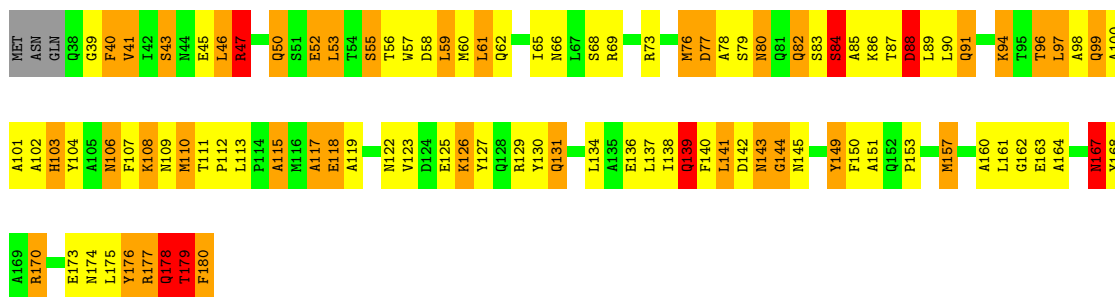
- Molecule 1: ASPARTATE RECEPTOR

Chain A: 



- Molecule 1: ASPARTATE RECEPTOR

Chain B: 



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	2238	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	2.49	63/1126 (5.6%)	2.50	66/1520 (4.3%)
1	B	2.49	58/1135 (5.1%)	2.45	69/1532 (4.5%)
All	All	2.49	121/2261 (5.4%)	2.48	135/3052 (4.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
All	All	0	9

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	125	GLU	CD-OE2	-13.04	1.11	1.25
1	A	130	TYR	CB-CG	11.69	1.69	1.51
1	A	136	GLU	CD-OE2	-10.71	1.13	1.25
1	B	52	GLU	CD-OE2	-10.42	1.14	1.25
1	B	162	GLY	N-CA	10.29	1.61	1.46
1	B	143	ASN	C-N	10.29	1.51	1.33
1	B	173	GLU	CD-OE1	10.11	1.36	1.25
1	A	70	SER	CB-OG	-10.03	1.29	1.42
1	A	57	TRP	CZ3-CH2	9.93	1.55	1.40
1	A	118	GLU	CD-OE2	-9.78	1.14	1.25
1	A	163	GLU	CD-OE2	-9.66	1.15	1.25
1	B	136	GLU	CD-OE1	-9.49	1.15	1.25
1	B	130	TYR	CE1-CZ	8.94	1.50	1.38
1	B	170	ARG	CD-NE	8.69	1.61	1.46
1	A	91	GLN	CG-CD	8.56	1.70	1.51
1	B	168	TYR	CG-CD1	-8.51	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	TRP	CD2-CE2	-8.29	1.31	1.41
1	B	125	GLU	CD-OE1	7.92	1.34	1.25
1	A	168	TYR	CE1-CZ	7.79	1.48	1.38
1	A	51	SER	CA-CB	7.60	1.64	1.52
1	A	57	TRP	CZ2-CH2	-7.50	1.23	1.37
1	B	91	GLN	CG-CD	7.43	1.68	1.51
1	A	103	HIS	CG-CD2	7.36	1.48	1.35
1	B	177	ARG	NE-CZ	7.35	1.42	1.33
1	A	168	TYR	CG-CD2	7.33	1.48	1.39
1	A	149	TYR	CD2-CE2	-7.32	1.28	1.39
1	B	40	PHE	CB-CG	7.27	1.63	1.51
1	B	130	TYR	CD1-CE1	-6.97	1.28	1.39
1	B	170	ARG	CZ-NH1	6.93	1.42	1.33
1	A	63	THR	CA-CB	6.88	1.71	1.53
1	A	82	GLN	CA-CB	6.84	1.69	1.53
1	A	52	GLU	CD-OE1	-6.79	1.18	1.25
1	B	102	ALA	C-N	-6.67	1.18	1.34
1	B	127	TYR	CG-CD1	6.67	1.47	1.39
1	A	72	ALA	CA-CB	-6.62	1.38	1.52
1	B	103	HIS	CA-CB	-6.61	1.39	1.53
1	A	150	PHE	C-O	6.54	1.35	1.23
1	B	104	TYR	CE2-CZ	-6.54	1.30	1.38
1	B	126	LYS	CA-CB	6.49	1.68	1.53
1	A	136	GLU	CD-OE1	6.46	1.32	1.25
1	B	177	ARG	CZ-NH2	-6.44	1.24	1.33
1	B	57	TRP	CA-CB	-6.34	1.40	1.53
1	A	149	TYR	CE1-CZ	-6.33	1.30	1.38
1	B	84	SER	C-O	-6.30	1.11	1.23
1	A	163	GLU	CG-CD	6.29	1.61	1.51
1	B	150	PHE	C-O	-6.29	1.11	1.23
1	B	167	ASN	CA-CB	6.25	1.69	1.53
1	A	140	PHE	CE2-CZ	6.24	1.49	1.37
1	B	149	TYR	CA-C	-6.23	1.36	1.52
1	A	168	TYR	CD1-CE1	-6.23	1.30	1.39
1	A	168	TYR	CD2-CE2	-6.23	1.30	1.39
1	A	120	SER	CA-CB	-6.20	1.43	1.52
1	B	52	GLU	CA-CB	-6.11	1.40	1.53
1	B	43	SER	CB-OG	6.08	1.50	1.42
1	A	57	TRP	CD2-CE2	-6.05	1.34	1.41
1	A	163	GLU	CD-OE1	6.01	1.32	1.25
1	A	145	ASN	CG-OD1	-6.00	1.10	1.24
1	B	39	GLY	CA-C	5.99	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	LYS	CE-NZ	-5.95	1.34	1.49
1	A	162	GLY	C-O	-5.95	1.14	1.23
1	A	176	TYR	CE1-CZ	5.95	1.46	1.38
1	A	176	TYR	CG-CD1	-5.95	1.31	1.39
1	B	150	PHE	CG-CD1	5.92	1.47	1.38
1	A	45	GLU	CA-CB	-5.92	1.41	1.53
1	B	57	TRP	CD1-NE1	-5.91	1.27	1.38
1	A	77	ASP	CG-OD2	-5.90	1.11	1.25
1	A	130	TYR	CG-CD1	-5.89	1.31	1.39
1	B	52	GLU	CG-CD	5.85	1.60	1.51
1	A	110	MET	CA-CB	-5.81	1.41	1.53
1	A	158	GLN	CA-CB	-5.81	1.41	1.53
1	B	50	GLN	CA-CB	-5.78	1.41	1.53
1	B	164	ALA	CA-CB	-5.77	1.40	1.52
1	A	86	LYS	N-CA	-5.75	1.34	1.46
1	A	42	ILE	CB-CG2	5.75	1.70	1.52
1	A	130	TYR	CD1-CE1	-5.67	1.30	1.39
1	B	163	GLU	CG-CD	5.67	1.60	1.51
1	A	108	LYS	CD-CE	5.67	1.65	1.51
1	A	176	TYR	CD1-CE1	5.66	1.47	1.39
1	B	176	TYR	CB-CG	5.64	1.60	1.51
1	A	73	ARG	CD-NE	-5.63	1.36	1.46
1	B	176	TYR	CD1-CE1	5.62	1.47	1.39
1	A	171	VAL	N-CA	-5.61	1.35	1.46
1	A	40	PHE	CA-CB	5.59	1.66	1.53
1	A	145	ASN	CG-ND2	5.53	1.46	1.32
1	B	83	SER	CB-OG	5.45	1.49	1.42
1	B	179	THR	N-CA	5.45	1.57	1.46
1	B	145	ASN	CG-ND2	5.44	1.46	1.32
1	B	112	PRO	C-O	5.43	1.34	1.23
1	B	80	ASN	CA-CB	5.43	1.67	1.53
1	A	157	MET	N-CA	5.42	1.57	1.46
1	B	150	PHE	CE2-CZ	5.42	1.47	1.37
1	A	154	THR	N-CA	-5.39	1.35	1.46
1	A	69	ARG	NE-CZ	-5.39	1.26	1.33
1	A	74	MET	C-N	5.38	1.46	1.34
1	A	116	MET	CA-CB	5.37	1.65	1.53
1	A	139	GLN	CG-CD	5.36	1.63	1.51
1	A	74	MET	CA-CB	5.36	1.65	1.53
1	A	94	LYS	C-O	5.35	1.33	1.23
1	A	170	ARG	CD-NE	5.31	1.55	1.46
1	B	109	ASN	C-N	5.30	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	GLU	CB-CG	5.29	1.62	1.52
1	A	57	TRP	CD1-NE1	-5.29	1.28	1.38
1	B	107	PHE	CG-CD1	5.29	1.46	1.38
1	B	163	GLU	CD-OE2	5.26	1.31	1.25
1	B	123	VAL	CB-CG2	-5.25	1.41	1.52
1	A	96	THR	CA-CB	5.25	1.67	1.53
1	B	52	GLU	CD-OE1	5.22	1.31	1.25
1	B	45	GLU	CA-CB	-5.22	1.42	1.53
1	B	131	GLN	C-O	5.22	1.33	1.23
1	B	118	GLU	CD-OE2	5.19	1.31	1.25
1	A	89	LEU	C-N	5.18	1.46	1.34
1	A	91	GLN	C-N	-5.16	1.22	1.34
1	B	180	PHE	N-CA	-5.12	1.36	1.46
1	A	177	ARG	CB-CG	-5.09	1.38	1.52
1	A	98	ALA	N-CA	-5.09	1.36	1.46
1	B	118	GLU	CA-CB	5.08	1.65	1.53
1	A	113	LEU	CA-CB	5.08	1.65	1.53
1	B	98	ALA	C-O	5.07	1.32	1.23
1	A	171	VAL	C-O	5.05	1.32	1.23
1	A	115	ALA	N-CA	5.04	1.56	1.46
1	B	57	TRP	CD2-CE3	-5.04	1.32	1.40

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	NE-CZ-NH2	15.15	127.88	120.30
1	A	170	ARG	NE-CZ-NH2	-14.34	113.13	120.30
1	B	129	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	B	127	TYR	CG-CD1-CE1	-12.87	111.01	121.30
1	A	57	TRP	CH2-CZ2-CE2	11.61	129.01	117.40
1	B	73	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	B	127	TYR	CB-CG-CD1	-11.55	114.07	121.00
1	A	130	TYR	CB-CG-CD2	-11.47	114.12	121.00
1	B	177	ARG	NE-CZ-NH2	10.72	125.66	120.30
1	B	129	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	A	171	VAL	CA-CB-CG2	-10.21	95.59	110.90
1	A	47	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	B	140	PHE	CB-CG-CD2	-10.00	113.80	120.80
1	A	107	PHE	CB-CG-CD1	9.81	127.67	120.80
1	A	168	TYR	CB-CG-CD2	-9.52	115.29	121.00
1	A	176	TYR	CB-CG-CD1	-9.11	115.53	121.00
1	B	57	TRP	CD1-CG-CD2	8.99	113.49	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	A	149	TYR	CG-CD1-CE1	-8.86	114.21	121.30
1	B	170	ARG	NE-CZ-NH2	8.81	124.71	120.30
1	B	168	TYR	CZ-CE2-CD2	-8.67	112.00	119.80
1	B	57	TRP	CE2-CD2-CG	-8.51	100.49	107.30
1	B	58	ASP	CB-CG-OD1	8.20	125.68	118.30
1	A	127	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	A	173	GLU	OE1-CD-OE2	-8.14	113.53	123.30
1	B	143	ASN	O-C-N	-8.02	109.56	123.20
1	A	47	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	176	TYR	CA-C-N	-7.77	100.11	117.20
1	A	168	TYR	CB-CG-CD1	7.76	125.66	121.00
1	B	179	THR	N-CA-C	-7.72	90.15	111.00
1	B	104	TYR	CB-CG-CD2	7.71	125.62	121.00
1	A	142	ASP	CB-CG-OD1	-7.57	111.48	118.30
1	A	40	PHE	CB-CG-CD2	-7.57	115.50	120.80
1	B	69	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	A	176	TYR	CD1-CG-CD2	7.30	125.94	117.90
1	A	40	PHE	CB-CG-CD1	7.21	125.85	120.80
1	A	180	PHE	CB-CG-CD2	-7.10	115.83	120.80
1	B	69	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	B	82	GLN	CA-C-N	-6.80	102.24	117.20
1	A	104	TYR	CB-CG-CD1	-6.79	116.92	121.00
1	B	57	TRP	CG-CD2-CE3	6.79	140.01	133.90
1	B	118	GLU	OE1-CD-OE2	-6.77	115.18	123.30
1	A	69	ARG	NH1-CZ-NH2	-6.68	112.05	119.40
1	B	143	ASN	CA-C-O	6.67	134.11	120.10
1	B	179	THR	CA-C-N	-6.61	102.65	117.20
1	B	110	MET	CA-CB-CG	-6.57	102.14	113.30
1	A	149	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	B	40	PHE	CB-CG-CD2	-6.51	116.24	120.80
1	A	104	TYR	CB-CG-CD2	6.48	124.89	121.00
1	B	58	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	B	57	TRP	CG-CD1-NE1	-6.47	103.63	110.10
1	A	39	GLY	N-CA-C	-6.44	96.99	113.10
1	A	127	TYR	CZ-CE2-CD2	-6.42	114.02	119.80
1	A	147	ASP	CB-CA-C	-6.27	97.86	110.40
1	B	157	MET	CG-SD-CE	-6.27	90.17	100.20
1	A	107	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	B	140	PHE	CG-CD2-CE2	-6.13	114.05	120.80
1	B	85	ALA	CB-CA-C	6.11	119.27	110.10
1	A	171	VAL	N-CA-CB	-6.09	98.10	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	THR	CA-CB-CG2	-6.03	103.95	112.40
1	B	62	GLN	CA-C-O	-6.03	107.44	120.10
1	A	42	ILE	CA-CB-CG2	-6.02	98.86	110.90
1	A	157	MET	O-C-N	6.01	132.32	122.70
1	B	173	GLU	OE1-CD-OE2	-6.00	116.11	123.30
1	B	87	THR	CA-C-N	-5.97	104.06	117.20
1	B	106	ASN	N-CA-CB	5.95	121.31	110.60
1	A	134	LEU	CB-CG-CD2	-5.93	100.92	111.00
1	B	139	GLN	CA-CB-CG	-5.90	100.42	113.40
1	A	113	LEU	CA-CB-CG	5.89	128.84	115.30
1	A	47	ARG	N-CA-C	-5.88	95.11	111.00
1	B	82	GLN	O-C-N	5.88	132.11	122.70
1	B	88	ASP	N-CA-CB	5.88	121.19	110.60
1	B	178	GLN	CA-C-N	-5.87	104.29	117.20
1	A	114	PRO	N-CA-C	5.86	127.33	112.10
1	A	170	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	177	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	129	ARG	O-C-N	-5.77	113.47	122.70
1	A	129	ARG	CA-CB-CG	5.73	126.00	113.40
1	B	141	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	A	176	TYR	CA-CB-CG	-5.72	102.53	113.40
1	A	111	THR	N-CA-C	-5.70	95.60	111.00
1	B	123	VAL	O-C-N	-5.69	113.59	122.70
1	A	178	GLN	CA-C-N	-5.67	104.72	117.20
1	B	56	THR	CA-CB-CG2	5.65	120.31	112.40
1	B	117	ALA	CA-C-N	5.65	129.63	117.20
1	A	176	TYR	CA-C-O	5.63	131.93	120.10
1	A	171	VAL	CA-CB-CG1	5.59	119.28	110.90
1	B	110	MET	CG-SD-CE	-5.54	91.34	100.20
1	A	76	MET	O-C-N	5.53	131.55	122.70
1	B	46	LEU	CA-C-N	5.51	129.32	117.20
1	A	167	ASN	CA-CB-CG	5.49	125.47	113.40
1	B	84	SER	CA-C-N	-5.48	105.14	117.20
1	A	49	GLN	CA-C-N	5.45	129.20	117.20
1	B	66	ASN	OD1-CG-ND2	-5.45	109.37	121.90
1	B	99	GLN	CA-CB-CG	5.43	125.36	113.40
1	B	178	GLN	O-C-N	5.43	131.39	122.70
1	A	110	MET	CG-SD-CE	-5.41	91.54	100.20
1	A	125	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	B	130	TYR	CZ-CE2-CD2	5.38	124.64	119.80
1	B	115	ALA	CA-C-N	-5.37	105.38	117.20
1	B	140	PHE	CD1-CG-CD2	5.35	125.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	77	ASP	CA-CB-CG	5.34	125.14	113.40
1	B	115	ALA	N-CA-CB	-5.33	102.64	110.10
1	B	52	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	A	80	ASN	CA-CB-CG	5.33	125.12	113.40
1	A	50	GLN	CB-CG-CD	5.32	125.42	111.60
1	B	144	GLY	O-C-N	-5.27	114.27	122.70
1	B	149	TYR	CG-CD2-CE2	5.27	125.52	121.30
1	B	176	TYR	CG-CD1-CE1	-5.26	117.09	121.30
1	A	135	ALA	CB-CA-C	-5.26	102.21	110.10
1	B	47	ARG	O-C-N	-5.25	114.30	122.70
1	A	180	PHE	CG-CD2-CE2	-5.24	115.03	120.80
1	B	103	HIS	N-CA-CB	5.22	119.99	110.60
1	A	57	TRP	CE3-CZ3-CH2	-5.19	115.49	121.20
1	B	127	TYR	CG-CD2-CE2	-5.19	117.15	121.30
1	A	146	MET	CA-C-N	5.18	128.59	117.20
1	B	61	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	57	TRP	NE1-CE2-CZ2	-5.14	124.75	130.40
1	B	86	LYS	O-C-N	5.12	130.89	122.70
1	A	128	GLN	OE1-CD-NE2	-5.11	110.14	121.90
1	A	130	TYR	CB-CG-CD1	5.11	124.06	121.00
1	B	86	LYS	CA-C-N	-5.11	105.96	117.20
1	B	96	THR	CA-CB-CG2	-5.10	105.25	112.40
1	A	57	TRP	CZ3-CH2-CZ2	-5.10	115.48	121.60
1	B	123	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	A	103	HIS	ND1-CG-CD2	-5.08	98.89	106.00
1	A	146	MET	CA-CB-CG	5.06	121.91	113.30
1	A	147	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	B	50	GLN	CB-CA-C	5.05	120.50	110.40
1	B	117	ALA	O-C-N	-5.04	114.63	122.70
1	B	84	SER	N-CA-C	-5.03	97.41	111.00
1	A	106	ASN	OD1-CG-ND2	-5.02	110.35	121.90
1	B	104	TYR	CG-CD1-CE1	-5.02	117.28	121.30
1	A	140	PHE	CB-CG-CD2	-5.02	117.29	120.80

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

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Mol	Chain	Res	Type	Group
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1110	0	1072	56	0
1	B	1119	0	1079	47	0
2	B	9	0	6	0	0
All	All	2238	0	2157	94	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 21.

All (94) 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
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: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:C	1:B:180:PHE:O	2.18	0.77
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:40:PHE:CZ	1:B:180:PHE:HB2	2.28	0.69

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD22	1:A:176:TYR:CZ	2.49	0.47
1:B:177:ARG:NE	1:B:179:THR:HG1	2.11	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:B:52:GLU:HG3	1:B:110:MET:HE3	1.99	0.44
1:A:177:ARG:NH2	1:A:180:PHE:HZ	2.16	0.44
1:A:74:MET:SD	1:A:146:MET:HE1	2.58	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: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:B:178:GLN:OE1	1:B:179:THR:C	2.56	0.43
1:A:149:TYR:HD2	1:A:150:PHE:CD2	2.36	0.43
1:B:52:GLU:HG3	1:B:110:MET:CE	2.48	0.43
1:A:141:LEU:CD2	1:A:146:MET:HE1	2.49	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
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: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: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 [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	140/146 (96%)	114 (81%)	16 (11%)	10 (7%)	1	5
1	B	141/146 (97%)	120 (85%)	15 (11%)	6 (4%)	2	15
All	All	281/292 (96%)	234 (83%)	31 (11%)	16 (6%)	1	10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	49	GLN
1	A	114	PRO
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/119 (97%)	89 (77%)	26 (23%)	1	4
1	B	116/119 (98%)	90 (78%)	26 (22%)	1	4
All	All	231/238 (97%)	179 (78%)	52 (22%)	1	4

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	48	GLN
1	A	52	GLU
1	A	54	THR
1	A	55	SER
1	A	60	MET
1	A	77	ASP
1	A	82	GLN
1	A	83	SER
1	A	84	SER
1	A	88	ASP
1	A	106	ASN
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	157	MET
1	A	163	GLU
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

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Mol	Chain	Res	Type
1	B	68	SER
1	B	76	MET
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	134	LEU
1	B	139	GLN
1	B	141	LEU
1	B	143	ASN
1	B	153	PRO
1	B	161	LEU
1	B	167	ASN
1	B	178	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	49	GLN
1	A	50	GLN
1	A	103	HIS
1	A	155	GLN
1	A	158	GLN
1	B	38	GLN
1	B	92	ASN
1	B	122	ASN
1	B	131	GLN
1	B	152	GLN
1	B	174	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	-	6,8,8	1.64	1 (16%)	8,10,10	1.41	2 (25%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	ASP	OD2-CG	-2.46	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ASP	O-C-CA	-2.27	114.12	122.14
2	B	1	ASP	OD2-CG-CB	2.20	121.13	114.07

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.