



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:45 AM UTC

PDB ID : 1LIH / pdb_00001lih
Title : THREE-DIMENSIONAL STRUCTURES OF THE LIGAND-BINDING DOMAIN OF THE BACTERIAL ASPARTATE RECEPTOR WITH AND WITHOUT A LIGAND
Authors : Kim, S.-H.; Scott, W.; Yeh, J.I.; Prive, G.G.; Milburn, M.
Deposited on : 1995-04-18
Resolution : 2.20 Å(reported)

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

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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

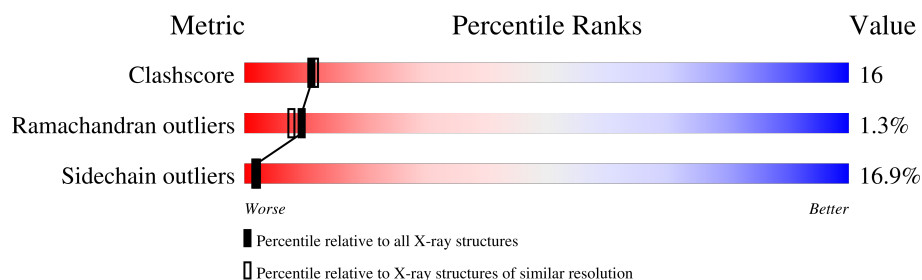
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

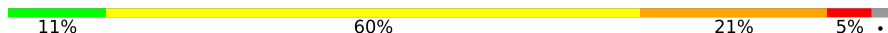
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	164	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PHN	A	1	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1373 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.

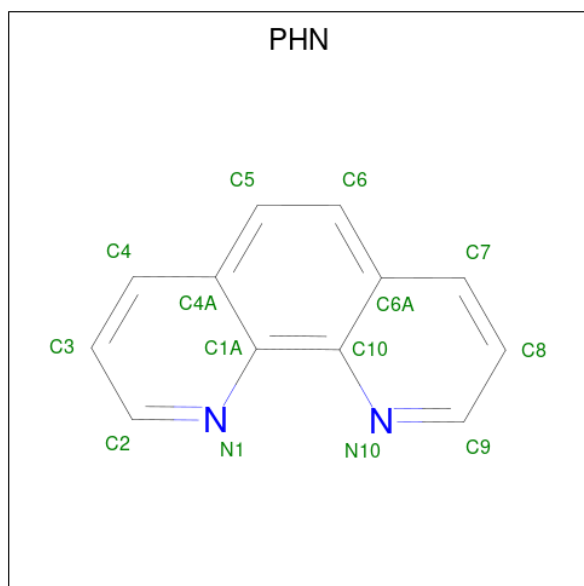
- Molecule 1 is a protein called ASPARTATE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	160	1243	765	221	247	10	78	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	CYS	ASN	conflict	UNP P02941

- Molecule 2 is 1,10-PHENANTHROLINE (CCD ID: PHN) (formula: C₁₂H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	14	12	2	0	0

- Molecule 3 is water.

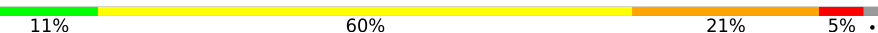
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total 116	O 116	0	0

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 RECEPTOR

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	80.03Å 80.03Å 155.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1373	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: PHN

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	3.31	161/1261 (12.8%)	2.89	139/1702 (8.2%)

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	4

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	MET	C-N	-16.97	1.10	1.33
1	A	35	HIS	CD2-NE2	-11.43	1.25	1.37
1	A	103	HIS	CD2-NE2	-10.75	1.26	1.37
1	A	101	ALA	N-CA	10.63	1.60	1.46
1	A	74	MET	CA-CB	-10.58	1.36	1.53
1	A	60	MET	N-CA	10.55	1.59	1.46
1	A	69	ARG	NE-CZ	10.51	1.44	1.33
1	A	47	ARG	CZ-NH1	10.11	1.46	1.32
1	A	135	ALA	CA-C	-9.68	1.40	1.52
1	A	139	GLN	CA-C	-9.44	1.40	1.52
1	A	159	ASN	CA-C	-9.28	1.40	1.52
1	A	132	ALA	N-CA	8.98	1.57	1.46
1	A	33	LEU	C-O	-8.90	1.13	1.24
1	A	34	GLN	N-CA	8.89	1.56	1.46
1	A	119	ALA	C-O	-8.87	1.13	1.24
1	A	56	THR	CA-CB	8.87	1.67	1.53
1	A	119	ALA	CA-CB	-8.73	1.39	1.53
1	A	27	GLY	CA-C	8.70	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	GLN	C-N	8.56	1.45	1.33
1	A	123	VAL	N-CA	-8.56	1.36	1.46
1	A	169	ALA	N-CA	8.56	1.56	1.46
1	A	93	ALA	CA-C	-8.53	1.41	1.52
1	A	85	ALA	C-O	8.49	1.33	1.24
1	A	65	ILE	C-O	8.39	1.33	1.24
1	A	47	ARG	C-O	8.38	1.33	1.24
1	A	154	THR	CA-CB	-8.34	1.40	1.53
1	A	51	SER	C-O	-8.21	1.14	1.24
1	A	162	GLY	C-O	8.20	1.33	1.23
1	A	49	GLN	CA-C	-8.08	1.42	1.52
1	A	50	GLN	CA-CB	-8.01	1.40	1.53
1	A	129	ARG	CZ-NH1	7.94	1.43	1.32
1	A	78	ALA	C-N	7.86	1.44	1.33
1	A	71	ALA	CA-C	7.78	1.63	1.52
1	A	54	THR	C-O	7.77	1.33	1.24
1	A	29	LEU	C-O	7.71	1.33	1.23
1	A	72	ALA	CA-CB	7.69	1.65	1.53
1	A	177	ARG	C-O	-7.69	1.14	1.24
1	A	145	ASN	C-N	-7.65	1.22	1.33
1	A	113	LEU	CA-C	7.65	1.63	1.53
1	A	145	ASN	CA-CB	-7.53	1.43	1.52
1	A	164	ALA	CA-C	7.52	1.62	1.52
1	A	134	LEU	C-O	-7.51	1.15	1.24
1	A	169	ALA	CA-CB	-7.48	1.41	1.53
1	A	147	ASP	CA-CB	-7.47	1.41	1.53
1	A	45	GLU	C-N	-7.44	1.24	1.33
1	A	73	ARG	NE-CZ	7.42	1.41	1.33
1	A	106	ASN	C-O	-7.42	1.15	1.24
1	A	57	TRP	CG-CD2	-7.41	1.30	1.43
1	A	112	PRO	CA-CB	-7.41	1.43	1.53
1	A	85	ALA	CA-C	-7.35	1.43	1.52
1	A	28	LEU	N-CA	7.35	1.56	1.46
1	A	35	HIS	CB-CG	7.29	1.60	1.50
1	A	100	ALA	C-N	-7.25	1.24	1.33
1	A	141	LEU	CA-C	-7.18	1.42	1.52
1	A	65	ILE	CA-CB	7.09	1.62	1.54
1	A	66	ASN	CG-OD1	7.06	1.36	1.23
1	A	143	ASN	C-N	7.03	1.43	1.33
1	A	26	GLY	CA-C	7.01	1.60	1.51
1	A	164	ALA	CA-CB	-7.01	1.42	1.53
1	A	91	GLN	CD-OE1	-7.01	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	PRO	N-CD	6.95	1.57	1.47
1	A	28	LEU	C-O	6.92	1.31	1.23
1	A	47	ARG	N-CA	-6.92	1.38	1.46
1	A	165	LEU	N-CA	-6.91	1.37	1.46
1	A	159	ASN	C-O	6.90	1.32	1.24
1	A	27	GLY	C-N	-6.89	1.25	1.33
1	A	155	GLN	C-O	-6.85	1.16	1.24
1	A	35	HIS	C-N	6.82	1.43	1.33
1	A	128	GLN	N-CA	-6.77	1.38	1.46
1	A	91	GLN	C-O	-6.75	1.16	1.24
1	A	35	HIS	CG-CD2	6.68	1.43	1.35
1	A	83	SER	C-O	6.64	1.32	1.24
1	A	178	GLN	N-CA	6.61	1.54	1.46
1	A	41	VAL	CA-C	6.58	1.61	1.52
1	A	178	GLN	CA-CB	-6.55	1.42	1.53
1	A	88	ASP	CA-CB	6.51	1.64	1.54
1	A	39	GLY	N-CA	-6.50	1.37	1.45
1	A	55	SER	C-O	6.49	1.32	1.24
1	A	151	ALA	N-CA	6.48	1.54	1.46
1	A	102	ALA	C-O	-6.44	1.16	1.24
1	A	99	GLN	CG-CD	6.43	1.68	1.52
1	A	123	VAL	CA-CB	6.41	1.62	1.54
1	A	118	GLU	C-O	-6.39	1.16	1.24
1	A	166	GLY	N-CA	6.28	1.53	1.45
1	A	140	PHE	CA-C	-6.27	1.44	1.52
1	A	129	ARG	C-O	-6.26	1.16	1.24
1	A	143	ASN	C-O	-6.25	1.15	1.24
1	A	117	ALA	CA-CB	-6.23	1.43	1.53
1	A	170	ARG	CA-C	-6.21	1.44	1.52
1	A	74	MET	C-O	-6.19	1.17	1.24
1	A	174	ASN	N-CA	6.18	1.53	1.46
1	A	126	LYS	CA-C	6.17	1.61	1.52
1	A	168	TYR	C-N	-6.05	1.26	1.33
1	A	163	GLU	CA-C	6.01	1.60	1.52
1	A	135	ALA	CA-CB	6.01	1.62	1.53
1	A	57	TRP	C-N	-6.01	1.26	1.33
1	A	33	LEU	N-CA	-5.97	1.39	1.46
1	A	170	ARG	NE-CZ	5.96	1.39	1.33
1	A	166	GLY	C-N	5.96	1.42	1.33
1	A	142	ASP	C-O	-5.91	1.16	1.24
1	A	33	LEU	CA-C	5.89	1.60	1.52
1	A	114	PRO	C-N	-5.86	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	LEU	CA-CB	-5.83	1.43	1.53
1	A	144	GLY	N-CA	-5.83	1.36	1.45
1	A	65	ILE	N-CA	-5.82	1.39	1.46
1	A	125	GLU	CD-OE2	-5.78	1.14	1.25
1	A	53	LEU	CA-C	5.78	1.60	1.52
1	A	181	ASP	C-O	-5.73	1.16	1.24
1	A	142	ASP	C-N	5.71	1.42	1.33
1	A	107	PHE	C-O	-5.71	1.17	1.24
1	A	103	HIS	CG-CD2	5.70	1.42	1.35
1	A	152	GLN	C-O	-5.69	1.17	1.24
1	A	126	LYS	CE-NZ	-5.69	1.32	1.49
1	A	123	VAL	C-N	5.68	1.41	1.34
1	A	37	GLN	CD-NE2	-5.68	1.21	1.33
1	A	91	GLN	CA-C	5.67	1.60	1.52
1	A	173	GLU	C-N	-5.66	1.26	1.33
1	A	147	ASP	N-CA	5.64	1.53	1.46
1	A	85	ALA	C-N	-5.62	1.25	1.33
1	A	34	GLN	CA-CB	-5.61	1.44	1.53
1	A	107	PHE	CA-C	5.58	1.59	1.52
1	A	50	GLN	N-CA	5.53	1.53	1.46
1	A	155	GLN	C-N	5.51	1.41	1.33
1	A	125	GLU	C-O	-5.50	1.17	1.24
1	A	131	GLN	CG-CD	5.50	1.65	1.52
1	A	77	ASP	CG-OD1	-5.49	1.15	1.25
1	A	130	TYR	CZ-OH	-5.47	1.26	1.38
1	A	159	ASN	CG-OD1	5.44	1.33	1.23
1	A	30	PHE	CG-CD2	-5.41	1.27	1.38
1	A	125	GLU	C-N	-5.40	1.26	1.33
1	A	167	ASN	C-O	-5.38	1.17	1.24
1	A	42	ILE	CA-C	-5.35	1.46	1.52
1	A	45	GLU	CD-OE1	-5.33	1.15	1.25
1	A	137	LEU	N-CA	-5.31	1.39	1.46
1	A	155	GLN	N-CA	5.28	1.52	1.46
1	A	150	PHE	CA-CB	5.28	1.62	1.53
1	A	34	GLN	C-O	5.23	1.30	1.24
1	A	171	VAL	CA-CB	5.22	1.61	1.54
1	A	100	ALA	N-CA	5.21	1.52	1.46
1	A	153	PRO	CA-CB	-5.20	1.47	1.53
1	A	163	GLU	C-N	-5.20	1.26	1.33
1	A	87	THR	C-O	5.19	1.30	1.24
1	A	133	ALA	C-O	-5.18	1.18	1.24
1	A	149	TYR	N-CA	5.17	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	ASN	N-CA	-5.13	1.40	1.46
1	A	103	HIS	CE1-NE2	-5.13	1.27	1.32
1	A	140	PHE	C-O	5.13	1.30	1.24
1	A	94	LYS	C-O	5.11	1.30	1.24
1	A	63	THR	C-O	5.11	1.30	1.24
1	A	42	ILE	N-CA	5.10	1.52	1.46
1	A	92	ASN	C-O	5.10	1.29	1.24
1	A	177	ARG	CZ-NH2	5.08	1.40	1.33
1	A	60	MET	CA-C	-5.07	1.46	1.52
1	A	63	THR	N-CA	-5.06	1.40	1.46
1	A	57	TRP	CD1-NE1	-5.05	1.27	1.37
1	A	171	VAL	C-O	5.05	1.30	1.24
1	A	65	ILE	C-N	-5.04	1.27	1.33
1	A	148	ALA	CA-C	5.03	1.59	1.52
1	A	56	THR	CA-C	5.01	1.59	1.52
1	A	45	GLU	N-CA	5.01	1.52	1.46
1	A	49	GLN	C-O	-5.01	1.18	1.24

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	MET	O-C-N	-22.08	89.93	121.72
1	A	87	THR	O-C-N	-20.95	94.73	122.59
1	A	26	GLY	CA-C-O	-12.02	110.08	121.38
1	A	61	LEU	O-C-N	-10.79	110.95	122.07
1	A	171	VAL	CA-C-O	-10.43	109.79	120.85
1	A	77	ASP	CA-CB-CG	-9.98	102.62	112.60
1	A	167	ASN	OD1-CG-ND2	-9.84	112.76	122.60
1	A	77	ASP	N-CA-C	9.73	123.68	110.55
1	A	37	GLN	CA-CB-CG	-8.91	96.27	114.10
1	A	57	TRP	CB-CG-CD1	-8.84	113.64	126.90
1	A	174	ASN	CA-CB-CG	-8.71	103.89	112.60
1	A	67	LEU	O-C-N	8.42	132.35	122.17
1	A	93	ALA	N-CA-C	-8.37	102.16	111.28
1	A	150	PHE	N-CA-C	8.32	121.48	111.82
1	A	123	VAL	O-C-N	-8.30	113.28	121.83
1	A	114	PRO	CA-C-N	8.19	133.70	120.60
1	A	114	PRO	C-N-CA	8.19	133.70	120.60
1	A	140	PHE	O-C-N	-8.10	113.53	122.12
1	A	154	THR	N-CA-C	7.99	119.99	111.28
1	A	184	ALA	CB-CA-C	-7.97	98.54	110.50
1	A	172	SER	CB-CA-C	-7.86	97.74	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	LEU	CA-C-O	-7.66	112.35	120.55
1	A	109	ASN	N-CA-C	7.62	121.68	112.38
1	A	174	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	A	171	VAL	N-CA-C	-7.54	103.11	110.72
1	A	95	THR	N-CA-CB	-7.50	99.09	110.12
1	A	92	ASN	N-CA-CB	7.48	120.85	110.01
1	A	117	ALA	N-CA-CB	-7.36	98.87	110.28
1	A	57	TRP	CB-CG-CD2	7.30	137.02	126.80
1	A	103	HIS	CA-CB-CG	-7.28	106.52	113.80
1	A	69	ARG	O-C-N	-7.16	113.46	122.27
1	A	95	THR	CB-CA-C	7.16	122.67	110.79
1	A	39	GLY	O-C-N	-7.09	114.55	122.28
1	A	107	PHE	O-C-N	7.08	129.37	122.07
1	A	177	ARG	CA-C-O	7.08	128.10	120.10
1	A	111	THR	CA-C-O	7.06	126.43	119.51
1	A	78	ALA	N-CA-C	-6.95	96.00	110.80
1	A	120	SER	O-C-N	-6.95	114.59	122.09
1	A	47	ARG	NH1-CZ-NH2	6.93	128.31	119.30
1	A	77	ASP	O-C-N	6.88	130.69	122.85
1	A	101	ALA	O-C-N	-6.87	113.46	122.39
1	A	123	VAL	N-CA-C	6.85	117.64	110.72
1	A	47	ARG	O-C-N	6.79	129.06	122.07
1	A	143	ASN	CA-C-O	6.75	127.96	119.12
1	A	63	THR	CA-C-O	-6.62	113.89	120.70
1	A	139	GLN	OE1-CD-NE2	-6.61	115.99	122.60
1	A	80	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	A	175	LEU	N-CA-C	-6.57	104.20	111.36
1	A	55	SER	CA-C-O	-6.56	112.42	119.97
1	A	149	TYR	N-CA-C	-6.54	103.05	111.02
1	A	125	GLU	O-C-N	6.48	128.77	122.03
1	A	34	GLN	CG-CD-NE2	6.42	126.03	116.40
1	A	30	PHE	CA-CB-CG	-6.38	107.42	113.80
1	A	81	GLN	CA-C-O	-6.38	111.39	120.51
1	A	54	THR	CA-CB-OG1	-6.32	100.12	109.60
1	A	122	ASN	N-CA-C	-6.31	104.50	111.82
1	A	97	LEU	CB-CA-C	-6.29	100.96	110.90
1	A	142	ASP	CA-CB-CG	-6.22	106.38	112.60
1	A	77	ASP	CA-C-O	6.20	129.12	121.81
1	A	86	LYS	CA-C-N	6.11	133.20	121.54
1	A	86	LYS	C-N-CA	6.11	133.20	121.54
1	A	92	ASN	CB-CA-C	-6.10	101.30	110.88
1	A	167	ASN	CB-CG-ND2	6.08	125.52	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	NE-CZ-NH1	-6.07	115.43	121.50
1	A	74	MET	N-CA-C	-6.07	104.57	111.07
1	A	92	ASN	O-C-N	-6.06	115.83	122.07
1	A	53	LEU	O-C-N	6.05	128.53	122.12
1	A	58	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	44	ASN	CA-C-O	-6.00	113.07	119.97
1	A	66	ASN	CA-CB-CG	5.99	118.59	112.60
1	A	105	ALA	O-C-N	-5.99	115.33	122.15
1	A	166	GLY	N-CA-C	-5.98	104.89	113.86
1	A	140	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	82	GLN	CG-CD-NE2	5.94	125.30	116.40
1	A	104	TYR	CG-CD1-CE1	-5.87	112.39	121.20
1	A	92	ASN	CA-C-N	5.81	128.06	120.28
1	A	92	ASN	C-N-CA	5.81	128.06	120.28
1	A	177	ARG	N-CA-C	5.79	118.37	111.71
1	A	128	GLN	N-CA-CB	-5.78	101.39	110.06
1	A	90	LEU	CB-CA-C	-5.78	99.58	110.67
1	A	112	PRO	N-CA-CB	5.75	108.44	103.27
1	A	34	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	A	161	LEU	N-CA-C	-5.70	105.15	111.36
1	A	183	SER	CA-C-N	5.70	131.95	121.70
1	A	183	SER	C-N-CA	5.70	131.95	121.70
1	A	30	PHE	N-CA-C	5.69	118.67	109.40
1	A	50	GLN	O-C-N	-5.67	116.11	122.12
1	A	112	PRO	N-CD-CG	-5.66	94.72	103.20
1	A	73	ARG	CA-C-O	5.65	126.54	120.55
1	A	74	MET	O-C-N	5.65	127.89	122.07
1	A	68	SER	O-C-N	-5.64	116.23	122.09
1	A	96	THR	CA-CB-OG1	5.63	118.05	109.60
1	A	91	GLN	CA-C-O	5.61	126.37	120.42
1	A	60	MET	O-C-N	-5.61	114.94	122.23
1	A	43	SER	N-CA-CB	5.60	118.84	110.22
1	A	143	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	112	PRO	CA-C-O	-5.55	115.29	121.23
1	A	148	ALA	O-C-N	5.52	129.06	122.27
1	A	158	GLN	CG-CD-OE1	-5.51	109.77	120.80
1	A	93	ALA	CA-C-O	-5.51	114.71	120.55
1	A	35	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	A	120	SER	CA-C-O	5.47	126.33	120.70
1	A	106	ASN	N-CA-C	-5.45	105.24	111.07
1	A	73	ARG	O-C-N	-5.45	116.34	122.12
1	A	71	ALA	CA-C-O	-5.41	114.79	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ASN	N-CA-C	-5.39	105.30	111.07
1	A	118	GLU	N-CA-CB	5.37	117.77	109.98
1	A	81	GLN	N-CA-CB	-5.34	101.46	110.49
1	A	62	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	A	159	ASN	CB-CG-ND2	-5.33	108.41	116.40
1	A	178	GLN	N-CA-C	-5.32	106.74	113.18
1	A	139	GLN	CB-CA-C	-5.32	101.81	110.85
1	A	125	GLU	CA-CB-CG	5.31	124.73	114.10
1	A	90	LEU	N-CA-CB	5.30	118.49	110.28
1	A	69	ARG	CD-NE-CZ	-5.29	116.99	124.40
1	A	89	LEU	O-C-N	5.29	128.18	122.15
1	A	158	GLN	CG-CD-NE2	5.26	124.29	116.40
1	A	25	MET	O-C-N	-5.25	114.60	123.00
1	A	97	LEU	N-CA-C	-5.23	105.50	111.14
1	A	106	ASN	CA-C-O	-5.22	115.34	120.82
1	A	129	ARG	NH1-CZ-NH2	-5.21	112.52	119.30
1	A	118	GLU	CB-CA-C	-5.21	102.88	110.95
1	A	127	TYR	N-CA-C	-5.21	105.52	111.14
1	A	64	ARG	O-C-N	-5.18	116.63	122.12
1	A	104	TYR	CB-CG-CD1	-5.17	113.04	120.80
1	A	27	GLY	O-C-N	5.15	128.33	122.67
1	A	59	LEU	CA-C-O	-5.14	112.53	119.11
1	A	71	ALA	N-CA-C	-5.12	105.13	111.33
1	A	103	HIS	CB-CA-C	-5.11	102.30	110.79
1	A	125	GLU	CA-C-N	-5.11	112.18	120.72
1	A	125	GLU	C-N-CA	-5.11	112.18	120.72
1	A	28	LEU	O-C-N	-5.11	115.64	122.38
1	A	43	SER	CB-CA-C	-5.09	101.21	110.63
1	A	94	LYS	CA-C-O	-5.08	115.03	120.42
1	A	103	HIS	ND1-CE1-NE2	5.06	113.46	108.40
1	A	54	THR	N-CA-C	-5.04	105.68	111.07
1	A	49	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	A	109	ASN	CA-CB-CG	5.03	117.62	112.60
1	A	184	ALA	CA-C-O	-5.02	112.27	120.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	69	ARG	Mainchain
1	A	76	MET	Mainchain
1	A	87	THR	Peptide,Mainchain

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	1243	0	1196	38	0
2	A	14	0	8	2	0
3	A	116	0	0	15	0
All	All	1373	0	1204	38	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 16.

All (38) 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:126:LYS:HD3	3:A:356:HOH:O	1.36	1.22
1:A:126:LYS:HB2	3:A:409:HOH:O	1.72	0.89
1:A:43:SER:OG	2:A:1:PHN:H9	1.84	0.78
1:A:25:MET:HB2	1:A:29:LEU:HD11	1.65	0.77
1:A:167:ASN:HA	3:A:391:HOH:O	1.84	0.77
1:A:43:SER:OG	2:A:1:PHN:C9	2.37	0.72
1:A:69:ARG:HB2	3:A:399:HOH:O	1.95	0.66
1:A:69:ARG:NH2	1:A:89:LEU:HD11	2.19	0.58
1:A:89:LEU:HG	3:A:399:HOH:O	2.03	0.57
1:A:113:LEU:HD22	3:A:390:HOH:O	2.04	0.57
1:A:164:ALA:HB2	3:A:356:HOH:O	2.04	0.57
1:A:116:MET:HE3	1:A:175:LEU:HD12	1.87	0.56
1:A:101:ALA:HB3	3:A:404:HOH:O	2.07	0.54
1:A:123:VAL:HA	3:A:409:HOH:O	2.07	0.53
1:A:34:GLN:HE22	1:A:38:GLN:HE21	1.56	0.53
1:A:102:ALA:N	3:A:404:HOH:O	2.42	0.52
1:A:34:GLN:HE22	1:A:38:GLN:NE2	2.08	0.51
1:A:110:MET:SD	3:A:307:HOH:O	2.60	0.50
1:A:26:GLY:HA2	3:A:304:HOH:O	2.11	0.49
1:A:126:LYS:HE3	1:A:129:ARG:NH2	2.27	0.48
1:A:101:ALA:N	3:A:404:HOH:O	2.46	0.48
1:A:126:LYS:N	1:A:126:LYS:HD2	2.31	0.45
1:A:116:MET:HE1	1:A:171:VAL:HG12	1.98	0.45
1:A:169:ALA:HA	3:A:418:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:O	1:A:128:GLN:HB2	2.18	0.44
1:A:153:PRO:HG2	1:A:157:MET:HE2	2.00	0.43
1:A:116:MET:CE	1:A:171:VAL:HG12	2.50	0.42
1:A:67:LEU:HD11	1:A:138:ILE:HG12	2.01	0.42
1:A:89:LEU:HA	1:A:92:ASN:OD1	2.19	0.42
1:A:69:ARG:HH21	1:A:89:LEU:HD11	1.84	0.41
1:A:126:LYS:HE3	1:A:129:ARG:HH22	1.84	0.41
1:A:133:ALA:HB1	1:A:152:GLN:NE2	2.36	0.41
1:A:65:ILE:O	1:A:68:SER:HB2	2.21	0.41
1:A:145:ASN:ND2	1:A:148:ALA:H	2.19	0.41
1:A:145:ASN:HD22	1:A:148:ALA:H	1.68	0.41
1:A:67:LEU:HD12	1:A:67:LEU:HA	1.92	0.40
1:A:170:ARG:HB3	3:A:391:HOH:O	2.20	0.40
1:A:89:LEU:HA	1:A:89:LEU:HD12	1.82	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	158/164 (96%)	146 (92%)	10 (6%)	2 (1%)	9 8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ALA
1	A	87	THR

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	130/134 (97%)	108 (83%)	22 (17%)	2 2

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	32	SER
1	A	33	LEU
1	A	46	LEU
1	A	59	LEU
1	A	61	LEU
1	A	67	LEU
1	A	77	ASP
1	A	79	SER
1	A	80	ASN
1	A	82	GLN
1	A	84	SER
1	A	89	LEU
1	A	97	LEU
1	A	111	THR
1	A	113	LEU
1	A	128	GLN
1	A	134	LEU
1	A	136	GLU
1	A	145	ASN
1	A	163	GLU
1	A	175	LEU

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	34	GLN
1	A	35	HIS
1	A	49	GLN

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Mol	Chain	Res	Type
1	A	103	HIS
1	A	106	ASN
1	A	145	ASN
1	A	152	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	PHN	A	1	-	16,16,16	2.41	8 (50%)	22,22,22	2.63	9 (40%)

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	PHN	A	1	-	-	-	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	PHN	C4A-C1A	-4.42	1.32	1.41
2	A	1	PHN	C5-C4A	-4.12	1.33	1.42
2	A	1	PHN	C2-N1	4.07	1.40	1.32
2	A	1	PHN	C3-C2	2.52	1.44	1.37
2	A	1	PHN	C7-C6A	-2.37	1.36	1.42
2	A	1	PHN	C4-C4A	-2.35	1.36	1.42
2	A	1	PHN	C9-N10	2.23	1.36	1.32
2	A	1	PHN	C1A-N1	-2.11	1.33	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	PHN	C1A-C10-N10	6.43	125.97	118.24
2	A	1	PHN	C3-C2-N1	-4.56	117.27	123.97
2	A	1	PHN	C5-C4A-C1A	3.64	125.55	118.55
2	A	1	PHN	C9-N10-C10	3.51	123.19	117.07
2	A	1	PHN	C6A-C10-N10	-3.50	116.34	122.50
2	A	1	PHN	C10-C1A-N1	-3.23	114.36	118.24
2	A	1	PHN	C8-C9-N10	-2.99	119.58	123.97
2	A	1	PHN	C6-C5-C4A	-2.87	117.10	121.34
2	A	1	PHN	C5-C4A-C4	-2.59	117.10	123.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	PHN	2	0

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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	76:MET	C	77:ASP	N	1.10

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.