Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 09:18 AM EST

PDB ID	:	1LIH
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.

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:

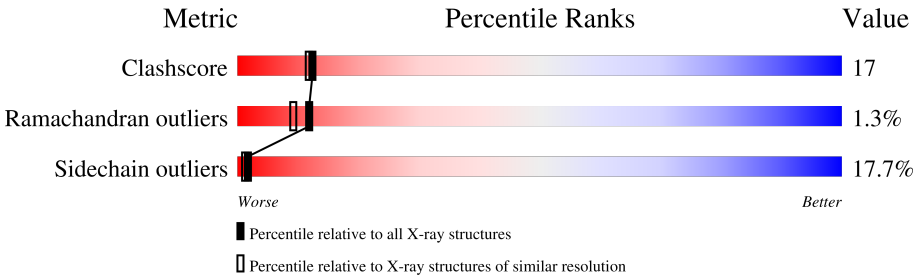
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	164	31% 47% 16%

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

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.

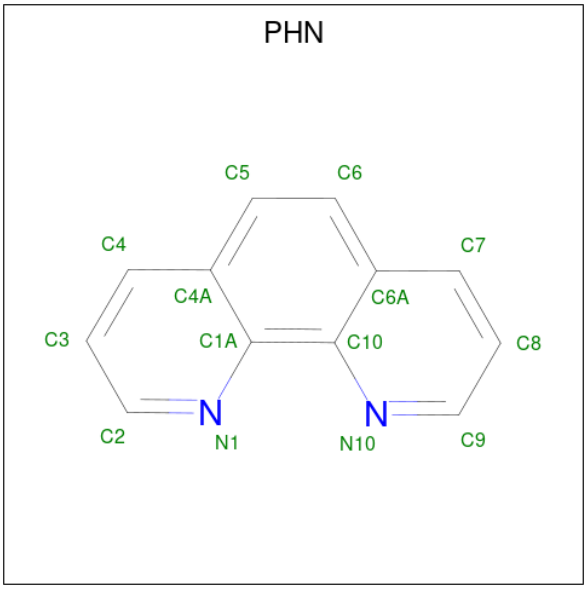
- Molecule 1 is a protein called ASPARTATE RECEPTOR.

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

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 (three-letter code: PHN) (formula: $C_{12}H_8N_2$).



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

- Molecule 3 is water.

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

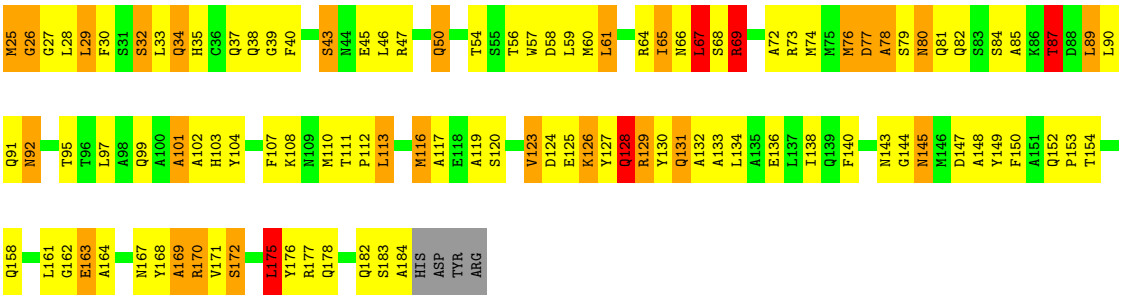
3 Residue-property plots (i)

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:



4 Data and refinement statistics (i)

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	2.54	72/1261 (5.7%)	2.41	66/1702 (3.9%)

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 (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	ARG	CZ-NH1	10.65	1.46	1.33
1	A	76	MET	C-N	-10.39	1.10	1.34
1	A	125	GLU	CD-OE2	-10.25	1.14	1.25
1	A	45	GLU	CD-OE1	-9.47	1.15	1.25
1	A	69	ARG	NE-CZ	8.89	1.44	1.33
1	A	129	ARG	CZ-NH1	8.31	1.43	1.33
1	A	104	TYR	CG-CD2	-7.87	1.28	1.39
1	A	127	TYR	CG-CD1	-7.81	1.28	1.39
1	A	57	TRP	CG-CD2	-7.79	1.30	1.43
1	A	74	MET	CA-CB	-7.73	1.36	1.53
1	A	130	TYR	CG-CD1	-7.66	1.29	1.39
1	A	176	TYR	CE1-CZ	-7.52	1.28	1.38
1	A	30	PHE	CG-CD2	-7.50	1.27	1.38
1	A	149	TYR	CG-CD2	7.48	1.48	1.39
1	A	99	GLN	CG-CD	7.43	1.68	1.51
1	A	27	GLY	CA-C	7.33	1.63	1.51
1	A	32	SER	CB-OG	7.24	1.51	1.42
1	A	153	PRO	N-CD	6.88	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ALA	N-CA	6.84	1.60	1.46
1	A	40	PHE	CG-CD2	6.74	1.48	1.38
1	A	126	LYS	CE-NZ	-6.71	1.32	1.49
1	A	130	TYR	CZ-OH	-6.64	1.26	1.37
1	A	60	MET	N-CA	6.62	1.59	1.46
1	A	45	GLU	CD-OE2	-6.55	1.18	1.25
1	A	149	TYR	CD1-CE1	-6.55	1.29	1.39
1	A	30	PHE	CE1-CZ	-6.52	1.25	1.37
1	A	144	GLY	N-CA	-6.45	1.36	1.46
1	A	131	GLN	CG-CD	6.42	1.65	1.51
1	A	104	TYR	CE1-CZ	-6.38	1.30	1.38
1	A	127	TYR	CE1-CZ	-6.30	1.30	1.38
1	A	57	TRP	CD1-NE1	-6.30	1.27	1.38
1	A	162	GLY	C-O	6.30	1.33	1.23
1	A	73	ARG	NE-CZ	6.28	1.41	1.33
1	A	91	GLN	CD-OE1	-6.23	1.10	1.24
1	A	168	TYR	CG-CD1	-6.23	1.31	1.39
1	A	72	ALA	CA-CB	6.21	1.65	1.52
1	A	119	ALA	CA-CB	-6.10	1.39	1.52
1	A	50	GLN	CA-CB	-6.01	1.40	1.53
1	A	66	ASN	CG-OD1	5.92	1.36	1.24
1	A	35	HIS	CD2-NE2	-5.76	1.25	1.38
1	A	163	GLU	CD-OE1	5.74	1.31	1.25
1	A	35	HIS	CB-CG	5.73	1.60	1.50
1	A	39	GLY	N-CA	-5.72	1.37	1.46
1	A	168	TYR	CG-CD2	5.68	1.46	1.39
1	A	80	ASN	CB-CG	5.66	1.64	1.51
1	A	147	ASP	CA-CB	-5.59	1.41	1.53
1	A	143	ASN	C-N	5.57	1.43	1.33
1	A	57	TRP	CE2-CZ2	-5.57	1.30	1.39
1	A	58	ASP	CB-CG	5.54	1.63	1.51
1	A	85	ALA	C-O	5.53	1.33	1.23
1	A	84	SER	CA-CB	5.53	1.61	1.52
1	A	47	ARG	C-O	5.47	1.33	1.23
1	A	103	HIS	CD2-NE2	-5.42	1.26	1.38
1	A	178	GLN	CA-CB	-5.41	1.42	1.53
1	A	65	ILE	C-O	5.40	1.33	1.23
1	A	158	GLN	CG-CD	5.40	1.63	1.51
1	A	56	THR	CA-CB	5.40	1.67	1.53
1	A	177	ARG	CZ-NH2	5.39	1.40	1.33
1	A	132	ALA	N-CA	5.36	1.57	1.46
1	A	29	LEU	C-O	5.30	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	GLN	N-CA	5.30	1.56	1.46
1	A	130	TYR	CB-CG	-5.27	1.43	1.51
1	A	26	GLY	CA-C	5.18	1.60	1.51
1	A	119	ALA	C-O	-5.16	1.13	1.23
1	A	123	VAL	N-CA	-5.15	1.36	1.46
1	A	169	ALA	CA-CB	-5.14	1.41	1.52
1	A	183	SER	CA-CB	-5.11	1.45	1.52
1	A	54	THR	C-O	5.10	1.33	1.23
1	A	130	TYR	CD1-CE1	5.09	1.47	1.39
1	A	108	LYS	CD-CE	5.05	1.63	1.51
1	A	170	ARG	NE-CZ	5.04	1.39	1.33
1	A	154	THR	CA-CB	-5.02	1.40	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76	MET	O-C-N	-20.48	89.93	122.70
1	A	87	THR	O-C-N	-17.48	94.73	122.70
1	A	104	TYR	CB-CG-CD1	-13.26	113.04	121.00
1	A	69	ARG	NE-CZ-NH1	11.15	125.87	120.30
1	A	104	TYR	CG-CD1-CE1	-11.13	112.39	121.30
1	A	64	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	A	87	THR	CA-C-N	10.73	140.81	117.20
1	A	57	TRP	CB-CG-CD1	-10.28	113.64	127.00
1	A	47	ARG	NE-CZ-NH1	-9.74	115.43	120.30
1	A	104	TYR	CZ-CE2-CD2	-9.36	111.38	119.80
1	A	69	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	A	77	ASP	CA-C-N	-8.80	97.84	117.20
1	A	47	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	A	140	PHE	CB-CG-CD2	-8.57	114.80	120.80
1	A	176	TYR	CZ-CE2-CD2	-8.44	112.20	119.80
1	A	47	ARG	NH1-CZ-NH2	8.10	128.31	119.40
1	A	57	TRP	CB-CG-CD2	8.02	137.02	126.60
1	A	117	ALA	N-CA-CB	-8.02	98.87	110.10
1	A	37	GLN	CA-CB-CG	-7.79	96.27	113.40
1	A	184	ALA	CB-CA-C	-7.71	98.54	110.10
1	A	40	PHE	CB-CG-CD2	-7.51	115.54	120.80
1	A	149	TYR	CB-CG-CD1	7.37	125.42	121.00
1	A	61	LEU	O-C-N	-7.34	110.95	122.70
1	A	58	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	127	TYR	CB-CG-CD1	-7.21	116.67	121.00
1	A	182	GLN	O-C-N	-6.92	111.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	25	MET	CA-C-N	6.65	129.51	116.20
1	A	172	SER	CB-CA-C	-6.51	97.74	110.10
1	A	73	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	A	129	ARG	NH1-CZ-NH2	-6.25	112.52	119.40
1	A	67	LEU	O-C-N	6.03	132.35	122.70
1	A	26	GLY	CA-C-N	6.01	128.21	116.20
1	A	140	PHE	CD1-CE1-CZ	5.98	127.28	120.10
1	A	158	GLN	CG-CD-OE1	-5.92	109.77	121.60
1	A	95	THR	N-CA-CB	-5.90	99.09	110.30
1	A	123	VAL	O-C-N	-5.89	113.28	122.70
1	A	26	GLY	CA-C-O	-5.84	110.08	120.60
1	A	107	PHE	CB-CG-CD1	-5.83	116.72	120.80
1	A	101	ALA	O-C-N	-5.78	113.46	122.70
1	A	69	ARG	O-C-N	-5.77	113.46	122.70
1	A	90	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	A	176	TYR	CE1-CZ-CE2	5.75	129.00	119.80
1	A	140	PHE	O-C-N	-5.73	113.53	122.70
1	A	64	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	A	92	ASN	N-CA-CB	5.70	120.85	110.60
1	A	112	PRO	N-CD-CG	-5.66	94.72	103.20
1	A	150	PHE	CG-CD1-CE1	-5.63	114.61	120.80
1	A	40	PHE	CG-CD2-CE2	-5.60	114.64	120.80
1	A	90	LEU	CB-CA-C	-5.59	99.58	110.20
1	A	43	SER	N-CA-CB	5.56	118.84	110.50
1	A	78	ALA	N-CA-C	-5.55	96.00	111.00
1	A	117	ALA	CB-CA-C	5.53	118.39	110.10
1	A	161	LEU	CB-CG-CD2	-5.53	101.60	111.00
1	A	175	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	57	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	A	140	PHE	CG-CD2-CE2	-5.28	114.99	120.80
1	A	127	TYR	CD1-CG-CD2	5.25	123.67	117.90
1	A	125	GLU	CA-CB-CG	5.15	124.73	113.40
1	A	128	GLN	N-CA-CB	-5.12	101.39	110.60
1	A	116	MET	CG-SD-CE	-5.10	92.03	100.20
1	A	39	GLY	O-C-N	-5.09	114.55	122.70
1	A	150	PHE	CD1-CG-CD2	5.09	124.91	118.30
1	A	81	GLN	N-CA-CB	-5.08	101.46	110.60
1	A	120	SER	O-C-N	-5.07	114.59	122.70
1	A	25	MET	O-C-N	-5.06	114.60	123.20

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	Mainchain,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	1243	0	1195	39	0
2	A	14	0	8	2	0
3	A	116	0	0	17	0
All	All	1373	0	1203	39	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 17.

All (39) 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:172:SER:OG	3:A:418:HOH:O	2.05	0.75
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	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:ALA:HA	3:A:418:HOH:O	2.17	0.44
1:A:124:ASP:O	1:A:128:GLN:HB2	2.18	0.44
1:A:116:MET:HE1	1:A:171:VAL:HG12	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:HD22	1:A:148:ALA:H	1.68	0.41
1:A:145:ASN:ND2	1:A:148:ALA:H	2.19	0.41
1:A:172:SER:CB	3:A:418:HOH:O	2.66	0.40
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%)	12 9

All (2) Ramachandran outliers are listed below:

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

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	130/134 (97%)	107 (82%)	23 (18%)	2 1

All (23) 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	50	GLN
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	89	LEU
1	A	97	LEU
1	A	111	THR
1	A	113	LEU
1	A	128	GLN
1	A	131	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 (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	38	GLN
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 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	PHN	A	1	-	16,16,16	2.29	8 (50%)	22,22,22	2.56	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	-4.32	1.32	1.41
2	A	1	PHN	C2-N1	3.92	1.40	1.32
2	A	1	PHN	C5-C4A	-3.69	1.33	1.41
2	A	1	PHN	C3-C2	2.45	1.44	1.37
2	A	1	PHN	C9-N10	2.14	1.36	1.32
2	A	1	PHN	C7-C6A	-2.12	1.36	1.41
2	A	1	PHN	C4-C4A	-2.10	1.36	1.41
2	A	1	PHN	C1A-N1	-2.09	1.33	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	PHN	C1A-C10-N10	6.32	125.97	118.23
2	A	1	PHN	C3-C2-N1	-4.35	117.27	123.94
2	A	1	PHN	C5-C4A-C1A	3.60	125.55	118.54
2	A	1	PHN	C6A-C10-N10	-3.49	116.34	122.51
2	A	1	PHN	C9-N10-C10	3.40	123.19	117.12
2	A	1	PHN	C10-C1A-N1	-3.16	114.36	118.23
2	A	1	PHN	C8-C9-N10	-2.84	119.58	123.94
2	A	1	PHN	C6-C5-C4A	-2.76	117.10	121.36
2	A	1	PHN	C5-C4A-C4	-2.60	117.10	123.19

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.